Lecture Notes in Mathematics

1954

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Quantum Potential Theory

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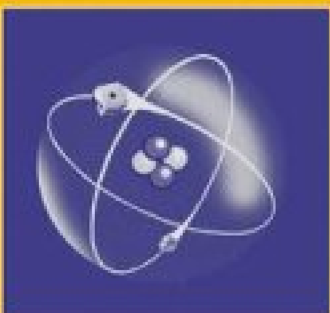

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Preface

This volume contains the notes of lectures given at the School "Quantum Potential Theory: Structure and Applications to Physics". This school was held at the Alfried Krupp Wissenschaftskolleg in Greifswald from February 26 to March 9, 2007. We thank the lecturers for the hard work they accomplished in preparing and giving these lectures and in writing these notes. Their lectures give an introduction to current research in their domains, which is essentially self-contained and should be accessible to Ph.D. students. We hope that this volume will help to bring together researchers from the areas of classical and quantum probability, functional analysis and operator algebras, and theoretical and mathematical physics, and contribute in this way to developing further the subject of quantum potential theory.

We are greatly indebted to the Alfried Krupp von Bohlen und Halbach-Stiftung for the financial support, without which the school would not have been possible. We are also very thankful for the support by the University of Greifswald and the University of Franche-Comté. One of the organisers (UF) was supported by a Marie Curie Outgoing International Fellowship of the EU (Contract Q-MALL MOIF-CT-2006-022137).

Special thanks go to Melanie Hinz who helped with the preparation and organisation of the school and who took care of all of the logistics.

Finally, we would like to thank all the students for coming to Greifswald and helping to make the school a success.

Sendai and Greifswald, June 2008

Uwe Franz
Michael Schürmann

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Introduction

The term potential theory comes from 19th century physics, where the fundamental forces like gravity or electrostatic forces were described as the gradients of potentials, i.e. functions which satisfy the Laplace equation. Hence potential theory was the study of solutions of the Laplace equation. Nowadays the fundamental forces in physics are described by systems of non-linear partial differential equations such as the Einstein equations and the Yang-Mills equations, and the Laplace equation arises only as a limiting case. Nevertheless, the Laplace equation is still used in applications in many areas of physics and engineering like heat conduction and electrostatics. And the term "potential theory" has survived as a convenient label for the theory of functions satisfying the Laplace equation, i.e. so-called harmonic functions.

In the 20th century, with the development of probability and stochastic processes, it was discovered that potential theory is intimately related to the theory of Markov processes, in particular diffusion processes and Brownian motion. The distributions of these processes evolve according to a heat equation, and invariant distributions satisfy a Laplace-type equation. Conversely, these processes can be used to express solutions of, e.g., the Laplace equation. For more details see Nicolas Privault's lecture "Potential Theory in Classical Probability" in this volume.

The notions of quantum stochastic processes and quantum Markov processes were introduced in the 1970's and allow to describe open quantum systems in close analogy to classical probability and classical Markov processes. Roughly speaking, one can now recognize two different trends in the subsequent development of the theory of quantum Markov processes. The first is guided by physical applications, studies concrete physically motivated models, and develops tools for filtering noisy quantum signals or controling noisy quantum systems. The second aims to develop a mathematical theory, by generalizing or extending key results of the theory of Markov processes to the quantum (or noncommutative) case, and by looking for analogues of important tools that greatly influenced the development of classical potential theory, like stochastic calculus, Dirichlet forms, or boundaries of random

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walks. In our school the first direction was represented by Luc Bouten's lecture "Applications of Controlled Quantum Processes in Quantum Optics", the second by Philippe Biane's lecture "Introduction to Random Walks on Noncommutative Spaces" and by Fabio Cipriani's lecture "Noncommutative Dirichlet Forms", see also the corresponding chapters of this book.

Besides providing important background material on operator algebras and noncommutative analogues of function spaces used in other lectures, Quanhua Xu's lecture on "Interactions between Quantum Probability and Operator Space Theory" shows how quantum probability can be applied to modern functional analysis. For example, a clever choice of sequences of quantum random variables plays an essential role in establishing key results like noncommutative Khintchine type inequalities.

Central questions from probabilistic potential theory like the computation of hitting times and the study of the asymptotic behaviour of a walk are also the main topic in Norio Konno's lecture on "Quantum Walks". These quantum walks are not quantum Markov processes in the sense of the lectures by Biane, Bouten, and Cipriani, but another type of quantum analogue of random walks and Markov chains, and many of the classical potential theoretical methods have interesting analogues adapted to this case. By giving an introduction and survey of this quickly developing field this lecture was an enrichment of the school and nicely complements the other chapters.

The goal of the School "Quantum Potential Theory: Structure and Applications to Physics" and these lecture notes is two-fold. First of all we want to provide an introduction to the rapidly developing theory of quantum Markov semigroups and quantum Markov processes with its manifold aspects ranging from functional analysis and probability theory to quantum physics. We hope that we have succeeded in preparing a monograph that is accessible to graduate students in mathematics and physics. But furthermore we also hope that this book will catch the interest of experienced mathematicians and physicists working in this field or related fields, in order to stimulate more communication between researchers working on "pure" and "applied" aspects. We believe that a strong collaboration between these communities will be to everybody's benefit. Keeping in mind the physical applications will help to sharpen the theoreticians' eye for the relevant questions and properties, and new powerful mathematical tools will allow to get a better and deeper understanding of concrete physical systems.

Potential Theory in Classical Probability

Nicolas Privault

Abstract These notes are an elementary introduction to classical potential theory and to its connection with probabilistic tools such as stochastic calculus and the Markov property. In particular we review the probabilistic interpretations of harmonicity, of the Dirichlet problem, and of the Poisson equation using Brownian motion and stochastic calculus.

1 Introduction

The origins of potential theory can be traced to the physical problem of reconstructing a repartition of electric charges inside a planar or a spatial domain, given the measurement of the electrical field created on the boundary of this domain.

In mathematical analytic terms this amounts to representing the values of a function h inside a domain given the data of the values of h on the boundary of the domain. In the simplest case of a domain empty of electric charges, the problem can be formulated as that of finding a harmonic function h on E (roughly speaking, a function with vanishing Laplacian, see § 2.2 below), given its values prescribed by a function f on the boundary ∂E, i.e. as the Dirichlet problem:

$$\begin{cases} \Delta h(y) = 0, & y \in E, \\ h(y) = f(y), & y \in \partial E. \end{cases}$$

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Close connections between the notion of potential and the Markov property have been observed at early stages of the development of the theory, see e.g. [Doo84] and references therein. Thus a number of potential theoretic problems have a probabilistic interpretation or can be solved by probabilistic methods.

These notes aim at gathering both analytic and probabilistic aspects of potential theory into a single document. We partly follow the point of view of Chung [Chu95] with complements on analytic potential theory coming from Helms [Hel69], some additions on stochastic calculus, and probabilistic applications found in Bass [Bas98].

More precisely, we proceed as follow. In Section 2 we give a summary of classical analytic potential theory: Green kernels, Laplace and Poisson equations in particular, following mainly Brelot [Bre65], Chung [Chu95] and Helms [Hel69]. Section 3 introduces the Markovian setting of semigroups which will be the main framework for probabilistic interpretations. A sample of references used in this domain is Ethier and Kurtz [EK86], Kallenberg [Kal02], and also Chung [Chu95]. The probabilistic interpretation of potential theory also makes significant use of Brownian motion and stochastic calculus. They are summarized in Section 4, see Protter [Pro05], Ikeda and Watanabe [IW89], however our presentation of stochastic calculus is given in the framework of normal martingales due to their links with quantum stochastic calculus, cf. Biane [Bia93]. In Section 5 we present the probabilistic connection between potential theory and Markov processes, following Bass [Bas98], Dynkin [Dyn65], Kallenberg [Kal02], and Port and Stone [PS78]. Our description of the Martin boundary in discrete time follows that of Revuz [Rev75].

2 Analytic Potential Theory

2.1 Electrostatic Interpretation

Let E denote a closed region of $\mathbb{R}^n$, more precisely a compact subset having a smooth boundary ∂E with surface measure σ. Gauss's law is the main tool for determining a repartition of electric charges inside E, given the values of the electrical field created on ∂E. It states that given a repartition of charges $q(dx)$ the flux of the electric field $\mathbf{U}$ across the boundary ∂E is proportional to the sum of electric charges enclosed in E. Namely we have

$$\int_E q(dx) = \epsilon_0 \int_{\partial E} \langle \mathbf{n}(x), \mathbf{U}(x) \rangle \sigma(dx), \tag{2.1}$$

where $q(dx)$ is a signed measure representing the distribution of electric charges, $\epsilon_0 > 0$ is the electrical permittivity constant, $\mathbf{U}(x)$ denotes the electric field at $x \in \partial E$, and $\mathbf{n}(x)$ represents the outer (i.e. oriented towards the exterior of E) unit vector orthogonal to the surface ∂E.

On the other hand the divergence theorem, which can be viewed as a particular case of the Stokes theorem, states that if $\mathbf{U} : E \to \mathbb{R}^n$ is a $\mathcal{C}^1$ vector field we have

$$\int_E \operatorname{div} \mathbf{U}(x) dx = \int_{\partial E} \langle \mathbf{n}(x), \mathbf{U}(x) \rangle \sigma(dx), \tag{2.2}$$

where the divergence $\operatorname{div} \mathbf{U}$ is defined as

$$\operatorname{div} \mathbf{U}(x) = \sum_{i=1}^n \frac{\partial \mathbf{U}_i}{\partial x_i}(x).$$

The divergence theorem (2.2) can be interpreted as a mathematical formulation of the Gauss law (2.1). Under this identification, $\operatorname{div} \mathbf{U}(x)$ is proportional to the density of charges inside E, which leads to the Maxwell equation

$$\epsilon_0 \operatorname{div} \mathbf{U}(x) dx = q(dx), \tag{2.3}$$

where $q(dx)$ is the distribution of electric charge at x and $\mathbf{U}$ is viewed as the induced electric field on the surface ∂E.

When $q(dx)$ has the density $q(x)$ at x, i.e. $q(dx) = q(x)dx$, and the field $\mathbf{U}(x)$ derives from a potential $V : \mathbb{R}^n \to \mathbb{R}_+$, i.e. when

$$\mathbf{U}(x) = \nabla V(x), \qquad x \in E,$$

Maxwell's equation (2.3) takes the form of the Poisson equation:

$$\epsilon_0 \Delta V(x) = q(x), \qquad x \in E, \tag{2.4}$$

where the Laplacian $\Delta = \operatorname{div} \nabla$ is given by

$$\Delta V(x) = \sum_{j=1}^n \frac{\partial^2 V}{\partial x_i^2}(x), \qquad x \in E.$$

In particular, when the domain E is empty of electric charges, the potential V satisfies the Laplace equation

$$\Delta V(x) = 0 \qquad x \in E.$$

As mentioned in the introduction, a typical problem in classical potential theory is to recover the values of the potential $V(x)$ inside E from its values on the boundary ∂E, given that $V(x)$ satisfies the Poisson equation (2.4). This can be achieved in particular by representing $V(x)$, $x \in E$, as an integral with respect to the surface measure over the boundary ∂E, or by direct solution of the Poisson equation for $V(x)$.

Consider for example the Newton potential kernel

$$V(x) = \frac{q}{\epsilon_0 s_n} \frac{1}{\|x-y\|^{n-2}}, \qquad x \in \mathbb{R}^n \setminus \{y\},$$

created by a single charge q at $y \in \mathbb{R}^n$, where $s_2 = 2\pi$, $s_3 = 4\pi$, and in general

$$s_n = \frac{2\pi^{n/2}}{\Gamma(n/2)}, \qquad n \geq 2,$$

is the surface of the unit $n-1$-dimensional sphere in $\mathbb{R}^n$.

The electrical field created by V is

$$\mathbf{U}(x) := \nabla V(x) = \frac{q}{\epsilon_0 s_n} \frac{x-y}{\|x-y\|^{n-1}}, \qquad x \in \mathbb{R}^n \setminus \{y\},$$

cf, Figure 1. Letting $B(y,r)$, resp. $S(y,r)$, denote the open ball, resp. the sphere, of center $y \in \mathbb{R}^n$ and radius $r > 0$, we have

$$\begin{aligned}\int_{B(y,r)} \Delta V(x) dx &= \int_{S(y,r)} \langle \mathbf{n}(x), \nabla V(x) \rangle \sigma(dx) \\ &= \int_{S(y,r)} \langle \mathbf{n}(x), \mathbf{U}(x) \rangle \sigma(dx) \\ &= \frac{q}{\epsilon_0},\end{aligned}$$

where σ denotes the surface measure on $S(y,r)$.
From this and the Poisson equation (2.4) we deduce that the repartition of electric charge is

$$q(dx) = q\delta_y(dx)$$

i.e. we recover the fact that the potential V is generated by a single charge located at y. We also obtain a version of the Poisson equation (2.4) in distribution sense:

$$\Delta_x \frac{1}{\|x-y\|^{n-2}} = s_n \delta_y(dx),$$

where the Laplacian Δ_x is taken with respect to the variable x. On the other hand, taking $E = B(0,r) \setminus B(0,\rho)$ we have $\partial E = S(0,r) \cup S(0,\rho)$ and

$$\begin{aligned}\int_E \Delta V(x) dx &= \int_{S(0,r)} \langle \mathbf{n}(x), \nabla V(x) \rangle \sigma(dx) + \int_{S(0,\rho)} \langle \mathbf{n}(x), \nabla V(x) \rangle \sigma(dx) \\ &= cs_n - cs_n = 0,\end{aligned}$$

hence

$$\Delta_x \frac{1}{\|x-y\|^{n-2}} = 0, \qquad x \in \mathbb{R}^n \setminus \{y\}.$$

The electrical permittivity ϵ_0 will be set equal to 1 in the sequel.

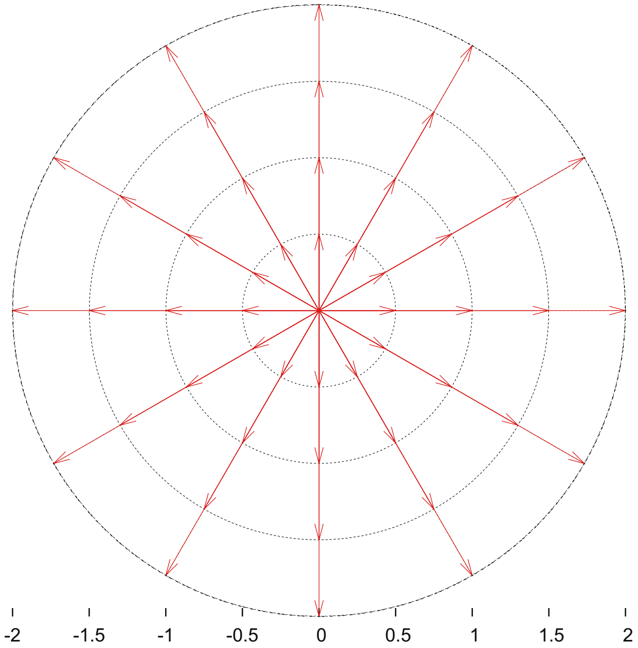

Fig. 1 Electrical field generated by a point mass at $y = 0$.

2.2 Harmonic Functions

The notion of harmonic function will be first introduced from the mean value property. Let

$$\sigma_r^x(dy) = \frac{1}{s_n r^{n-1}} \sigma(dy)$$

denote the normalized surface measure on $S(x,r)$, and recall that

$$\int f(x)dx = s_n \int_0^\infty r^{n-1} \int_{S(y,r)} f(z) \sigma_r^y(dz) dr.$$

Definition 2.1. A continuous real-valued function on an open subset O of $\mathbb{R}^n$ is said to be *harmonic*, resp. superharmonic, in O if one has

$$f(x) = \int_{S(x,r)} f(y) \sigma_r^x(dy),$$

resp.

$$f(x) \geq \int_{S(x,r)} f(y) \sigma_r^x(dy),$$

for all $x \in O$ and $r > 0$ such that $B(x,r) \subset O$.

Next we show the equivalence between the mean value property and the vanishing of the Laplacian.

Proposition 2.2. *A $\mathcal{C}^2$ function f is harmonic, resp. superharmonic, on an open subset O of $\mathbb{R}^n$ if and only if it satisfies the Laplace equation*

$$\Delta f(x) = 0, \qquad x \in O,$$

resp. the partial differential inequality

$$\Delta f(x) \leq 0, \qquad x \in O.$$

Proof. In spherical coordinates, using the divergence formula and the identity

$$\begin{aligned}\frac{d}{dr}\int_{S(0,1)} f(y+rx)\sigma_1^0(dx) &= \int_{S(0,1)} \langle x, \nabla f(y+rx)\rangle \sigma_1^0(dx) \\ &= \frac{r}{s_n}\int_{B(0,1)} \Delta f(y+rx)dx,\end{aligned}$$

yields

$$\begin{aligned}\int_{B(y,r)} \Delta f(x)dx &= r^{n-1}\int_{B(0,1)} \Delta f(y+rx)dx \\ &= s_n r^{n-2}\int_{S(0,1)} \langle x, \nabla f(y+rx)\rangle \sigma_1^0(dx) \\ &= s_n r^{n-2}\frac{d}{dr}\int_{S(0,1)} f(y+rx)\sigma_1^0(dx) \\ &= s_n r^{n-2}\frac{d}{dr}\int_{S(y,r)} f(x)\sigma_r^y(dx).\end{aligned}$$

If f is harmonic, this shows that

$$\int_{B(y,r)} \Delta f(x)dx = 0,$$

for all $y \in E$ and $r > 0$ such that $B(y,r) \subset O$, hence $\Delta f = 0$ on O. Conversely, if $\Delta f = 0$ on O then

$$\int_{S(y,r)} f(x)\sigma_r^y(dx)$$

is constant in r, hence

$$f(y) = \lim_{\rho\to 0}\int_{S(y,\rho)} f(x)\sigma_\rho^y(dx) = \int_{S(y,r)} f(x)\sigma_r^y(dx), \qquad r > 0.$$

The proof is similar in the case of superharmonic functions. □

The fundamental harmonic functions based at $y \in \mathbb{R}^n$ are the functions which are harmonic on $\mathbb{R}^n \backslash \{y\}$ and depend only on $r = \|x-y\|$, $y \in \mathbb{R}^n$. They satisfy the Laplace equation

$$\Delta h(x) = 0, \qquad x \in \mathbb{R}^n,$$

in spherical coordinates, with

$$\Delta h(r) = \frac{d^2 h}{dr^2}(r) + \frac{(n-1)}{r}\frac{dh}{dr}(r).$$

In case $n = 2$, the fundamental harmonic functions are given by the logarithmic potential

$$h_y(x) = \begin{cases} -\dfrac{1}{s_2} \log \|x-y\|, & x \neq y, \\ \\ +\infty, & x = y, \end{cases} \tag{2.5}$$

and by the Newton potential kernel in case $n \geq 3$:

$$h_y(x) = \begin{cases} \dfrac{1}{(n-2)s_n} \dfrac{1}{\|x-y\|^{n-2}}, & x \neq y, \\ \\ +\infty, & x = y. \end{cases} \tag{2.6}$$

More generally, for $a \in \mathbb{R}$ and $y \in \mathbb{R}^n$, the function

$$x \mapsto \|x-y\|^a,$$

is superharmonic on $\mathbb{R}^n$, $n \geq 3$, if and only if $a \in [2-n, 0]$, and harmonic when $a = 2 - n$.

We now focus on the Dirichlet problem on the ball $E = B(y, r)$. We consider

$$h_0(r) = -\frac{1}{s_2}\log(r), \qquad r > 0,$$

in case $n = 2$, and

$$h_0(r) = \frac{1}{(n-2)s_n r^{n-2}}, \qquad r > 0,$$

if $n \geq 3$, and let

$$x^* := y + \frac{r^2}{\|y-x\|^2}(x-y)$$

denote the inverse of $x \in B(y,r)$ with respect to the sphere $S(y,r)$. Note the relation

$$\begin{aligned}\|z - x^*\| &= \left\| z - y - \frac{r^2}{\|y-x\|^2}(x-y) \right\| \\ &= \frac{r}{\|x-y\|} \left\| \frac{\|x-y\|}{r}(z-y) - \frac{r}{\|y-x\|}(x-y) \right\|,\end{aligned}$$

hence for all $z \in S(y,r)$ and $x \in B(y,r)$,

$$\|z - x^*\| = r\frac{\|x-z\|}{\|x-y\|}, \tag{2.7}$$

since

$$\left\| \|x-y\| \frac{z-y}{\|z-y\|} - r\frac{x-y}{\|y-x\|} \right\| = \|x-z\|.$$

The function $z \mapsto h_x(z)$ is not $\mathcal{C}^2$, hence not harmonic, on $\bar{B}(y,r)$. Instead of h_x we will use $z \mapsto h_{x^*}(z)$, which is harmonic on a neighborhood of $\bar{B}(y,r)$, to construct a solution of the Dirichlet problem on $B(y,r)$.

Lemma 2.3. *The solution of the Dirichlet problem* (2.10) *for* $E = B(y,r)$ *with boundary condition* h_x, $x \in B(y,r)$, *is given by*

$$x \mapsto h_0\left(\frac{\|y-x\|\|z-x^*\|}{r}\right), \qquad z \in B(y,r).$$

Proof. We have if $n \geq 3$:

$$\begin{aligned}h_0\left(\frac{\|y-x\|\|z-x^*\|}{r}\right) &= \frac{r^{n-2}}{(n-2)s_n\|x-y\|^{n-2}}\frac{1}{\|z-x^*\|^{n-2}} \\ &= \frac{r^{n-2}}{\|x-y\|^{n-2}}h_{x^*}(z),\end{aligned}$$

and if $n = 2$:

$$\begin{aligned}h_0\left(\frac{\|y-x\|\|z-x^*\|}{r}\right) &= -\frac{1}{s_2}\log\left(\frac{\|y-x\|\|z-x^*\|}{r}\right) \\ &= h_{x^*}(y) - \frac{1}{s_2}\log\left(\frac{\|y-x\|}{r}\right).\end{aligned}$$

This function is harmonic in $z \in B(y,r)$ and is equal to h_x on $S(y,r)$ from (2.7). □

Figure 3 represents the solution of the Dirichlet problem with boundary condition h_x on $S(y,r)$ for $n = 2$ as obtained after truncation of Figure 2.

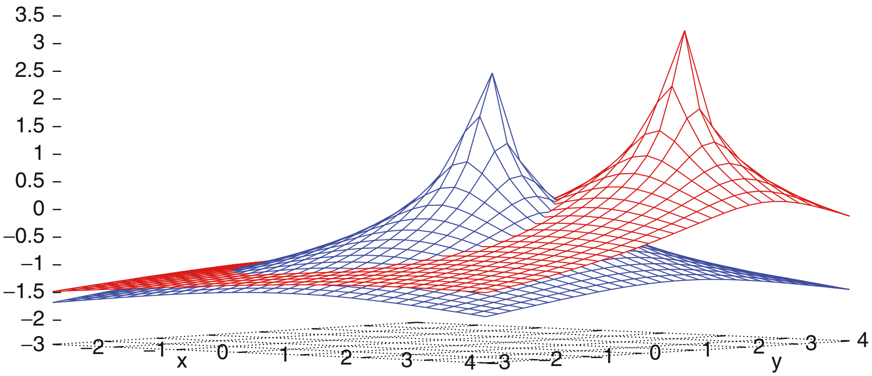

Fig. 2 Graph of h_x and of $h_0(\|y-x\|\|z-x^*\|/r)$ when $n=2$.

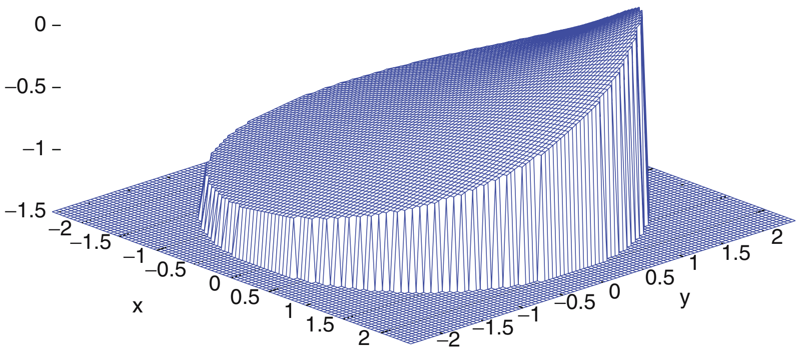

Fig. 3 Solution of the Dirichlet problem.

2.3 Representation of a Function on E from its Values on ∂E

As mentioned in the introduction, it can be of interest to compute a repartition of charges inside a domain E from the values of the field generated on the boundary ∂E.

In this section we present the representation formula for the values of an harmonic function inside an arbitrary domain E as an integral over its boundary ∂E, that follows from the Green identity. This formula uses a kernel which can be explicitly computed in some special cases, e.g. when $E = B(y,r)$ is an open ball, in which case it is called the Poisson formula, cf. Section 2.4 below.

Assume that E is an open domain in $\mathbb{R}^n$ with smooth boundary ∂E and let

$$\partial_n f(x) = \langle \mathbf{n}(x), \nabla f(x) \rangle$$

denote the normal derivative of f on ∂E.

Applying the divergence theorem (2.2) to the products $u(x)\nabla v(x)$ and $v(x)\nabla u(x)$, where u, v are $\mathcal{C}^2$ functions on E, yields Green's identity:

$$\int_E (u(x)\Delta v(x) - v(x)\Delta u(x))dx = \int_{\partial E} (u(x)\partial_n v(x) - v(x)\partial_n u(x))d\sigma(x). \quad (2.8)$$

On the other hand, taking $u = 1$ in the divergence theorem yields Gauss's integral theorem

$$\int_{\partial E} \partial_n v(x) d\sigma(x) = 0, \quad (2.9)$$

provided v is harmonic on E.

In the next definition, h_x denotes the fundamental harmonic function defined in (2.5) and (2.6).

Definition 2.4. The Green kernel $G^E(\cdot,\cdot)$ on E is defined as

$$G^E(x, y) := h_x(y) - w_x(y), \qquad x, y \in E,$$

where for all $x \in \mathbb{R}^n$, w_x is a smooth solution to the Dirichlet problem

$$\begin{cases} \Delta w_x(y) = 0, & y \in E, \\ w_x(y) = h_x(y), & y \in \partial E. \end{cases} \quad (2.10)$$

In the case of a general boundary ∂E, the Dirichlet problem may have no solution, even when the boundary value function f is continuous. Note that since $(x, y) \mapsto h_x(y)$ is symmetric, the Green kernel is also symmetric in two variables, i.e.

$$G^E(x, y) = G^E(y, x), \qquad x, y \in E,$$

and $G^E(\cdot,\cdot)$ vanishes on the boundary ∂E. The next proposition provides an integral representation formula for $\mathcal{C}^2$ functions on E using the Green kernel. In the case of harmonic functions, it reduces to a representation from the values on the boundary ∂E, cf. Corollary 2.6 below.

Proposition 2.5. *For all $\mathcal{C}^2$ functions u on E we have*

$$u(x) = \int_{\partial E} u(z)\partial_n G^E(x, z)\sigma(dz) + \int_E G^E(x, z)\Delta u(z)dz, \qquad x \in E. \quad (2.11)$$

Proof. We do the proof in case $n \geq 3$, the case $n = 2$ being similar. Given $x \in E$, apply Green's identity (2.8) to the functions u and h_x, where h_x is harmonic on $E \backslash B(x, r)$ for $r > 0$ small enough, to obtain

$$\begin{aligned} &\int_{E\backslash B(x,r)} h_x(y)\Delta u(y)dy - \int_{\partial E} (h_x(y)\partial_n u(y) - u(y)\partial_n h_x(y))d\sigma(y) \\ &\quad = \frac{1}{n-2}\int_{S(x,r)} \left(\frac{1}{s_n r^{n-2}}\partial_n u(y) + \frac{n-2}{s_n r^{n-1}} u(y)\right) d\sigma(y), \end{aligned}$$

since

$$y \mapsto \partial_n \frac{1}{\|y-x\|^{n-2}} = \frac{\partial}{\partial \rho} \rho^{2-n}_{|\rho=r} = -\frac{n-2}{r^{n-1}}.$$

In case u is harmonic, from the Gauss integral theorem (2.9) and the mean value property of u we get

$$\begin{aligned}\int_{E\setminus B(x,r)} h_x(y)\Delta u(y)dy - \int_{\partial E} (h_x(y)\partial_n u(y) - u(y)\partial_n h_x(y))d\sigma(y) \\ = \int_{S(x,r)} u(y)\sigma_r^x(dy) \\ = u(x).\end{aligned}$$

In the general case we need to pass to the limit as r tends to 0, which gives the same result:

$$u(x) = \int_{E\setminus B(x,r)} h_x(y)\Delta u(y)dy + \int_{\partial E} (u(y)\partial_n h_x(y) - h_x(y)\partial_n u(y))d\sigma(y). \tag{2.12}$$

Our goal is now to avoid using the values of the derivative term $\partial_n u(y)$ on ∂E in the above formula. To this end we note that from Green's identity (2.8) we have

$$\begin{aligned}\int_E w_x(y)\Delta u(y)dy &= \int_{\partial E} (w_x(y)\partial_n u(y) - u(y)\partial_n w_x(y))d\sigma(y) \\ &= \int_{\partial E} (h_x(y)\partial_n u(y) - u(y)\partial_n w_x(y))d\sigma(y) \qquad (2.13)\end{aligned}$$

for any smooth solution w_x to the Dirichlet problem (2.10). Taking the difference between (2.12) and (2.13) yields

$$\begin{aligned}u(x) &= \int_E (h_x(y) - w_x(y))\Delta u(y)dy + \int_{\partial E} u(y)\partial_n(h_x(y) - w_x(y))d\sigma(y) \\ &= \int_E G^E(x,y)\Delta u(y)dy + \int_{\partial E} u(y)\partial_n G^E(x,y)d\sigma(y), \qquad x \in E.\end{aligned}$$

□

Using (2.5) and (2.6), Relation (2.11) can be reformulated as

$$\begin{aligned}u(x) = \frac{1}{(n-2)s_n}\int_{\partial E}\left(u(z)\partial_n \frac{1}{\|x-z\|^{n-2}} - \frac{1}{\|x-z\|^{n-2}}\partial_n u(z)\right)\sigma(dz) \\ + \frac{1}{(n-2)s_n}\int_E \frac{1}{\|x-z\|^{n-2}}\Delta u(z)dz, \qquad x \in B(y,r),\end{aligned}$$

if $n \geq 3$, and if $n = 2$:

$$u(x) = -\frac{1}{s_2} \int_{\partial E} (u(z)\partial_n \log \|x - z\| - (\log \|x - z\|)\partial_n u(z))\sigma(dz)$$
$$- \int_E (\log \|x - z\|) \Delta u(z) dz, \qquad x \in B(y, r).$$

Corollary 2.6. *When u is harmonic on E we get*

$$u(x) = \int_{\partial E} u(y)\partial_n G^E(x, y) d\sigma(y), \qquad x \in E. \tag{2.14}$$

As a consequence of Lemma 2.3, the Green kernel $G^{B(y,r)}(\cdot, y)$ relative to the ball $B(y, r)$ is given for $x \in B(y, r)$ by

$$G^{B(y,r)}(x, z) = \begin{cases} -\dfrac{1}{s_2} \log \left(\dfrac{r}{\|y - x\|} \dfrac{\|z - x\|}{\|z - x^*\|} \right), & z \in B(y, r) \backslash \{x\}, \quad x \neq y, \\ -\dfrac{1}{s_2} \log \left(\dfrac{\|z - y\|}{r} \right), & z \in B(y, r) \backslash \{x\}, \quad x = y, \\ +\infty, & z = x, \end{cases}$$

if $n = 2$, cf. Figure 4 and

$$G^{B(y,r)}(x, z) = \begin{cases} \dfrac{1}{(n-2)s_n} \left(\dfrac{1}{\|z - x\|^{n-2}} - \dfrac{r^{n-2}}{\|x - y\|^{n-2}} \dfrac{1}{\|z - x^*\|^{n-2}} \right), \\ z \in B(y, r) \backslash \{x\}, \quad x \neq y, \\ \dfrac{1}{(n-2)s_n} \left(\dfrac{1}{\|z - y\|^{n-2}} - \dfrac{1}{r^{n-2}} \right), \\ z \in B(y, r) \backslash \{x\}, \quad x = y, \\ +\infty, \qquad z = x, \end{cases}$$

if $n \geq 3$.

The Green kernel on $E = \mathbb{R}^n$, $n \geq 3$, is obtained by letting r go to infinity:

$$G^{\mathbb{R}^n}(x, z) = \frac{1}{(n-2)s_n \|z - x\|^{n-2}} = h_x(z) = h_z(x), \qquad x, z \in \mathbb{R}^n. \tag{2.15}$$

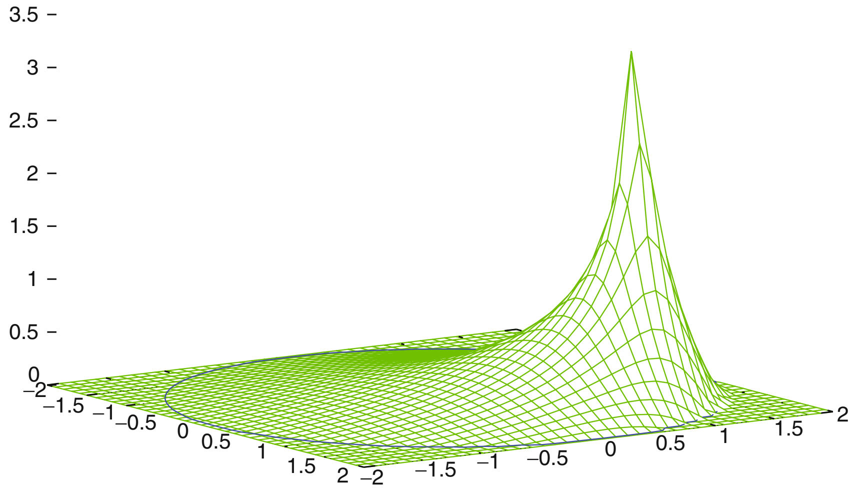

Fig. 4 Graph of $z \mapsto G(x,z)$ with $x \in E = B(y,r)$ and $n = 2$.

2.4 Poisson Formula

Given u a sufficiently integrable function on $S(y,r)$ we let $\mathcal{I}_u^{B(y,r)}(x)$ denote the Poisson integral of u over $S(y,r)$, defined as:

$$\mathcal{I}_u^{B(y,r)}(x) = \frac{1}{s_n r}\int_{S(y,r)} \frac{r^2 - \|y-x\|^2}{\|z-x\|^n} u(z)\sigma(dz), \qquad x \in B(y,r).$$

Next is the Poisson formula obtained as a consequence of Proposition 2.5.

Theorem 2.7. *Let $n \geq 2$. If u has continuous second partial derivatives on $E = \bar{B}(y,r)$ then for all $x \in B(y,r)$ we have*

$$u(x) = \mathcal{I}_u^{B(y,r)}(x) + \int_{B(y,r)} G^{B(y,r)}(x,z)\Delta u(z)dz. \tag{2.16}$$

Proof. We use the relation

$$u(x) = \int_{S(y,r)} u(z)\partial_n G^{B(y,r)}(x,z)\sigma(dz) + \int_{B(y,r)} G^{B(y,r)}(x,z)\Delta u(z)dz,$$

$x \in B(y,r)$, and the fact that

$$\begin{aligned} z \mapsto \partial_n G^{B(y,r)}(x,z) &= -\frac{1}{s_2}\partial_n \log\left(\frac{\|y-x\|}{r}\frac{\|z-x^*\|}{\|z-x\|}\right) \\ &= \frac{1}{(n-2)}\frac{r^2-\|x-y\|^2}{s_n r\|z-x\|^2} \end{aligned}$$

if $n = 2$, and similarly for $n \geq 3$. □

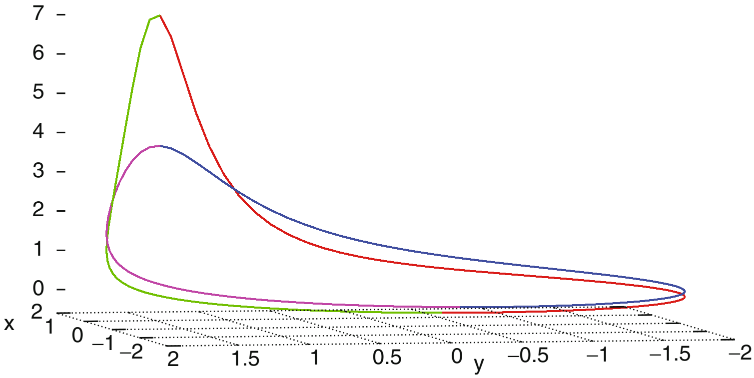

Fig. 5 Poisson kernel graphs on $S(y,r)$ for $n=2$ for two values of $x \in B(y,r)$.

When u is harmonic on a neighborhood of $\bar{B}(y,r)$ we obtain the Poisson representation formula of u on $E = \bar{B}(y,r)$ using the values of u on the sphere $\partial E = S(y,r)$, as a consequence of Theorem 2.7.

Corollary 2.8. *Assume that u is harmonic on a neighborhood of $\bar{B}(y,r)$. We have*

$$u(x) = \frac{1}{s_n r} \int_{S(y,r)} \frac{r^2 - \|y-x\|^2}{\|z-x\|^n} u(z)\sigma(dz), \qquad x \in B(y,r), \tag{2.17}$$

for all $n \geq 2$.

Similarly, Theorem 2.7 also shows that

$$u(x) \leq \mathcal{I}_u^{B(y,r)}(x), \qquad x \in B(y,r),$$

when u is superharmonic on $B(y,r)$. Note also that when $x=y$, Relation (2.17) recovers the mean value property of harmonic functions:

$$u(y) = \frac{1}{s_n r^{n-1}} \int_{S(y,r)} u(z)\sigma(dz),$$

and the corresponding inequality for superharmonic functions.

The function

$$z \mapsto \frac{r^2 - \|x-y\|^2}{\|x-z\|^n}$$

is called the Poisson kernel on $S(y,r)$ at $x \in B(y,r)$ cf. Figure 5.
A direct calculation shows that the Poisson kernel is harmonic on $\mathbb{R}^n \setminus (S(y,r) \cup \{z\})$:

$$\Delta_x \frac{r^2 - \|y-x\|^2}{\|z-x\|^n} = 0, \qquad x \notin S(y,r) \cup \{z\}, \tag{2.18}$$

hence all Poisson integrals are harmonic functions on $B(y,r)$. Moreover Theorem 2.17 of du Plessis [dP70] asserts that for any $z \in S(y,r)$, letting x tend to z without entering $S(y,r)$ we have

$$\lim_{x \to z} \mathcal{I}_u^{B(y,r)}(x) = u(z).$$

Hence the Poisson integral solves the Dirichlet problem (2.10) on $B(y,r)$.

Proposition 2.9. *Given f a continuous function on $S(y,r)$, the Poisson integral*

$$\mathcal{I}_f^{B(y,r)}(x) = \frac{1}{s_n r} \int_{S(y,r)} \frac{r^2 - \|x-y\|^2}{\|x-z\|^n} f(z)\sigma(dz), \qquad x \in B(y,r),$$

provides a solution of the Dirichlet problem

$$\begin{cases} \Delta w(x) = 0, & x \in B(y,r), \\ w(x) = f(x), & x \in S(y,r), \end{cases}$$

with boundary condition f.

Recall that the Dirichlet problem on $B(y,r)$ may not have a solution when the boundary condition f is not continuous.

In particular, from Lemma 2.3 we have

$$\mathcal{I}_{h_x}^{B(y,r)}(z) = \frac{r^{n-2}}{\|x-y\|^{n-2}} h_{x^*}(z), \qquad x \in B(y,r),$$

for $n \geq 3$, and

$$\mathcal{I}_{h_x}^{B(y,r)}(z) = h_{x^*}(z) - \frac{1}{s_2} \log\left(\frac{\|x-y\|}{r}\right), \qquad x \in B(y,r),$$

for $n = 2$, where x^* denotes the inverse of x with respect to $S(y,r)$. This function solves the Dirichlet problem with boundary condition h_x, and the corresponding Green kernel satisfies

$$G^{B(y,r)}(x,z) = h_x(z) - \mathcal{I}_{h_x}^{B(y,r)}(z), \qquad x, z \in B(y,r).$$

When $x = y$ the solution $\mathcal{I}_{h_y}^{B(y,r)}(z)$ of the Dirichlet problem on $B(y,r)$ with boundary condition h_y is constant and equal to $(n-2)^{-1} s_n^{-1} r^{2-n}$ on $B(y,r)$, and we have the identity

$$\frac{1}{s_n r^{n-1}} \int_{S(y,r)} \frac{r^2 - \|y-z\|^2}{\|x-z\|^n} \sigma(dx) = r^{2-n}, \qquad z \in B(y,r),$$

for $n \geq 3$, cf. Figure 6.

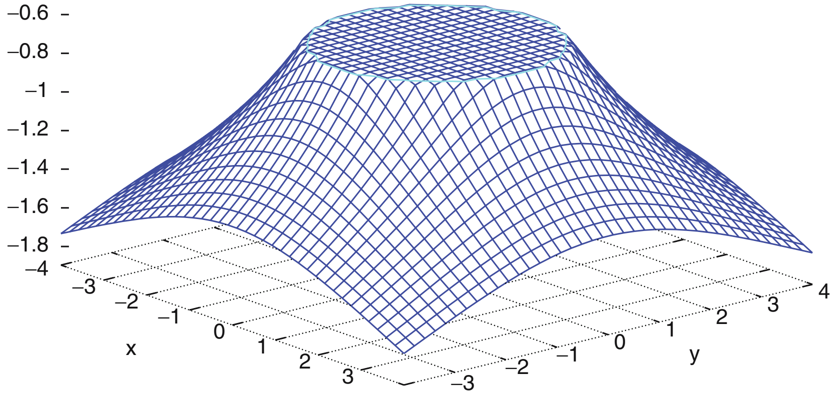

Fig. 6 Reduced of h_x relative to $D = \mathbb{R}^2 \backslash B(y, r)$ with $x = y$.

2.5 Potentials and Balayage

In electrostatics, the function $x \mapsto h_y(x)$ represents the Newton potential created at $x \in \mathbb{R}^n$ by a charge at $y \in E$, and the function

$$x \mapsto \int_E h_y(x) q(dy)$$

represents the sum of all potentials generated at $x \in \mathbb{R}^n$ by a distribution $q(dy)$ of charges inside E. In particular, when $E = \mathbb{R}^n$, $n \geq 3$, this sum equals

$$x \mapsto \int_{\mathbb{R}^n} G^{\mathbb{R}^n}(x, y) q(dy)$$

from (2.15), and the general definition of potentials originates from this interpretation.

Definition 2.10. Given a measure μ on E, the Green potential of μ is defined as the function

$$x \mapsto G^E \mu(x) := \int_E G^E(x, y) \mu(dy),$$

where $G^E(x, y)$ is the Green kernel on E.

Potentials will be used in the construction of superharmonic functions, cf. Proposition 5.1 below. Conversely, it is natural to ask whether a superharmonic function can be represented as the potential of a measure. In general, recall (cf. Proposition 2.5) the relation

$$u(x) = \int_{\partial E} u(z) \partial_n G^E(x, z) \sigma(dz) + \int_E G^E(x, z) \Delta u(z) dz, \qquad x \in E, \quad (2.19)$$

which yields, if $E = B(y, r)$:

$$u(x) = \mathcal{I}_u^E(x) + \int_E G^E(x, z)\Delta u(z)dz, \qquad x \in B(y, r), \tag{2.20}$$

where the Poisson integral $\mathcal{I}_u^E$ is harmonic from (2.18). Relation (2.20) can be seen as a decomposition of u into the sum of a harmonic function on $B(y, r)$ and a potential. The general question of representing superharmonic functions as potentials is examined next in Theorem 2.12 below, with application to the construction of Martin boundaries in Section 2.6.

Definition 2.11. Consider

i) an open subset E of $\mathbb{R}^n$ with Green kernel G^E,
ii) a subset D of E, and
iii) a non-negative superharmonic function u on E.

The infimum on E over all non-negative superharmonic function on E which are (pointwise) greater than u on D is called the reduced function of u relative to D, and denoted by $\mathfrak{R}_u^D$.

In other terms, letting Φ_u denote the set of non-negative superharmonic functions v on E such that $v \geq u$ on D, we have

$$\mathfrak{R}_u^D := \inf\{v \in \Phi_u\}.$$

The lower regularization

$$\hat{\mathfrak{R}}_u^D(x) := \liminf_{y \to x} \mathfrak{R}_u^D(y), \qquad x \in E,$$

is called the *balayage* of u, and is also a superharmonic function.

In case $D = \mathbb{R}^n \backslash B(y, r)$, the reduced function of h_y relative to D is given by

$$\mathfrak{R}_{h_y}^D(z) = h_y(z)\mathbf{1}_{\{z \notin B(y,r)\}} + h_0(r)\mathbf{1}_{\{z \in B(y,r)\}}, \qquad z \in \mathbb{R}^n, \tag{2.21}$$

cf. Figure 7. More generally if v is superharmonic then $\mathfrak{R}_v^D = \mathcal{I}_v^{B(y,r)}$ on $\mathbb{R}^2 \backslash D = B(y, r)$, cf. p. 62 and p. 100 of Brelot [Bre65]. Hence if $D = B^c(y, r) = \mathbb{R}^n \backslash B(y, r)$ and $x \in B(y, r)$, we have

$$\begin{aligned}
\mathfrak{R}_{h_x}^{B^c(y,r)}(z) &= \mathcal{I}_{h_x}^{B(y,r)}(z) \\
&= h_0\left(\frac{\|x - y\|\|z - x^*\|}{r}\right) \\
&= \frac{r^{n-2}}{(n-2)s_n\|x - y\|^{n-2}} \frac{1}{\|z - x^*\|^{n-2}}, \qquad z \in B(y, r).
\end{aligned}$$

Using Proposition 2.5 and the identity

$$\Delta \mathfrak{R}_{h_y}^{B^c(y,r)} = \sigma_r^y,$$

in distribution sense, we can represent $\mathfrak{R}_{h_y}^{B^c(y,r)}$ on $E = B(y,R)$, $R > r$, as

$$\begin{aligned}
&\mathfrak{R}_{h_y}^{B^c(y,r)}(x) \\
&= \int_{S(y,R)} \mathfrak{R}_{h_y}^{B^c(y,r)}(z) \partial_n G^{B(y,R)}(x,z)\sigma(dz) + \int_{B(y,R)} G^{B(y,R)}(x,z)\sigma_r^y(dz) \\
&= h_0(R) + \int_{S(y,r)} G^{B(y,R)}(x,z)\sigma_r^y(dz), \qquad x \in B(y,R).
\end{aligned}$$

Letting R go to infinity yields

$$\begin{aligned}
\mathfrak{R}_{h_y}^{B^c(y,r)}(x) &= \int_{S(y,r)} G^{\mathbb{R}^n}(x,z)\sigma_r^y(dz) \\
&= \int_{S(y,r)} h_x(z)\sigma_r^y(dz) \\
&= h_x(y), \qquad x \notin B(y,r),
\end{aligned}$$

since h_x is harmonic on $\mathbb{R}^n \backslash B(y,r)$, and

$$\begin{aligned}
\mathfrak{R}_{h_y}^{B^c(y,r)}(x) &= \int_{S(y,r)} h_0\left(\frac{\|y-x\|\|z-x^*\|}{r}\right)\sigma_r^y(dz) \\
&= h_0\left(\frac{\|y-x\|\|y-x^*\|}{r}\right) \\
&= h_0(r), \qquad x \in B(y,r),
\end{aligned}$$

which recovers the decomposition (2.21).
More generally we have the following result, for which we refer to Theorem 7.12 of Helms [Hel69].

Theorem 2.12. *If D is a compact subset of E and u is a non-negative superharmonic function on E then $\hat{\mathfrak{R}}_u^D$ is a potential, i.e. there exists a measure μ on E such that*

$$\hat{\mathfrak{R}}_u^D(x) = \int_E G^E(x,y)\mu(dy), \qquad x \in E. \tag{2.22}$$

If moreover $\mathfrak{R}_v^D$ is harmonic on D then μ is supported by ∂D, cf. Theorem 6.9 in Helms [Hel69].

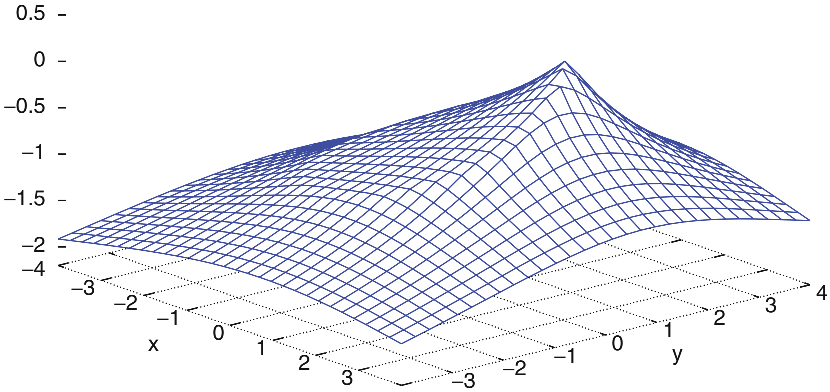

Fig. 7 Reduced of h_x relative to $D = \mathbb{R}^2 \backslash B(y,r)$ with $x \in B(y,r) \backslash \{y\}$.

2.6 Martin Boundary

The Martin boundary theory extends the Poisson integral representation described in Section 2.4 to arbitrary open domains with a non smooth boundary, or having no boundary. Given E a connected open subset of $\mathbb{R}^n$, the Martin boundary ΔE of E is defined in an abstract sense as $\Delta E := \hat{E} \backslash E$, where $\hat{E}$ is a suitable compactification of E. Our aim is now to show that every non-negative harmonic function on E admits an integral representation using its values on the boundary ΔE.

For this, let u be non-negative and harmonic on E, and consider an increasing sequence $(E_n)_{n\in\mathbb{N}}$ of open sets with smooth boundaries $(\partial E_n)_{n\in\mathbb{N}}$ and compact closures, such that

$$E = \bigcup_{n=0}^{\infty} E_n.$$

Then the balayage $\mathfrak{R}_u^{E_n}$ of u relative to E_n coincides with u on E_n, and from Theorem 2.12 it can be represented as

$$\mathfrak{R}_u^{E_n}(x) = \int_{E_n} G^E(x,y) d\mu_n(y)$$

where μ_n is a measure supported by ∂E_n. Note that since

$$\mathfrak{R}_u^{E_n}(x) = u(x), \qquad x \in E_k, \quad k \geq n,$$

and

$$\lim_{n\to\infty} G^E(x,y)_{|y\in\partial E_n} = 0, \qquad x \in E,$$

the total mass of μ_n has to increase to infinity:

$$\lim_{n\to\infty} \mu_n(E_n) = \infty.$$

For this reason one decides to renormalize μ_n by fixing $x_0 \in E_1$ and letting

$$\tilde{\mu}_n(dy) := G^E(x_0, y)\mu_n(dy), \qquad n \in \mathbb{N},$$

so that $\tilde{\mu}_n$ has total mass

$$\tilde{\mu}_n(E_n) = u(x_0) < \infty,$$

independently of $n \in \mathbb{N}$. Next, let the kernel K_{x_0} be defined as

$$K_{x_0}(x, y) := \frac{G^E(x, y)}{G^E(x_0, y)}, \qquad x, y \in E,$$

with the relation

$$\hat{\mathfrak{R}}_u^{E_n}(x) = \int_{E_n} K_{x_0}(x, y) d\tilde{\mu}_n(y).$$

The construction of the Martin boundary $\varDelta E$ of E relies on the following theorem by Constantinescu and Cornea, cf. Helms [Hel69], Chapter 12.

Theorem 2.13. *Let E denote a non-compact, locally compact space and consider a family $\varPhi$ of continuous mappings*

$$f : E \to [-\infty, \infty].$$

Then there exists a unique compact space $\hat{E}$ in which E is everywhere dense, such that:

a) every $f \in \varPhi$ can be extended to a function f^* on $\hat{E}$ by continuity,
b) the extended functions separate the points of the boundary $\varDelta E = \hat{E} \backslash E$ in the sense that if $x, y \in \varDelta E$ with $x \neq y$, there exists $f \in \varPhi$ such that $f^*(x) \neq f^*(y)$.

The Martin space is then defined as the unique compact space $\hat{E}$ in which E is everywhere dense, and such that the functions

$$\{y \mapsto K_{x_0}(x, y) \ : \ x \in E\}$$

admit continuous extensions which separate the boundary $\hat{E} \backslash E$. Such a compactification $\hat{E}$ of E exists and is unique as a consequence of the Constantinescu-Cornea Theorem 2.13, applied to the family

$$\varPhi := \{x \mapsto K_{x_0}(x, z) \ : \ z \in E\}.$$

In this way the Martin boundary of E is defined as

$$\varDelta E := \hat{E} \backslash E.$$

The Martin boundary is unique up to an homeomorphism, namely if x_0, $x_0' \in E$, then

$$K_{x_0'}(x,z) = \frac{K_{x_0}(x,z)}{K_{x_0}(x_0',z)}$$

and

$$K_{x_0}(x,z) = \frac{K_{x_0'}(x,z)}{K_{x_0'}(x_0,z)}$$

may have different limits in $\hat{E}'$ which still separate the boundary ΔE. For this reason, in the sequel we will drop the index x_0 in $K_{x_0}(x,z)$. In the next theorem, the Poisson representation formula is extended to Martin boundaries.

Theorem 2.14. *Any non-negative harmonic function h on E can be represented as*

$$h(x) = \int_{\Delta E} K(z,x)\nu(dz), \qquad x \in E,$$

where ν is a non-negative Radon measure on ΔE.

Proof. Since $\tilde{\mu}_n(E_n)$ is bounded (actually it is constant) in $n \in \mathbb{N}$ we can extract a subsequence $(\tilde{\mu}_{n_k})_{k\in\mathbb{N}}$ converging vaguely to a measure μ on $\hat{E}$, i.e.

$$\lim_{k\to\infty} \int_{\hat{E}} f(x)\tilde{\mu}_{n_k}(dx) = \int_{\hat{E}} f(x)\mu(dx), \qquad f \in \mathcal{C}_c(E),$$

see e.g. Ex. 10, p. 81 of Hirsch and Lacombe [HL99]. The continuity of $z \mapsto K(x,z)$ in $z \in \hat{E}$ then implies

$$\begin{aligned} h(x) &= \lim_{n\to\infty} \hat{\mathfrak{R}}_u^{E_n}(x) \\ &= \lim_{k\to\infty} \hat{\mathfrak{R}}_u^{E_{n_k}}(x) \\ &= \lim_{k\to\infty} \int_{\hat{E}} K(z,x)\nu_{n_k}(dz) \\ &= \int_{\hat{E}} K(z,x)\mu(dz), \qquad x \in E. \end{aligned}$$

Finally, ν is supported by ΔE since for all $f \in \mathcal{C}_c(E_n)$,

$$\int_E f(x)\mu(dx) = \lim_{k\to\infty} \int_{E_k} f(x)\tilde{\mu}_{n_k}(dx) = 0.$$

□

When $E = B(y,r)$ one can check by explicit calculation that

$$\lim_{\zeta\to z} K_y(x,\zeta) = \frac{r^2 - \|x-y\|^2}{\|z-x\|^n}, \qquad z \in S(y,r),$$

is the Poisson kernel on $S(y,r)$. In this case we have

$$\mu = \sigma_r^y,$$

which is the normalized surface measure on $S(y,r)$, and the Martin boundary $\Delta B(y,r)$ of $B(y,r)$ equals its usual boundary $S(y,r)$.

3 Markov Processes

3.1 Markov Property

Let $\mathcal{C}_0(\mathbb{R}^n)$ denote the class of continuous functions tending to 0 at infinity. Recall that f is said to tend to 0 at infinity if for all $\varepsilon > 0$ there exists a compact subset K of $\mathbb{R}^n$ such that $|f(x)| \leq \varepsilon$ for all $x \in \mathbb{R}^n \backslash K$.

Definition 3.1. An $\mathbb{R}^n$-valued stochastic process, i.e. a family $(X_t)_{t\in\mathbb{R}_+}$ of random variables on a probability space $(\Omega, \mathcal{F}, P)$, is a Markov process if for all $t \in \mathbb{R}_+$ the σ-fields

$$\mathcal{F}_t^+ := \sigma(X_s \ : \ s \geq t)$$

and

$$\mathcal{F}_t := \sigma(X_s \ : \ 0 \leq s \leq t).$$

are conditionally independent given X_t.

The above condition can be restated by saying that for all $A \in \mathcal{F}_t^+$ and $B \in \mathcal{F}_t$ we have

$$P(A \cap B \mid X_t) = P(A \mid X_t) P(B \mid X_t),$$

cf. Chung [Chu95]. This definition naturally entails that:

i) $(X_t)_{t\in\mathbb{R}_+}$ is adapted with respect to $(\mathcal{F}_t)_{t\in\mathbb{R}_+}$, i.e. X_t is $\mathcal{F}_t$-measurable, $t \in \mathbb{R}_+$, and
ii) X_u is conditionally independent of $\mathcal{F}_t$ given X_t, for all $u \geq t$, i.e.

$$\mathbb{E}[f(X_u) \mid \mathcal{F}_t] = \mathbb{E}[f(X_u) \mid X_t], \qquad 0 \leq t \leq u,$$

for any bounded measurable function f on $\mathbb{R}^n$.

In particular,

$$P(X_u \in A \mid \mathcal{F}_t) = \mathbb{E}[\mathbf{1}_A(X_u) \mid \mathcal{F}_t] = \mathbb{E}[\mathbf{1}_A(X_u) \mid X_t] = P(X_u \in A \mid X_t),$$

$A \in \mathcal{B}(\mathbb{R}^n)$. Processes with independent increments provide simple examples of Markov processes. Indeed, if $(X_t)_{t\in\mathbb{R}^n}$ has independent increments, then for all bounded measurable functions f, g we have

$$\begin{aligned}
&\mathbb{E}[f(X_{t_1},\dots,X_{t_n})g(X_{s_1},\dots,X_{s_n}) \mid X_t] \\
&= \mathbb{E}[f(X_{t_1}-X_t+x,\dots,X_{t_n}-X_t+x) \\
&\quad \times g(X_{s_1}-X_t+x,\dots,X_{s_n}-X_t+x)]_{x=X_t} \\
&= \mathbb{E}[f(X_{t_1}-X_t+x,\dots,X_{t_n}-X_t+x)]_{x=X_t} \\
&\quad \times \mathbb{E}[g(X_{s_1}-X_t+x,\dots,X_{s_n}-X_t+x)]_{x=X_t} \\
&= \mathbb{E}[f(X_{t_1},\dots,X_{t_n}) \mid X_t]\mathbb{E}[g(X_{s_1},\dots,X_{s_n}) \mid X_t],
\end{aligned}$$

$0 \le s_1 < \cdots < s_n < t < t_1 < \cdots < t_n$.

In discrete time, a sequence $(X_n)_{n\in\mathbb{N}}$ of random variables is said to be a Markov chain if for all $n \in \mathbb{N}$, the σ-algebras

$$\mathcal{F}_n = \sigma(\{X_k \ : \ k \le n\})$$

and

$$\mathcal{F}_n^+ = \sigma(\{X_k \ : \ k \ge n\})$$

are independent conditionally to X_n. In particular, for every $\mathcal{F}_n^+$-measurable bounded random variable F we have

$$\mathbb{E}[F \mid \mathcal{F}_n] = \mathbb{E}[F \mid X_n], \qquad n \in \mathbb{N}.$$

3.2 Transition Kernels and Semigroups

A transition kernel is a mapping $P(x, dy)$ such that

i) for every $x \in E$, $A \mapsto P(x, A)$ is a probability measure, and
ii) for every $A \in \mathcal{B}(E)$, the mapping $x \mapsto P(x, A)$ is a measurable function.

The transition kernel $\mu_{s,t}$ associated to a Markov process $(X_t)_{t\in\mathbb{R}_+}$ is defined as

$$\mu_{s,t}(x, A) = P(X_t \in A \mid X_s = x) \qquad 0 \le s \le t,$$

and we have

$$\mu_{s,t}(X_s, A) = P(X_t \in A \mid X_s) = P(X_t \in A \mid \mathcal{F}_s), \qquad 0 \le s \le t.$$

The transition operator $(T_{s,t})_{0\le s\le t}$ associated to $(X_t)_{t\in\mathbb{R}_+}$ is defined as

$$T_{s,t}f(x) := \mathbb{E}[f(X_t) \mid X_s = x] = \int_{\mathbb{R}^n} f(y)\mu_{s,t}(x, dy), \qquad x \in \mathbb{R}^n.$$

Letting $p_{s,t}(x)$ denote the density of $X_t - X_s$ we have

$$\mu_{s,t}(x, A) = \int_A p_{s,t}(y - x)dy, \qquad A \in \mathcal{B}(\mathbb{R}^n),$$

and

$$T_{s,t}f(x) = \int_{\mathbb{R}^n} f(y)p_{s,t}(y-x)dy.$$

In discrete time, a sequence $(X_n)_{n\in\mathbb{N}}$ of random variables is called a homogeneous Markov chain with transition kernel P if

$$\mathbb{E}[f(X_n) \mid \mathcal{F}_m] = P^{n-m}f(X_m), \qquad 0 \leq m \leq n. \tag{3.1}$$

In the sequel we will assume that $(X_t)_{t\in\mathbb{R}_+}$ is time homogeneous, i.e. $\mu_{s,t}$ depends only on the difference $t-s$, and we will denote it by μ_{t-s}. In this case the family $(T_{0,t})_{t\in\mathbb{R}_+}$ is denoted by $(T_t)_{t\in\mathbb{R}_+}$. It defines a transition semigroup associated to $(X_t)_{t\in\mathbb{R}_+}$, with

$$T_tf(x) = \mathbb{E}[f(X_t) \mid X_0 = x] = \int_{\mathbb{R}^n} f(y)\mu_t(x,dy), \qquad x \in \mathbb{R}^n,$$

and satisfies the semigroup property

$$\begin{aligned}
T_tT_sf(x) &= \mathbb{E}[T_sf(X_t) \mid X_0 = x] \\
&= \mathbb{E}[\mathbb{E}[f(X_{t+s}) \mid X_s] \mid X_0 = x] \\
&= \mathbb{E}[\mathbb{E}[f(X_{t+s}) \mid \mathcal{F}_s] \mid X_0 = x] \\
&= \mathbb{E}[f(X_{t+s}) \mid X_0 = x] \\
&= T_{t+s}f(x),
\end{aligned}$$

which can be formulated as the Chapman-Kolmogorov equation

$$\mu_{s+t}(x,A) = \mu_s * \mu_t(x,A) = \int_{\mathbb{R}^n} \mu_s(x,dy)\mu_t(y,A). \tag{3.2}$$

By induction, using (3.2) we obtain

$$\begin{aligned}
&P_x((X_{t_1},\ldots,X_{t_n}) \in B_1 \times \cdots \times B_n) \\
&\qquad = \int_{B_1} \cdots \int_{B_n} \mu_{0,t_1}(x,dx_1)\cdots\mu_{t_{n-1},t_n}(x_{n-1},dx_n)
\end{aligned}$$

for $0 < t_1 < \cdots < t_n$ and $B_1,\ldots,B_n$ Borel subsets of $\mathbb{R}^n$.

If $(X_t)_{t\in\mathbb{R}_+}$ is a homogeneous Markov processes with independent increments, the density $p_t(x)$ of X_t satisfies the convolution property

$$p_{s+t}(x) = \int_{\mathbb{R}^n} p_s(y-x)p_t(y)dy, \qquad x \in \mathbb{R}^n,$$

which is satisfied in particular by processes with stationary and independent increments such as Lévy processes. A typical example of a probability density satisfying such a convolution property is the Gaussian density, i.e.

$$p_t(x) = \frac{1}{(2\pi t)^{n/2}} \exp\left(-\frac{1}{2t}\|x\|^2_{\mathbb{R}^n}\right), \qquad x \in \mathbb{R}^n.$$

From now on we assume that $(T_t)_{t\in\mathbb{R}_+}$ is a strongly continuous Feller semigroup, i.e. a family of positive contraction operators on $\mathcal{C}_0(\mathbb{R}^n)$ such that

i) $T_{s+t} = T_s T_t$, $s, t \geq 0$,

ii) $T_t(\mathcal{C}_0(\mathbb{R}^n)) \subset \mathcal{C}_0(\mathbb{R}^n)$,

iii) $T_t f(x) \to f(x)$ as $t \to 0$, $f \in \mathcal{C}_0(\mathbb{R}^n)$, $x \in \mathbb{R}^n$.

The resolvent of $(T_t)_{t\in\mathbb{R}_+}$ is defined as

$$R_\lambda f(x) := \int_0^\infty e^{-\lambda t} T_t f(x) dt, \qquad x \in \mathbb{R}^n,$$

i.e.

$$R_\lambda f(x) = \mathbb{E}_x \left[\int_0^\infty e^{-\lambda t} f(X_t) dt\right], \qquad x \in \mathbb{R}^n,$$

for sufficiently integrable f on $\mathbb{R}^n$, where $\mathbb{E}_x$ denotes the conditional expectation given that $\{X_0 = x\}$. It satisfies the resolvent equation

$$R_\lambda - R_\mu = (\mu - \lambda) R_\lambda R_\mu, \qquad \lambda, \mu > 0.$$

We refer to [Kal02] for the following result.

Theorem 3.2. *Let $(T_t)_{t\in\mathbb{R}_+}$ be a Feller semigroup on $\mathcal{C}_0(\mathbb{R}^n)$ with resolvent R_λ, $\lambda > 0$. Then there exists an operator A with domain $\mathcal{D} \subset \mathcal{C}_0(\mathbb{R}^n)$ such that*

$$R_\lambda^{-1} = \lambda I - A, \qquad \lambda > 0. \tag{3.3}$$

The operator A is called the generator of $(T_t)_{t\in\mathbb{R}_+}$ and it characterizes $(T_t)_{t\in\mathbb{R}_+}$. Furthermore, the semigroup $(T_t)_{t\in\mathbb{R}_+}$ is differentiable in t for all $f \in \mathcal{D}$ and it satisfies the forward and backward Kolmogorov equations

$$\frac{dT_t f}{dt} = T_t A f, \qquad \text{and} \qquad \frac{dT_t f}{dt} = A T_t f.$$

Note that the integral

$$\begin{aligned} \int_0^\infty p_t(x,y) dt &= \frac{\Gamma(n/2 - 1)}{2\pi^{n/2}\|x - y\|^{n-2}} \\ &= \frac{n-2}{2 s_n \|x - y\|^{n-2}} \\ &= (n/2 - 1) h_y(x) \end{aligned}$$

of the Gaussian transition density function is proportional to the Newton potential kernel $x \mapsto 1/\|x-y\|^{n-2}$ for $n \geq 3$. Hence the resolvent $R_0 f$ associated to the Gaussian semigroup $T_t f(x) = \int_{\mathbb{R}^n} f(y) p_t(x,y)dy$ is a potential in the sense of Definition 2.10, since:

$$\begin{aligned}
R_0 f(x) &= \int_0^\infty T_t f(x) dt \\
&= \mathbb{E}_x \left[\int_0^\infty f(B_t) dt \right] \\
&= \int_{\mathbb{R}^n} f(y) \int_0^\infty p_t(x,y) dt dy \\
&= \frac{n-2}{2 s_n} \int_{\mathbb{R}^n} \frac{f(y)}{\|x-y\|^{n-2}} dy.
\end{aligned}$$

More generally, for $\lambda > 0$ we have

$$\begin{aligned}
R_\lambda f(x) &= (\lambda I - A)^{-1} f(x) \\
&= \int_0^\infty e^{-\lambda t} T_t f(x) dt \\
&= \int_0^\infty e^{-\lambda t} e^{tA} f(x) dt \\
&= \int_0^\infty e^{-\lambda t} T_t f(x) dt \\
&= \int_0^\infty \int_{\mathbb{R}^n} f(y) e^{-\lambda t} p_t(x,y) dy dt \\
&= \int_{\mathbb{R}^n} f(y) g^\lambda(x,y) dy, \qquad x \in \mathbb{R}^n,
\end{aligned}$$

where $g^\lambda(x,y)$ is the λ-potential kernel defined as

$$g^\lambda(x,y) := \int_0^\infty e^{-\lambda t} p_t(x,y) dt, \tag{3.4}$$

and $R_\lambda f$ is also called a λ-potential.

Recall that the Hille-Yosida theorem also allows one to construct a strongly continuous semigroup from a generator A.

In another direction it is possible to associate a Markov process to any time homogeneous transition function satisfying $\mu_0(x,dy) = \delta_x(dy)$ and the Chapman-Kolmogorov equation (3.2), cf. e.g. Theorem 4.1.1 of Ethier and Kurtz [EK86].

3.3 Hitting Times

Definition 3.3. An a.s. non-negative random variable τ is called a stopping time with respect to a filtration $\mathcal{F}_t$ if

$$\{\tau \le t\} \in \mathcal{F}_t, \qquad t > 0.$$

The σ-algebra $\mathcal{F}_\tau$ is defined as the collection of measurable sets A such that

$$A \cap \{\tau < t\} \in \mathcal{F}_t$$

for all $t > 0$. Note that for all $s > 0$ we have

$$\{\tau < s\},\ \{\tau \le s\},\ \{\tau > s\},\ \{\tau \ge s\} \in \mathcal{F}_\tau.$$

Definition 3.4. One says that the process $(X_t)_{t\in\mathbb{R}_+}$ has the strong Markov property if for any P-a.s. finite $\mathcal{F}_t$-stopping time τ we have

$$\mathbb{E}[f(X(\tau+t)) \mid \mathcal{F}_\tau] = \mathbb{E}[f(X(t)) \mid X_0 = x]_{x=X_\tau} = T_t f(X_\tau), \tag{3.5}$$

for all bounded measurable f.

The hitting time τ_B of a Borel set $B \subset \mathbb{R}^n$ is defined as

$$\tau_B = \inf\{t > 0 \ : \ X_t \in B\},$$

with the convention $\inf \emptyset = +\infty$. A set B such that $P_x(\tau_B < \infty) = 0$ for all $x \in \mathbb{R}^n$ is said to be *polar*.

In discrete time it can be easily shown that hitting times are stopping times, from the relation

$$\{\tau_B \le n\}^c = \{\tau_B > n\} = \bigcap_{k=0}^{n} \{X_k \notin B\} \in \mathcal{F}_n,$$

however in continuous time the situation is more complicated. From e.g. Lemma 7.6 of Kallenberg [Kal02], we have that τ_B is a stopping time provided B is closed and $(X_t)_{t\in\mathbb{R}_+}$ is continuous, or B is open and $(X_t)_{t\in\mathbb{R}_+}$ is right-continuous.

Definition 3.5. The last exit time from B is denoted by l_B and defined as

$$l_B = \sup\{t > 0 \ : \ X_t \in B\},$$

with $l_B = 0$ if $\tau_B = +\infty$.

We say that B is recurrent if $P_x(l_B = +\infty) = 1$, $x \in \mathbb{R}^n$, and that B is transient if $l_B < \infty$, P-a.s., i.e. $P_x(l_B = +\infty) = 0$, $x \in \mathbb{R}^n$.

3.4 Dirichlet Forms

Before turning to a presentation of stochastic calculus we briefly describe the notion of Dirichlet form, which provides a functional analytic interpretation of the Dirichlet problem. A Dirichlet form is a positive bilinear form $\mathcal{E}$ defined on a domain $\mathbb{D}$ dense in a Hilbert space H of real-valued functions, such that

i) the space $\mathbb{D}$, equipped with the norm

$$\|f\|_{\mathbb{D}} := \sqrt{\|f\|_H^2 + \mathcal{E}(f,f)},$$

is a Hilbert space, and
ii) for any $f \in \mathbb{D}$ we have $\min(f,1) \in \mathbb{D}$ and

$$\mathcal{E}(\min(f,1), \min(f,1)) \leq \mathcal{E}(f,f).$$

The classical example of Dirichlet form is given by $H = L^2(\mathbb{R}^n)$ and

$$\mathcal{E}(f,g) := \int_{\mathbb{R}^n} \sum_{i=1}^n \frac{\partial f}{\partial x_i}(x) \frac{\partial g}{\partial x_i}(x) dx.$$

The generator $\mathcal{L}$ of $\mathcal{E}$ is defined by $\mathcal{L}f = g$, $f \in \mathbb{D}$, if for all $h \in \mathbb{D}$ we have

$$\mathcal{E}(f,h) = -\langle g, h \rangle_H.$$

It is known, cf. e.g. Bouleau and Hirsch [BH91], that a self-ajoint operator $\mathcal{L}$ on $H = L^2(\mathbb{R}^n)$ with domain $\mathrm{Dom}(\mathcal{L})$ is the generator of a Dirichlet form if and only if

$$\langle \mathcal{L}f, (f-1)^+ \rangle_{L^2(\mathbb{R}^n)} \leq 0, \qquad f \in \mathrm{Dom}(\mathcal{L}).$$

On the other hand, $\mathcal{L}$ is the generator of a strongly continuous semigroup $(P_t)_{t\in\mathbb{R}_+}$ on $H = L^2(\mathbb{R}^n)$ if and only if $(P_t)_{t\in\mathbb{R}_+}$ is sub-Markovian, i.e. for all $f \in L^2(\mathbb{R}^n)$,

$$0 \leq f \leq 1 \Longrightarrow 0 \leq P_t f \leq 1, \qquad t \in \mathbb{R}_+.$$

We refer to Ma and Röckner [MR92] for more details on the connection between stochastic processes and Dirichlet forms. Coming back to the Dirichlet problem

$$\begin{cases} \Delta u = 0, & x \in D, \\ \\ u(x) = 0, & x \in \partial D. \end{cases}$$

If f and g are $\mathcal{C}^1$ with compact support in D we have

$$\int_D g(x) \Delta f(x) dx = -\sum_{i=1}^n \int_D \frac{\partial f}{\partial x_i}(x) \frac{\partial g}{\partial x_i}(x) dx = -\mathcal{E}(f,g).$$

Here, $\mathbb{D}$ is the subspace of functions in $L^2(\mathbb{R}^n)$ whose derivative in distribution sense belongs to $L^2(\mathbb{R}^n)$, with norm

$$\|f\|_{\mathbb{D}}^2 = \int_{\mathbb{R}^n} |f(x)|^2 dx + \int_{\mathbb{R}^n} \sum_{i=1}^{n} \left| \frac{\partial f}{\partial x_i}(x) \right|^2 dx.$$

Hence the Dirichlet problem for f can be formulated as

$$\mathcal{E}(f, g) = 0,$$

for all g in the completion of $\mathcal{C}_c^\infty(D)$ with respect to the $\|\cdot\|_{\mathbb{D}}$-norm. Finally we mention the notion of capacity of an open set A, defined as

$$C(A) := \inf\{\|u\|_{\mathbb{D}} \ : \ u \in \mathbb{D} \text{ and } u \geq 1 \text{ on } A\}.$$

The notion of zero-capacity set is finer than that of zero-measure sets and gives rise to the notion of properties that hold in the quasi-everywhere sense, cf. Bouleau and Hirsch [BH91].

4 Stochastic Calculus

4.1 Brownian Motion and the Poisson Process

Let $(\Omega, \mathcal{F}, P)$ be a probability space and $(\mathcal{F}_t)_{t\in\mathbb{R}_+}$ a filtration, i.e. an increasing family of sub σ-algebras of $\mathcal{F}$. We assume that $(\mathcal{F}_t)_{t\in\mathbb{R}_+}$ is continuous on the right, i.e.

$$\mathcal{F}_t = \bigcap_{s>t} \mathcal{F}_s, \qquad t \in \mathbb{R}_+.$$

Recall that a process $(M_t)_{t\in\mathbb{R}_+}$ in $L^1(\Omega)$ is called an $\mathcal{F}_t$-martingale if $\mathbb{E}[M_t|\mathcal{F}_s] = M_s$, $0 \leq s \leq t$.

For example, if $(X_t)_{t\in[0,T]}$ is a (non homogeneous) Markov process with semigroup $(P_{s,t})_{0\leq s\leq t\leq T}$ satisfying

$$P_{s,t}f(X_s) = \mathbb{E}[f(X_t) \mid X_s] = \mathbb{E}[f(X_t) \mid \mathcal{F}_s], \quad 0 \leq s \leq t \leq T,$$

on $\mathcal{C}_b^2(\mathbb{R}^n)$ functions, with

$$P_{s,t} \circ P_{t,u} = P_{s,u}, \qquad 0 \leq s \leq t \leq u \leq T,$$

then $(P_{t,T}f(X_t))_{t\in[0,T]}$ is an $\mathcal{F}_t$-martingale:

$$\begin{aligned} \mathbb{E}[P_{t,T}f(X_t) \mid \mathcal{F}_s] &= \mathbb{E}[\mathbb{E}[f(X_T) \mid \mathcal{F}_t] \mid \mathcal{F}_s] \\ &= \mathbb{E}[f(X_T) \mid \mathcal{F}_s] \\ &= P_{s,T}f(X_s), \qquad 0 \leq s \leq t \leq T. \end{aligned}$$

Definition 4.1. A martingale $(M_t)_{t\in\mathbb{R}_+}$ in $L^2(\Omega)$ (i.e. $\mathbb{E}[|M_t|^2] < \infty$, $t \in \mathbb{R}_+$) and such that

$$\mathbb{E}[(M_t - M_s)^2|\mathcal{F}_s] = t - s, \qquad 0 \le s < t, \tag{4.1}$$

is called a normal martingale.

Every square-integrable process $(M_t)_{t\in\mathbb{R}_+}$ with centered independent increments and generating the filtration $(\mathcal{F}_t)_{t\in\mathbb{R}_+}$ satisfies

$$\mathbb{E}[(M_t - M_s)^2|\mathcal{F}_s] = \mathbb{E}[(M_t - M_s)^2], \qquad 0 \le s \le t,$$

hence the following remark.

Remark 4.2. A square-integrable process $(M_t)_{t\in\mathbb{R}_+}$ with centered independent increments is a normal martingale if and only if

$$\mathbb{E}[(M_t - M_s)^2] = t - s, \qquad 0 \le s \le t.$$

In our presentation of stochastic integration we will restrict ourselves to normal martingales. As will be seen in the next sections, this family contains Brownian motion and the standard compensated Poisson process as particular cases.

Remark 4.3. A martingale $(M_t)_{t\in\mathbb{R}_+}$ is normal if and only if $(M_t^2 - t)_{t\in\mathbb{R}_+}$ is a martingale, i.e.

$$\mathbb{E}[M_t^2 - t|\mathcal{F}_s] = M_s^2 - s, \qquad 0 \le s < t.$$

Proof. This follows from the equalities

$$\begin{aligned}
&\mathbb{E}[(M_t - M_s)^2|\mathcal{F}_s] - (t - s) \\
&= \mathbb{E}[M_t^2 - M_s^2 - 2(M_t - M_s)M_s|\mathcal{F}_s] - (t - s) \\
&= \mathbb{E}[M_t^2 - M_s^2|\mathcal{F}_s] - 2M_s\mathbb{E}[M_t - M_s|\mathcal{F}_s] - (t - s) \\
&= \mathbb{E}[M_t^2|\mathcal{F}_s] - t - (\mathbb{E}[M_s^2|\mathcal{F}_s] - s).
\end{aligned}$$

□

Throughout the remainder of this chapter, $(M_t)_{t\in\mathbb{R}_+}$ will be a normal martingale.

We now turn to the Brownian motion and the compensated Poisson process as the fundamental examples of normal martingales. Our starting point is now a family $(\xi_n)_{n\in\mathbb{N}}$ of independent standard (i.e. centered and with unit variance) Gaussian random variables under $\gamma_\mathbb{N}$, constructed as the canonical projections from $(\mathbb{R}^\mathbb{N}, \mathcal{B}_{\mathbb{R}^\mathbb{N}}, \gamma_\mathbb{N})$ into $\mathbb{R}$. The measure $\gamma_\mathbb{N}$ is characterized by its Fourier transform

$$\begin{aligned}\alpha \mapsto \mathbb{E}\left[\mathrm{e}^{i\langle \xi,\alpha\rangle_{\ell^2(\mathbb{N})}}\right] &= \mathbb{E}\left[\mathrm{e}^{i\sum_{n=0}^\infty \xi_n\alpha_n}\right] \\ &= \prod_{n=0}^\infty \mathrm{e}^{-\alpha_n^2/2} \\ &= \mathrm{e}^{-\frac{1}{2}\|\alpha\|^2_{\ell^2(\mathbb{N})}}, \qquad \alpha \in \ell^2(\mathbb{N}),\end{aligned}$$

i.e. $\langle \xi, \alpha\rangle_{\ell^2(\mathbb{N})}$ is a centered Gaussian random variable with variance $\|\alpha\|^2_{\ell^2(\mathbb{N})}$. Let $(e_n)_{n\in\mathbb{N}}$ denote an orthonormal basis of $L^2(\mathbb{R}_+)$.

Definition 4.4. Given $u \in L^2(\mathbb{R}_+)$ with decomposition

$$u = \sum_{n=0}^\infty \langle u, e_n\rangle e_n,$$

we let $J_1 : L^2(\mathbb{R}_+) \longrightarrow L^2(\mathbb{R}^\mathbb{N}, \gamma^\mathbb{N})$ be defined as

$$J_1(u) = \sum_{n=0}^\infty \xi_n \langle u, e_n\rangle.$$

We have the isometry property

$$\begin{aligned}\mathbb{E}[|J_1(u)|^2] &= \sum_{k=0}^\infty |\langle u, e_n\rangle|^2 \mathbb{E}[|\xi_n|^2] \\ &= \sum_{k=0}^\infty |\langle u, e_n\rangle|^2 \\ &= \|u\|^2_{L^2(\mathbb{R}_+)},\end{aligned} \tag{4.2}$$

and

$$\begin{aligned}\mathbb{E}\left[\mathrm{e}^{iJ_1(u)}\right] &= \prod_{n=0}^\infty \mathbb{E}\left[\mathrm{e}^{i\xi_n\langle u, e_n\rangle}\right] \\ &= \prod_{n=0}^\infty \mathrm{e}^{-\frac{1}{2}\langle u,e_n\rangle^2_{L^2(\mathbb{R}_+)}} \\ &= \exp\left(-\frac{1}{2}\|u\|^2_{L^2(\mathbb{R}_+)}\right),\end{aligned}$$

hence $J_1(u)$ is a centered Gaussian random variable with variance $\|u\|^2_{L^2(\mathbb{R}_+)}$. Next is a constructive approach to the definition of Brownian motion, using the decomposition

$$\mathbf{1}_{[0,t]} = \sum_{n=0}^\infty e_n \int_0^t e_n(s)ds.$$

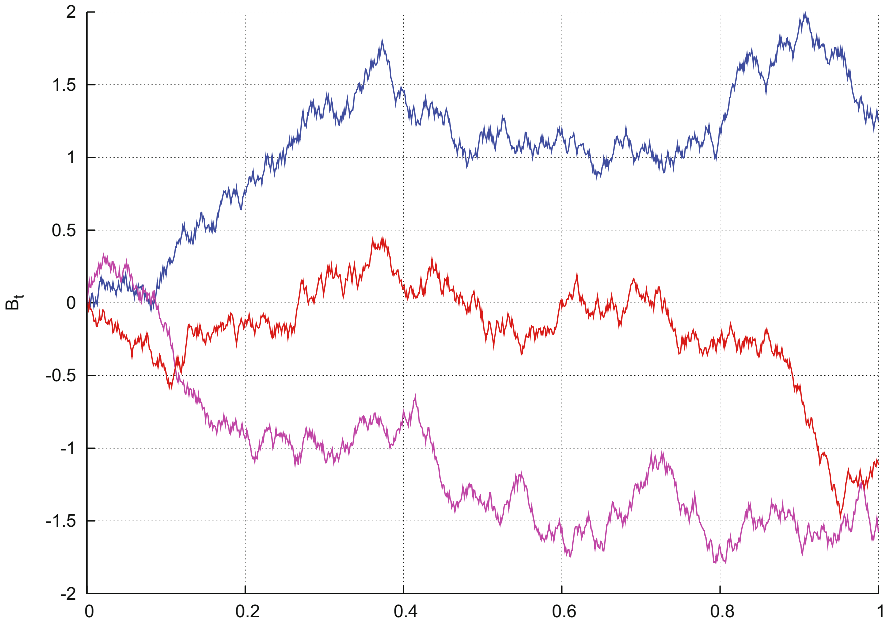

Fig. 8 Sample paths of one-dimensional Brownian motion.

Definition 4.5. For all $t \in \mathbb{R}_+$, let

$$B_t(\omega) := J_1(\mathbf{1}_{[0,t]}) = \sum_{n=0}^{\infty} \xi_n(\omega) \int_0^t e_n(s)ds. \tag{4.3}$$

Clearly, $B_t - B_s = J_1(\mathbf{1}_{[s,t]})$ is a Gaussian centered random variable with variance:

$$\mathbb{E}[(B_t - B_s)^2] = \mathbb{E}[|J_1(\mathbf{1}_{[s,t]})|^2] = \|\mathbf{1}_{[s,t]}\|^2_{L^2(\mathbb{R}_+)} = t - s, \tag{4.4}$$

cf. Figure 8. Moreover, the isometry formula (4.2) shows that if $u_1, \ldots, u_n$ are orthogonal in $L^2(\mathbb{R}_+)$ then $J_1(u_1), \ldots, J_1(u_n)$ are also mutually orthogonal in $L^2(\Omega)$, hence from Corollary 16.1 of Jacod and Protter [JP00], we get the following.

Proposition 4.6. *Let $u_1, \ldots, u_n$ be an orthogonal family in $L^2(\mathbb{R}_+)$, i.e.*

$$\langle u_i, u_j \rangle_{L^2(\mathbb{R}_+)} = 0, \qquad 1 \le i \ne j \le n.$$

Then $(J_1(u_1), \ldots, J_1(u_n))$ is a vector of independent Gaussian centered random variables with respective variances $\|u_1\|^2_{L^2(\mathbb{R}_+)}, \ldots, \|u_1\|^2_{L^2(\mathbb{R}_+)}$.

As a consequence of Proposition 4.6, $(B_t)_{t\in\mathbb{R}_+}$ has centered independent increments hence it is a martingale.

Moreover, from Relation (4.4) and Remark 4.2 we deduce the following proposition.

Proposition 4.7. *The Brownian motion* $(B_t)_{t\in\mathbb{R}_+}$ *is a* normal *martingale.*

The n-dimensional Brownian motion will be constructed as $(B_t^1,\dots,B_t^n)_{t\in\mathbb{R}_+}$ where $(B_t^1)_{t\in\mathbb{R}_+},\dots,(B_t^n)_{t\in\mathbb{R}_+}$ are independent copies of $(B_t)_{t\in\mathbb{R}_+}$, cf. Figure 9 and Figure 10 below.

The compensated Poisson process provides a second example of normal martingale. Let now $(\tau_n)_{n\geq 1}$ denote a sequence of independent and identically exponentially distributed random variables, with parameter $\lambda > 0$, i.e.

$$\mathbb{E}[f(\tau_1,\dots,\tau_n)] = \lambda^n \int_0^\infty \cdots \int_0^\infty \mathrm{e}^{-\lambda(s_1+\cdots+s_n)} f(s_1,\dots,s_n)ds_1\cdots ds_n,$$

for all sufficiently integrable measurable $f : \mathbb{R}_+^n \to \mathbb{R}$. Let also

$$T_n = \tau_1 + \cdots + \tau_n, \qquad n \geq 1.$$

We now consider the canonical point process associated to the family $(T_k)_{k\geq 1}$ of jump times.

Definition 4.8. The point process $(N_t)_{t\in\mathbb{R}_+}$ defined as

$$N_t := \sum_{k=1}^{\infty} \mathbf{1}_{[T_k,\infty)}(t), \qquad t \in \mathbb{R}_+ \tag{4.5}$$

is called the standard Poisson point process.

The process $(N_t)_{t\in\mathbb{R}_+}$ has independent increments which are distributed according to the Poisson law, i.e. for all $0 \leq t_0 \leq t_1 < \cdots < t_n$,

$$(N_{t_1} - N_{t_0}, \dots, N_{t_n} - N_{t_{n-1}})$$

is a vector of independent Poisson random variables with respective parameters

$$(\lambda(t_1 - t_0), \dots, \lambda(t_n - t_{n-1})).$$

We have $\mathbb{E}[N_t] = \lambda t$ and $\mathrm{V}ar[N_t] = \lambda t$, $t \in \mathbb{R}_+$, hence according to Remark 4.2, the process $\lambda^{-1/2}(N_t - \lambda t)$ is a normal martingale.

Compound Poisson processes provide other examples of normal martingales. Given $(Y_k)_{k\geq 1}$ a sequence of independent identically distributed random variables, define the compound Poisson process as

$$X_t = \sum_{k=1}^{N_t} Y_k, \qquad t \in \mathbb{R}_+.$$

The compensated compound Poisson martingale defined as

$$M_t := \frac{X_t - \lambda t \mathbb{E}[Y_1]}{\sqrt{\lambda \mathrm{Var}[Y_1]}}, \qquad t \in \mathbb{R}_+,$$

is a normal martingale.

4.2 Stochastic Integration

In this section we construct the Itô stochastic integral of square-integrable adapted processes with respect to normal martingales. The filtration $(\mathcal{F}_t)_{t\in\mathbb{R}_+}$ is generated by $(M_t)_{t\in\mathbb{R}_+}$:

$$\mathcal{F}_t = \sigma(M_s \ : \ 0 \leq s \leq t), \qquad t \in \mathbb{R}_+.$$

A process $(X_t)_{t\in\mathbb{R}_+}$ is said to be $\mathcal{F}_t$-adapted if X_t is $\mathcal{F}_t$-measurable for all $t \in \mathbb{R}_+$.

Definition 4.9. Let $L^p_{ad}(\Omega \times \mathbb{R}_+)$, $p \in [1, \infty]$, denote the space of $\mathcal{F}_t$-adapted processes in $L^p(\Omega \times \mathbb{R}_+)$.

Stochastic integrals will be first constructed as integrals of simple predictable processes.

Definition 4.10. Let $\mathcal{S}$ be a space of random variables dense in $L^2(\Omega, \mathcal{F}, P)$. Consider the space $\mathcal{P}$ of simple predictable processes $(u_t)_{t\in\mathbb{R}_+}$ of the form

$$u_t = \sum_{i=1}^{n} F_i \mathbf{1}_{(t^n_{i-1}, t^n_i]}(t), \qquad t \in \mathbb{R}_+, \tag{4.6}$$

where F_i is $\mathcal{F}_{t^n_{i-1}}$-measurable, $i = 1, \ldots, n$.

One easily checks that the set $\mathcal{P}$ of simple predictable processes forms a linear space. On the other hand, from Lemma 1.1 of Ikeda and Watanabe [IW89], p. 22 and p. 46, the space $\mathcal{P}$ of simple predictable processes is dense in $L^p_{ad}(\Omega \times \mathbb{R}_+)$ for all $p \geq 1$.

Proposition 4.11. *The stochastic integral with respect to the normal martingale $(M_t)_{t\in\mathbb{R}_+}$, defined on simple predictable processes $(u_t)_{t\in\mathbb{R}_+}$ of the form (4.6) by*

$$\int_0^\infty u_t dM_t := \sum_{i=1}^{n} F_i (M_{t_i} - M_{t_{i-1}}), \tag{4.7}$$

extends to $u \in L^2_{ad}(\Omega \times \mathbb{R}_+)$ via the isometry formula

$$\mathbb{E}\left[\int_0^\infty u_t dM_t \int_0^\infty v_t dM_t\right] = \mathbb{E}\left[\int_0^\infty u_t v_t dt\right]. \tag{4.8}$$

Proof. We start by showing that the isometry (4.8) holds for the simple predictable process $u = \sum_{i=1}^n G_i \mathbf{1}_{(t_{i-1},t_i]}$, with $0 = t_0 < t_1 < \cdots t_n$:

$$\begin{aligned}
&\mathbb{E}\left[\left(\int_0^\infty u_t dM_t\right)^2\right] = \mathbb{E}\left[\left(\sum_{i=1}^n G_i(M_{t_i} - M_{t_{i-1}})\right)^2\right] \\
&= \mathbb{E}\left[\sum_{i=1}^n |G_i|^2 (M_{t_i} - M_{t_{i-1}})^2\right] \\
&\quad +2\mathbb{E}\left[\sum_{1\le i<j\le n} G_i G_j (M_{t_i} - M_{t_{i-1}})(M_{t_j} - M_{t_{j-1}})\right] \\
&= \sum_{i=1}^n \mathbb{E}[\mathbb{E}[|G_i|^2 (M_{t_i} - M_{t_{i-1}})^2 | \mathcal{F}_{t_{i-1}}]] \\
&\quad +2 \sum_{1\le i<j\le n} \mathbb{E}[\mathbb{E}[G_i G_j (M_{t_i} - M_{t_{i-1}})(M_{t_j} - M_{t_{j-1}}) | \mathcal{F}_{t_{j-1}}]] \\
&= \sum_{i=1}^n \mathbb{E}[|G_i|^2 \mathbb{E}[(M_{t_i} - M_{t_{i-1}})^2 | \mathcal{F}_{t_{i-1}}]] \\
&\quad +2 \sum_{1\le i<j\le n} \mathbb{E}[G_i G_j (M_{t_i} - M_{t_{i-1}}) \mathbb{E}[(M_{t_j} - M_{t_{j-1}}) | \mathcal{F}_{t_{j-1}}]] \\
&= \mathbb{E}\left[\sum_{i=1}^n |G_i|^2 (t_i - t_{i-1})\right] \\
&= \mathbb{E}[\|u\|^2_{L^2(\mathbb{R}_+)}].
\end{aligned}$$

The stochastic integral operator extends to $L^2_{ad}(\Omega \times \mathbb{R}_+)$ by density and a Cauchy sequence argument, applying the isometry (4.8). □

Proposition 4.12. *For any* $u \in L^2_{ad}(\Omega \times \mathbb{R}_+)$ *we have*

$$\mathbb{E}\left[\int_0^\infty u_s dM_s \Big| \mathcal{F}_t\right] = \int_0^t u_s dM_s, \qquad t \in \mathbb{R}_+.$$

In particular, $\int_0^t u_s dM_s$ *is* $\mathcal{F}_t$*-measurable,* $t \in \mathbb{R}_+$.

Proof. Let $u \in \mathcal{P}$ have the form $u = G\mathbf{1}_{(a,b]}$, where G is bounded and $\mathcal{F}_a$-measurable.

i) If $0 \le a \le t$ we have

$$\begin{aligned}
\mathbb{E}\left[\int_0^\infty u_s dM_s \Big| \mathcal{F}_t\right] &= \mathbb{E}\left[G(M_b - M_a) | \mathcal{F}_t\right] \\
&= G\mathbb{E}\left[(M_b - M_a) | \mathcal{F}_t\right]
\end{aligned}$$

$$
\begin{aligned}
&= G\mathbb{E}\left[(M_b - M_t)|\mathcal{F}_t\right] + G\mathbb{E}\left[(M_t - M_a)|\mathcal{F}_t\right] \\
&= G(M_t - M_a) \\
&= \int_0^\infty \mathbf{1}_{[0,t]}(s) u_s dM_s.
\end{aligned}
$$

ii) If $0 \le t \le a$ we have for all bounded $\mathcal{F}_t$-measurable random variable F:

$$
\mathbb{E}\left[F \int_0^\infty u_s dM_s\right] = \mathbb{E}\left[FG(M_b - M_a)\right] = 0,
$$

hence

$$
\mathbb{E}\left[\int_0^\infty u_s dM_s \Big| \mathcal{F}_t\right] = \mathbb{E}\left[G(M_b - M_a)|\mathcal{F}_t\right] = 0 = \int_0^\infty \mathbf{1}_{[0,t]}(s) u_s dM_s.
$$

This statement is extended by linearity and density, since from the continuity of the conditional expectation on L^2 we have:

$$
\begin{aligned}
&\mathbb{E}\left[\left(\int_0^t u_s dM_s - \mathbb{E}\left[\int_0^\infty u_s dM_s \Big| \mathcal{F}_t\right]\right)^2\right] \\
&= \lim_{n\to\infty} \mathbb{E}\left[\left(\int_0^t u_s^n dM_s - \mathbb{E}\left[\int_0^\infty u_s dM_s \Big| \mathcal{F}_t\right]\right)^2\right] \\
&= \lim_{n\to\infty} \mathbb{E}\left[\left(\mathbb{E}\left[\int_0^\infty u_s^n dM_s - \int_0^\infty u_s dM_s \Big| \mathcal{F}_t\right]\right)^2\right] \\
&\le \lim_{n\to\infty} \mathbb{E}\left[\mathbb{E}\left[\left(\int_0^\infty u_s^n dM_s - \int_0^\infty u_s dM_s\right)^2 \Big| \mathcal{F}_t\right]\right] \\
&\le \lim_{n\to\infty} \mathbb{E}\left[\left(\int_0^\infty (u_s^n - u_s) dM_s\right)^2\right] \\
&= \lim_{n\to\infty} \mathbb{E}\left[\int_0^\infty |u_s^n - u_s|^2 ds\right] \\
&= 0.
\end{aligned}
$$

□

In particular, since $\mathcal{F}_0 = \{\emptyset, \Omega\}$, the Itô integral is a centered random variable by Proposition 4.12, i.e.

$$
\mathbb{E}\left[\int_0^\infty u_s dM_s\right] = 0. \tag{4.9}
$$

The following is an immediate corollary of Proposition 4.12.

Corollary 4.13. *The indefinite stochastic integral* $\left(\int_0^t u_s dM_s\right)_{t\in\mathbb{R}_+}$ *of* $u \in L^2_{ad}(\Omega \times \mathbb{R}_+)$ *is a martingale, i.e.:*

$$\mathbb{E}\left[\int_0^t u_r dM_r \Big| \mathcal{F}_s\right] = \int_0^s u_r dM_r, \qquad 0 \le s \le t.$$

Clearly, from Definitions 4.5 and (4.7), $J_1(u)$ coincides with the single stochastic integral $I_1(u)$ with respect to $(B_t)_{t\in\mathbb{R}_+}$.

On the other hand, since the standard compensated Poisson martingale $(M_t)_{t\in\mathbb{R}_+} = (N_t - t)_{t\in\mathbb{R}_+}$ is a normal martingale, the integral

$$\int_0^T u_t dM_t$$

is also defined in the Itô sense, i.e. as an $L^2(\Omega)$-limit of stochastic integrals of simple adapted processes.

4.3 Quadratic Variation

We now introduce the notion of quadratic variation for normal martingales.

Definition 4.14. The quadratic variation of $(M_t)_{t\in\mathbb{R}_+}$ is the process $([M,M]_t)_{t\in\mathbb{R}_+}$ defined as

$$[M,M]_t = M_t^2 - 2\int_0^t M_s dM_s, \qquad t \in \mathbb{R}_+. \tag{4.10}$$

Let now

$$\pi^n = \{0 = t_0^n < t_1^n < \cdots < t_{n-1}^n < t_n^n = t\}$$

denote a family of subdivision of $[0,t]$, such that $|\pi^n| := \max_{i=1,\dots,n} |t_i^n - t_{i-1}^n|$ converges to 0 as n goes to infinity.

Proposition 4.15. *We have*

$$[M,M]_t = \lim_{n\to\infty} \sum_{i=1}^n (M_{t_i^n} - M_{t_{i-1}^n})^2, \quad t \ge 0,$$

where the limit exists in $L^2(\Omega)$ *and is independent of the sequence* $(\pi^n)_{n\in\mathbb{N}}$ *of subdivisions chosen.*

Proof. As an immediate consequence of the definition 4.7 of the stochastic integral, we have

$$M_s(M_t - M_s) = \int_s^t M_s dM_r, \qquad 0 \le s \le t,$$

and

$$[M, M]_{t_i^n} - [M, M]_{t_{i-1}^n} = M_{t_i^n}^2 - M_{t_{i-1}^n}^2 - 2 \int_{t_{i-1}^n}^{t_i^n} M_s dM_s$$
$$= (M_{t_i^n} - M_{t_{i-1}^n})^2 + 2 \int_{t_{i-1}^n}^{t_i^n} (M_{t_{i-1}^n} - M_s) dM_s,$$

hence

$$\begin{aligned}
&\mathbb{E}\left[\left([M, M]_t - \sum_{i=1}^n (M_{t_i^n} - M_{t_{i-1}^n})^2\right)^2\right] \\
&= \mathbb{E}\left[\left(\sum_{i=1}^n [M, M]_{t_i^n} - [M, M]_{t_{i-1}^n} - (M_{t_i^n} - M_{t_{i-1}^n})^2\right)^2\right] \\
&= 4\mathbb{E}\left[\left(\sum_{i=1}^n \int_0^t \mathbf{1}_{(t_{i-1}^n, t_i^n]}(s)(M_s - M_{t_{i-1}^n}) dM_s\right)^2\right] \\
&= 4\mathbb{E}\left[\sum_{i=1}^n \int_{t_{i-1}^n}^{t_i^n} (M_s - M_{t_{i-1}^n})^2 ds\right] \\
&= 4\mathbb{E}\left[\sum_{i=1}^n \int_{t_{i-1}^n}^{t_i^n} (s - t_{i-1}^n)^2 ds\right] \\
&\leq 4t|\pi|.
\end{aligned}$$

□

Proposition 4.16. *The quadratic variation of Brownian motion* $(B_t)_{t \in \mathbb{R}_+}$ *is*

$$[B, B]_t = t, \quad t \in \mathbb{R}_+.$$

Proof. (cf. e.g. Protter [Pro05], Theorem I-28). For every subdivision $\{0 = t_0^n < \cdots < t_n^n = t = t\}$ we have, by independence of the increments of Brownian motion:

$$\begin{aligned}
&\mathbb{E}\left[\left(t - \sum_{i=1}^n (B_{t_i^n} - B_{t_{i-1}^n})^2\right)^2\right] \\
&= \mathbb{E}\left[\left(\sum_{i=1}^n (B_{t_i^n} - B_{t_{i-1}^n})^2 - (t_i^n - t_{i-1}^n)\right)^2\right] \\
&= \sum_{i=1}^n (t_i^n - t_{i-1}^n)^2 \mathbb{E}\left[\left(\frac{(B_{t_i^n} - B_{t_{i-1}^n})^2}{t_i^n - t_{i-1}^n} - 1\right)^2\right]
\end{aligned}$$

$$= \mathbb{E}[(Z^2 - 1)^2] \sum_{i=0}^{n} (t_i^n - t_{i-1}^n)^2$$
$$\leq t|\pi|\mathbb{E}[(Z^2 - 1)^2],$$

where Z is a standard Gaussian random variable. □

A simple analysis of the Poisson paths shows that the quadratic variation of the compensated Poisson process $(M_t)_{t\in\mathbb{R}_+} = (N_t - t)_{t\in\mathbb{R}_+}$ is

$$[M, M]_t = N_t, \qquad t \in \mathbb{R}_+.$$

Similarly for the compensated compound Poisson martingale

$$M_t := \frac{X_t - \lambda t \mathbb{E}[Y_1]}{\sqrt{\lambda \mathrm{Var}[Y_1]}}, \qquad t \in \mathbb{R}_+,$$

we have

$$[M, M]_t = \sum_{k=1}^{N_t} |Y_k|^2, \qquad t \in \mathbb{R}_+.$$

Definition 4.17. The angle bracket $\langle M, M\rangle_t$ is the unique increasing process such that

$$M_t^2 - \langle M, M\rangle_t, \qquad t \in \mathbb{R}_+,$$

is a martingale.

As a consequence of Remark 4.3 we have

$$\langle M, M\rangle_t = t, \qquad t \in \mathbb{R}_+,$$

for every normal martingale. Moreover,

$$[M, M]_t - \langle M, M\rangle_t, \qquad t \in \mathbb{R}_+,$$

is also a martingale as a consequence of Remark 4.3 and Proposition 4.12, since by Definition 4.14 we have

$$[M, M]_t - \langle M, M\rangle_t = [M, M]_t - t = M_t^2 - t - 2\int_0^t M_s dM_s, \qquad t \in \mathbb{R}_+. \tag{4.11}$$

Definition 4.18. We say that the martingale $(M_t)_{t\in\mathbb{R}_+}$ has the predictable representation property if any square-integrable martingale $(X_t)_{t\in\mathbb{R}_+}$ with respect to $(\mathcal{F}_t)_{t\in\mathbb{R}_+}$ can be represented as

$$X_t = X_0 + \int_0^t u_s dM_s, \qquad t \in \mathbb{R}_+, \tag{4.12}$$

where $(u_t)_{t\in\mathbb{R}_+} \in L^2_{ad}(\Omega \times \mathbb{R}_+)$ is an adapted process such that $u\mathbf{1}_{[0,T]} \in L^2(\Omega \times \mathbb{R}_+)$ for all $T > 0$.

It is known that Brownian motion and the compensated Poisson process have the predictable representation property. This is however not true of compound Poisson processes in general.

Definition 4.19. An equation of the form

$$[M, M]_t = t + \int_0^t \phi_s dM_s, \quad t \in \mathbb{R}_+, \tag{4.13}$$

where $(\phi_t)_{t\in\mathbb{R}_+}$ is a square-integrable adapted process, is called a structure equation, cf. Emery [É90].

As a consequence of (4.11) and (4.12) we have the following proposition.

Proposition 4.20. *Assume that $(M_t)_{t\in\mathbb{R}_+}$ is in $L^4(\Omega)$ and has the predictable representation property. Then $(M_t)_{t\in\mathbb{R}_+}$ satisfies the structure equation* (4.13), *i.e. there exists a square-integrable adapted process $(\phi_t)_{t\in\mathbb{R}_+}$ such that*

$$[M, M]_t = t + \int_0^t \phi_s dM_s, \qquad t \in \mathbb{R}_+.$$

Proof. Since $([M, M]_t - t)_{t\in\mathbb{R}_+}$ is a martingale, the predictable representation property shows the existence of a square-integrable adapted process $(\phi_t)_{t\in\mathbb{R}_+}$ such that

$$[M, M]_t - t = \int_0^t \phi_s dM_s, \qquad t \in \mathbb{R}_+.$$

□

In particular,

a) the Brownian motion $(B_t)_{t\in\mathbb{R}_+}$ satisfies the structure equation (4.13) with $\phi_t = 0$, since the quadratic variation of $(B_t)_{t\in\mathbb{R}_+}$ is $[B, B]_t = t$, $t \in \mathbb{R}_+$. Informally we have $\Delta B_t = \pm\sqrt{\Delta t}$ with equal probabilities 1/2.

b) The compensated Poisson martingale $(M_t)_{t\in\mathbb{R}_+} = \lambda(N_t - t/\lambda^2)_{t\in\mathbb{R}_+}$, where $(N_t)_{t\in\mathbb{R}_+}$ is a standard Poisson process with intensity $1/\lambda^2$ satisfies the structure equation (4.13) with $\phi_t = \lambda \in \mathbb{R}$, $t \in \mathbb{R}_+$, since

$$[M, M]_t = \lambda^2 N_t = t + \lambda M_t, \qquad t \in \mathbb{R}_+.$$

In this case, $\Delta M_t \in \{0, \lambda\}$ with respective probabilities $1 - \lambda^{-2}\Delta t$ and $\lambda^{-2}\Delta t$.

The Azéma martingales correspond to $\phi_t = \beta M_t$, $\beta \in [-2, 0)$, and provide examples of processes having the chaos representation property, but whose increments are not independent, cf. Emery [É90]. Note that not all normal martingales have the predictable representation property. For instance, the compensated compound Poisson martingales do not satisfy a structure equation and do not have the predictable representation property in general.

4.4 Itô's Formula

We consider a normal martingale $(M_t)_{t\in\mathbb{R}_+}$ satisfying the structure equation

$$d[M,M]_t = dt + \phi_t dM_t.$$

Such an equation is satisfied in particular if $(M_t)_{t\in\mathbb{R}_+}$ has the predictable representation property, cf. Proposition 4.20.

The following is a statement of Itô's formula for normal martingales, cf. Émery [É90], Proposition 2, p. 70.

Proposition 4.21. *Assume that $\phi \in L^\infty_{ad}(\mathbb{R}_+ \times \Omega)$. Let $(X_t)_{t\in\mathbb{R}_+}$ be a process given by*

$$X_t = X_0 + \int_0^t u_s dM_s + \int_0^t v_s ds, \tag{4.14}$$

where $(u_s)_{s\in\mathbb{R}_+}, (v_s)_{s\in\mathbb{R}_+}$ are adapted processes in $L^2_{ad}([0,t]\times\Omega)$ for all $t > 0$. We have for $f \in \mathcal{C}^{1,2}(\mathbb{R}_+ \times \mathbb{R})$:

$$\begin{aligned} f(t,X_t) - f(0,X_0) &= \int_0^t \frac{f(s,X_{s^-} + \phi_s u_s) - f(s,X_{s^-})}{\phi_s} dM_s \qquad (4.15)\\ &+ \int_0^t \frac{f(s,X_s + \phi_s u_s) - f(s,X_s) - \phi_s u_s \frac{\partial f}{\partial x}(s,X_s)}{\phi_s^2} ds \\ &+ \int_0^t \frac{\partial f}{\partial x}(s,X_s) v_s ds + \int_0^t \frac{\partial f}{\partial s}(s,X_s) ds. \end{aligned}$$

If $\phi_s = 0$, the terms

$$\frac{f(X_{s^-} + \phi_s u_s) - f(X_{s^-})}{\phi_s}$$

and

$$\frac{f(X_s + \phi_s u_s) - f(X_s) - \phi_s u_s f'(X_s)}{\phi_s^2}$$

can be replaced by their respective limits $u_s f'(X_{s^-})$ and $\frac{1}{2}u_s^2 f''(X_{s^-})$ as $\phi_s \to 0$.

Examples

i) For the d-dimensional Brownian motion $(B_t)_{t\in\mathbb{R}_+}$, $\phi = 0$ and the Itô formula reads

$$f(B_t) = f(B_0) + \int_0^t \langle \nabla f(B_s), dB_s\rangle + \frac{1}{2}\int_0^t \Delta f(B_s) ds,$$

for all $\mathcal{C}^2$ functions f, hence

$$\begin{aligned} T_t f(x) &= \mathbb{E}_x[f(B_t)] \\ &= \mathbb{E}_x\left[f(x) + \int_0^t \langle \nabla f(B_s), dB_s\rangle + \frac{1}{2}\int_0^t \Delta f(B_s)ds\right] \\ &= \mathbb{E}_x\left[f(x) + \frac{1}{2}\int_0^t \Delta f(B_s)ds\right] \\ &= f(x) + \frac{1}{2}\int_0^t \mathbb{E}_x\left[\Delta f(B_s)\right]ds \\ &= f(x) + \frac{1}{2}\int_0^t T_s\Delta f(x)ds, \end{aligned}$$

and as a Markov process, $(B_t)_{t\in\mathbb{R}_+}$ has generator $\frac{1}{2}\Delta$.
ii) For the compensated Poisson process $(N_t - t)_{t\in\mathbb{R}_+}$ we have $\phi_s = 1$, $s \in \mathbb{R}_+$, hence

$$\begin{aligned} f(N_t - t) = f(0) &+ \int_0^t (f(1 + N_{s^-} - s) - f(N_{s^-} - s))d(N_s - s) \\ &+ \int_0^t (f(1 + N_s - s) - f(N_s - s) - f'(N_s - s))ds, \end{aligned}$$

which can actually be recovered by elementary calculus. Hence the generator of the compensated Poisson process is

$$\mathcal{L}f(x) = f(x+1) - f(x) - f'(x).$$

From Itô's formula we have for any stopping time τ and $\mathcal{C}^2$ function u, under suitable integrability conditions:

$$\begin{aligned} \mathbb{E}_x[u(B_\tau)] &= u(x) + \mathbb{E}_x\left[\int_0^\tau \langle \nabla u(B_s), dB_s\rangle\right] + \frac{1}{2}\mathbb{E}_x\left[\int_0^\tau \Delta u(B_s)ds\right] \\ &= u(x) + \mathbb{E}_x\left[\int_0^\infty \mathbf{1}_{\{s\le\tau\}}\langle \nabla u(B_s), dB_s\rangle\right] + \frac{1}{2}\mathbb{E}_x\left[\int_0^\tau \Delta u(B_s)ds\right] \\ &= u(x) + \frac{1}{2}\mathbb{E}_x\left[\int_0^\tau \Delta u(B_s)ds\right], \end{aligned} \tag{4.16}$$

which is called Dynkin's formula, cf. Dynkin [Dyn65], Theorem 5.1. Let now

$$\sigma : \mathbb{R}_+ \times \mathbb{R}^n \to \mathbb{R}^d \otimes \mathbb{R}^n$$

and

$$b : \mathbb{R}_+ \times \mathbb{R}^n \to \mathbb{R}$$

satisfy the global Lipschitz condition

$$\|\sigma(t,x)-\sigma(t,y)\|^2+\|b(t,x)-b(t,y)\|^2 \leq K^2\|x-y\|^2,$$

$t \in \mathbb{R}_+$, $x, y \in \mathbb{R}^n$. Then there exists (cf. e.g. [Pro05], Theorem V-7) a unique strong solution to the stochastic differential equation

$$X_t = X_0 + \int_0^t \sigma(s, X_s)dB_s + \int_0^t b(s, X_s)ds,$$

and $(X_t)_{t\in\mathbb{R}_+}$ is a Markov process with generator

$$\mathcal{L} = \frac{1}{2}\sum_{i,j=1}^n a_{i,j}(t,x)\frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i=1}^n b_i(t,x)\frac{\partial}{\partial x_i},$$

where $a = \sigma^T\sigma$.

4.5 Killed Brownian Motion

Let D be a domain in $\mathbb{R}^2$. The transition operator of the Brownian motion $(B_t^D)_{t\in[0,\tau_{\partial D}]}$ killed on ∂D is defined as

$$q_t^D(x, A) = P_x(B_t^D \in A,\ \tau_{\partial D} > t),$$

where

$$\tau_{\partial D} = \inf\{t > 0 \ :\ B_t \in \partial D\}$$

is the first hitting time of ∂D by $(B_t)_{t\in\mathbb{R}_+}$. By the strong Markov property of Definition 3.4 we have

$$\begin{aligned}
P_x(B_t \in A) &= P_x(B_t \in A, t < \tau_{\partial D}) + P_x(B_t \in A, t \geq \tau_{\partial D}) \\
&= q_t^D(x, A) + P_x(B_t \in A, t \geq \tau_{\partial D}) \\
&= q_t^D(x, A) + \mathbb{E}_x[\mathbf{1}_{\{B_t\in A\}}\mathbf{1}_{\{t\geq\tau_{\partial D}\}}] \\
&= q_t^D(x, A) + \mathbb{E}_x[\mathbb{E}[\mathbf{1}_{\{B_t\in A\}}\mathbf{1}_{\{t\geq\tau_{\partial D}\}} \mid \mathcal{F}_{\tau_{\partial D}}]] \\
&= q_t^D(x, A) + \mathbb{E}_x[\mathbf{1}_{\{t\geq\tau_{\partial D}\}}\mathbb{E}[\mathbf{1}_{\{B_t\in A\}}\mathbf{1}_{\{t\geq\tau_{\partial D}\}} \mid \mathcal{F}_{\tau_{\partial D}}]] \\
&= q_t^D(x, A) + \mathbb{E}_x[\mathbf{1}_{\{t\geq\tau_{\partial D}\}}\mathbb{E}[\mathbf{1}_{\{B_{t-\tau_{\partial D}}\in A\}} \mid B_0 = x]_{x=B_{\tau_{\partial D}}}] \\
&= q_t^D(x, A) + \mathbb{E}_x[T_{t-\tau_{\partial D}}\mathbf{1}_A(B^D_{\tau_{\partial D}})\mathbf{1}_{\{t\geq\tau_{\partial D}\}}],
\end{aligned}$$

hence

$$q_t^D(x, A) = P_x(B_t \in A) - \mathbb{E}_x[T_{t-\tau_{\partial D}}\mathbf{1}_A(B^D_{\tau_{\partial D}})\mathbf{1}_{\{t\geq\tau_{\partial D}\}}],$$

and the killed process has the transition densities

$$p_t^D(x, y) := p_t(x, y) - \mathbb{E}_x[p_{t-\tau_{\partial D}}(B^D_{\tau_{\partial D}}, y)\mathbf{1}_{\{t\geq\tau_{\partial D}\}}], \qquad x, y \in D,\ t > 0. \tag{4.17}$$

The Green kernel is defined as

$$g_D(x,y) := \int_0^\infty p_t^D(x,y)dt,$$

and the associated Green potential is

$$G_D\mu(x) = \int_0^\infty g_D(x,y)\mu(dy),$$

with in particular

$$G_D f(x) := \mathbb{E}\left[\int_0^{\tau_{\partial D}} f(B_t)dt\right]$$

when $\mu(dx) = f(x)dx$ has density f with respect to the Lebesgue measure.

When $D = \mathbb{R}^n$ we have $\tau_{\partial D} = \infty$ a.s. hence $G_{\mathbb{R}^n} = G$.

Theorem 4.22. *The function $(x,y) \mapsto g_D(x,y)$ is symmetric and continuous on D^2, and $x \mapsto g_D(x,y)$ is harmonic on $D\backslash\{y\}$, $y \in D$.*

Proof. For all bounded domains A in $\mathbb{R}^n$, the function $G_D\mathbf{1}_A$ defined as

$$G_D\mathbf{1}_A(x) = \int_{\mathbb{R}^n} g_D(x,y)\mathbf{1}_A(y)dy = \mathbb{E}_x\left[\int_0^{\tau_{\partial D}} \mathbf{1}_A(B_t)dt\right]$$

has the mean value property in $D\backslash\bar{A}$, and the property extends to g_D by linear combinations and an limiting argument. □

From (4.17), the associated λ-potential kernel (3.4) is given by

$$g^\lambda(x,y) = \int_0^\infty e^{-\lambda t}p_t(x,y)dt = g_D^\lambda(x,y) + \int g^\lambda(z,y)h_D^\lambda(x,dz), \tag{4.18}$$

where

$$g_D^\lambda(x,y) := \int_0^\infty e^{-\lambda t}q_t^D(x,y)dt,$$

and

$$h_D^\lambda(x,A) = \mathbb{E}_x[e^{-\lambda\tau_{\partial D}}\mathbf{1}_{\{B^D_{\tau_{\partial D}}\in A\}}\mathbf{1}_{\{\tau_{\partial D}<\infty\}}].$$

5 Probabilistic Interpretations

5.1 Harmonicity

We start by two simple examples on the connection between harmonic functions and stochastic calculus. First, we show that Proposition 2.2, i.e. the fact that harmonic functions satisfy the mean value property, can be recovered using stochastic calculus. Let

$$\tau_r = \inf\{t \in \mathbb{R}_+ \ : \ B_t \in S(x,r)\}$$

denote the first exit time of $(B_t)_{t\in\mathbb{R}_+}$ from the open ball $B(x,r)$.

Due to the spatial symmetry of Brownian motion, B_{τ_r} is uniformly distributed on $S(x,r)$, hence

$$\mathbb{E}_x[u(B_{\tau_r})] = \int_{S(x,r)} u(x)\sigma_x^r(dy),$$

where σ_x^r denotes the uniform surface measure on the sphere $S(x,r)$.

On the other hand, from Dynkin's formula (4.16) we have

$$\mathbb{E}_x[u(B_{\tau_r})] = u(x) + \frac{1}{2}\mathbb{E}_x\left[\int_0^{\tau_r} \Delta u(B_s)ds\right].$$

Hence the condition $\Delta u = 0$ implies the mean value property

$$u(x) = \int_{S(x,r)} u(y)\sigma_y^r(dy), \tag{5.1}$$

and similarly the condition $\Delta u \leq 0$ implies

$$u(x) \geq \int_{S(x,r)} u(y)\sigma_y^r(dy). \tag{5.2}$$

From Remark 3, page 134 of Dynkin [Dyn65], for all $n \geq 1$ we have

$$\frac{1}{2}\Delta u(x) = \lim_{n\to\infty} \frac{\mathbb{E}_x[u(B_{\tau_{1/n}})] - u(x)}{\mathbb{E}_x[\tau_{1/n}]}, \tag{5.3}$$

which shows conversely that (5.1), resp. (5.2), implies $\Delta u \leq 0$, resp $\Delta u = 0$, which recovers Proposition 2.2.

Next, we recover the superharmonicity property of the potential

$$\begin{aligned} R_0 f(x) &= \int_0^\infty T_t f(x)dt \qquad (5.4)\\ &= \mathbb{E}_x\left[\int_0^\infty f(B_t)dt\right] \\ &= \int_0^\infty \int_{\mathbb{R}^n} f(y)p_t(x,y)dtdy \\ &= \frac{n-2}{2}\int_{\mathbb{R}^n} h_x(y)f(y)dy, \qquad x \in \mathbb{R}^n. \end{aligned}$$

Proposition 5.1. *Let f be a non-negative function on $\mathbb{R}^n$. Then the potential $R_0 f$ given in* (5.4) *is a superharmonic function provided it is $\mathcal{C}^2$ on $\mathbb{R}^n$.*

Proof. For all $r > 0$, using the strong Markov property (3.5) we have

$$\begin{aligned} g(x) &= \mathbb{E}_x \left[\int_0^{\tau_r} f(B_t)dt \right] + \mathbb{E}_x \left[\int_{\tau_r}^{\infty} f(B_t)dt \right] \\ &= \mathbb{E}_x \left[\int_0^{\tau_r} f(B_t)dt \right] + \mathbb{E}_x \left[\mathbb{E} \left[\int_{\tau_r}^{\infty} f(B_t)dt \Big| B_{\tau_r} \right] \right] \\ &= \mathbb{E}_x \left[\int_0^{\tau_r} f(B_t)dt \right] + \mathbb{E}_x [g(B_{\tau_r})] \\ &\geq \mathbb{E}_x [g(B_{\tau_r})] \\ &= \int_{S(x,r)} g(y)\sigma_x^r(dy), \end{aligned}$$

which shows that g is Δ-superharmonic from Proposition 2.2. □

Other non-negative superharmonic functionals can also be constructed by convolution, i.e. if f is Δ-superharmonic and g is non-negative and sufficiently integrable, then

$$x \mapsto \int_{\mathbb{R}^n} g(y) f(x-y) dy$$

is non-negative and Δ-superharmonic.

We now turn to an example in discrete time, with the notation of (3.1). Here a function f is called harmonic when $(I - P)f = 0$, and superharmonic if $(I - P)f \geq 0$.

Proposition 5.2. *A function f is superharmonic if and only if the sequence $(f(X_n))_{n\in\mathbb{N}}$ is a supermartingale.*

Proof. We have

$$\begin{aligned} \mathbb{E}[f(X_m) \mid \mathcal{F}_n] &= \mathbb{E}[f(X_{m-n}) \mid X_0 = x]_{x=X_n} \\ &= P_{m-n} f(X_n) \\ &\leq f(X_n). \end{aligned}$$

□

5.2 Dirichlet Problem

In this section we revisit the Dirichlet problem using probabilistic tools.

Theorem 5.3. *Consider an open domain in $\mathbb{R}^n$ and f a function on $\mathbb{R}^n$, and assume that the Dirichlet problem*

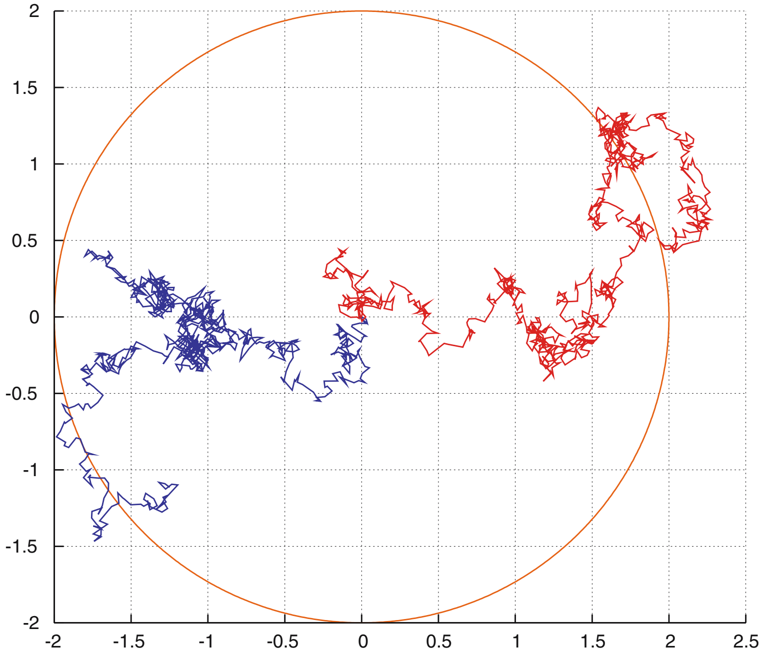

Fig. 9 Sample paths of a two-dimensional Brownian motion.

$$\begin{cases} \Delta u = 0, & x \in D, \\ u(x) = f(x), & x \in \partial D, \end{cases}$$

has a $\mathcal{C}^2$ *solution* u. *Then we have*

$$u(x) = \mathbb{E}_x[f(B_{\tau_{\partial D}})], \qquad x \in \bar{D},$$

where

$$\tau_{\partial D} = \inf\{t > 0 \ : \ B_t \in \partial D\}$$

is the first hitting time of ∂D *by* $(B_t)_{t \in \mathbb{R}_+}$.

Proof. For all $r > 0$ such that $B(x, r) \subset D$ we have

$$\begin{aligned} u(x) &= \mathbb{E}_x[f(B_{\tau_{\partial D}})] \\ &= \mathbb{E}_x[\mathbb{E}[f(B_{\tau_{\partial D}}) \mid B_{\tau_r}]] \\ &= \mathbb{E}_x[u(B_{\tau_r})] \\ &= \int_{S(x,r)} u(y) \sigma_x^r(dy), \qquad x \in \bar{D}, \end{aligned}$$

hence u has the mean value property, thus $\Delta u = 0$ by Proposition 2.2. $\square$

5.3 Poisson Equation

In the next theorem we show that the resolvent

$$\begin{aligned} R_\lambda f(x) &= \mathbb{E}_x\left[\int_0^\infty e^{-\lambda t} f(B_t)dt\right] \\ &= \int_0^\infty e^{-\lambda t} T_t f(x)dt, \qquad x \in \mathbb{R}^n, \end{aligned}$$

solves the Poisson equation. This is consistent with the fact that $R_\lambda = (\lambda I - \Delta/2)^{-1}$, cf. Relation (3.3) in Theorem 3.2.

Theorem 5.4. *Let $\lambda > 0$ and f a non-negative function on $\mathbb{R}^n$, and assume that the Poisson equation*

$$\frac{1}{2}\Delta u(x) - \lambda u(x) = -f(x), \qquad x \in \mathbb{R}^n, \tag{5.5}$$

has a $\mathcal{C}_b^2$ solution u. Then we have

$$u(x) = \mathbb{E}_x\left[\int_0^\infty e^{-\lambda t} f(B_t)dt\right], \qquad x \in \mathbb{R}^n.$$

Proof. By Itô's formula,

$$\begin{aligned} e^{-\lambda t}u(B_t) &= u(B_0) + \int_0^t e^{-\lambda s}\langle \nabla u(B_s), dB_s\rangle \\ &\quad + \frac{1}{2}\int_0^t e^{-\lambda s}\Delta u(B_s)ds - \lambda\int_0^t e^{-\lambda s}u(B_s)ds \\ &= u(B_0) + \int_0^t e^{-\lambda s}\langle \nabla u(B_s), dB_s\rangle - \frac{1}{2}\int_0^t e^{-\lambda s} f(B_s)ds, \end{aligned}$$

hence by taking expectations on both sides and using (4.9) we have

$$e^{-\lambda t}\mathbb{E}_x[u(B_t)] = u(x) - \frac{1}{2}\mathbb{E}_x\left[\int_0^t e^{-\lambda s} f(B_s)ds\right],$$

and letting t tend to infinity we get

$$0 = u(x) - \frac{1}{2}\mathbb{E}_x\left[\int_0^\infty e^{-\lambda s} f(B_s)ds\right].$$

□

When $\lambda = 0$, a similar result holds under the addition of a boundary condition on a smooth domain D.

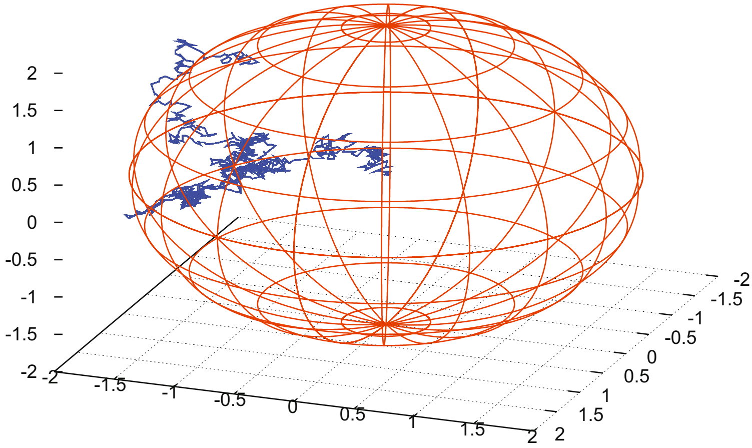

Fig. 10 Sample paths of a three-dimensional Brownian motion.

Theorem 5.5. *Let f a non-negative function on $\mathbb{R}^n$, and assume that the Poisson equation*

$$\begin{cases} \frac{1}{2}\Delta u(x) = -f(x), & x \in D, \\ u(x) = 0, & x \in \partial D, \end{cases} \tag{5.6}$$

has a $\mathcal{C}_b^2$ solution u. Then we have

$$u(x) = \mathbb{E}_x\left[\int_0^{\tau_{\partial D}} f(B_t)dt\right], \qquad x \in D.$$

Proof. Similarly to the proof of Theorem 5.4 we have

$$\begin{aligned} u(B_t) &= u(B_0) + \int_0^t \langle \nabla u(B_s), dB_s \rangle + \frac{1}{2}\int_0^t \Delta u(B_s)ds \\ &= u(B_0) + \int_0^t \langle \nabla u(B_s), dB_s \rangle - \int_0^t f(B_s)ds, \end{aligned}$$

hence

$$0 = \mathbb{E}_x[u(B_{\tau_{\partial D}})] = u(x) - \mathbb{E}_x\left[l\int_0^{\tau_{\partial D}} f(B_s)ds\right].$$

We easily check that the boundary condition $u(x) = 0$ is satisfied on $x \in \partial D$ since $\tau_{\partial D} = 0$ a.s. given that $B_0 \in \partial D$. $\square$

The probabilistic interpretation of the solution of the Poisson equation can also be formulated in terms of a Brownian motion killed at the boundary ∂D, cf. Section 4.5.

Proposition 5.6. *The solution u of* (5.6) *is given by*

$$u(x) = G_D f(x) = \int_{\mathbb{R}^n} g_D(x,y) f(y) dy, \qquad x \in D,$$

where g_D and $G_D f$ are the Green kernel and the Green potential of Brownian motion killed on ∂D.

Proof. We first need to show that the function g_D is the fundamental solution of the Poisson equation. We have

$$\begin{aligned}
\mathbb{E}_x\left[\int_0^{\tau_{\partial D}} \mathbf{1}_A(B_t)dt\right] &= \mathbb{E}_x\left[\int_0^{\tau_{\partial D}} \mathbf{1}_A(B_t^D)dt\right] \\
&= \mathbb{E}_x\left[\int_0^{\tau_{\partial D}} \mathbf{1}_{\{B_t^D \in A\}}dt\right] \\
&= \mathbb{E}_x\left[\int_0^{\infty} \mathbf{1}_{\{B_t^D \in A\}}dt\right] \\
&= \int_0^\infty P_x(B_t^D \in A)dt \\
&= \int_0^\infty q_t^D(x,A)dt \\
&= \int_0^\infty \int_A p_t^D(x,y)dydt \\
&= G_D \mathbf{1}_A(x) \\
&= \int_{\mathbb{R}^n} g_D(x,y)\mathbf{1}_A(y)dy,
\end{aligned}$$

hence

$$u(x) = \mathbb{E}_x\left[\int_0^{\tau_{\partial D}} f(B_t^D)dt\right] = G_D f(x) = \int_{\mathbb{R}^n} g_D(x,y)f(y)dy.$$

□

The solution of (5.6) can also be expressed using the λ-potential kernel g^λ.

Proposition 5.7. *The solution u of* (5.5) *can be represented as*

$$\begin{aligned}
u(x) &= \int_0^\infty e^{-\lambda t} \int_{\mathbb{R}^n} q_t^D(x,y) f(y) dy dt \\
&\quad + \int_{\mathbb{R}^n} f(y) \int_{\mathbb{R}^n} g^\lambda(z,y) \mathbb{E}_x[e^{-\lambda \tau_{\partial D}} \mathbf{1}_{\{B^D_{\tau_{\partial D}} \in dz\}} \mathbf{1}_{\{\tau_{\partial D} < \infty\}}] dy,
\end{aligned}$$

$x \in D$.

Proof. From (4.18) we have

$$\begin{aligned}
u(x) &= R_\lambda f(x) \\
&= \int_{\mathbb{R}^n} g^\lambda(x,y) f(y) dy \\
&= \int_{\mathbb{R}^n} g_D^\lambda(x,y) f(y) dy + \int_{\mathbb{R}^n} f(y) \int_{\mathbb{R}^n} g^\lambda(z,y) h_D^\lambda(x,dz) dy \\
&= \int_0^\infty e^{-\lambda t} \int_{\mathbb{R}^n} q_t^D(x,y) f(y) dy dt \\
&\quad + \int_{\mathbb{R}^n} f(y) \int_{\mathbb{R}^n} g^\lambda(z,y) \mathbb{E}_x[e^{-\lambda \tau_{\partial D}} \mathbf{1}_{\{B^D_{\tau_{\partial D}} \in dz\}} \mathbf{1}_{\{\tau_{\partial D} < \infty\}}] dy.
\end{aligned}$$

□

In discrete time, the potential kernel of P is defined as

$$G = \sum_{n=0}^\infty P^n,$$

and satisfies

$$Gf(x) = \mathbb{E}_x\left[\sum_{n=0}^\infty f(X_n)\right],$$

i.e.

$$G\mathbf{1}_A(x) = \sum_{n=0}^\infty P_x(\{X_n \in A\}).$$

The Poisson equation with second member f is here the equation

$$(I-P)u = f.$$

Let

$$\tau_D = \inf\{n \geq 1 \ : \ X_n \in D\}$$

denote the hitting time of $D \subset E$. Then the function

$$u(x) := \mathbb{E}_x\left[\sum_{k=1}^{\tau_D} f(X_k)\right], \qquad x \in E,$$

solves the Poisson equation

$$\begin{cases} (I-P)u(x) = f(x), & x \in E, \\ u(x) = 0, & x \in D. \end{cases}$$

5.4 Cauchy Problem

This section presents a version of the Feynman-Kac formula. Consider the partial differential equation (PDE)

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x) = \dfrac{1}{2}\Delta u(t,x) - V(x)u(t,x) \\ \\ u(0,x) = f(x). \end{cases} \tag{5.7}$$

Proposition 5.8. *Assume that $f, V \in \mathcal{C}_b(\mathbb{R}^n)$ and V is non-negative. Then the solution of (5.7) is given by*

$$u(t,x) = \mathbb{E}_x\left[\exp\left(-\int_0^t V(B_s)ds\right)f(B_t)\right], \qquad t \in \mathbb{R}_+, \quad x \in \mathbb{R}^n. \tag{5.8}$$

Proof. Let

$$\tilde{T}_t f(x) = \mathbb{E}_x\left[\exp\left(-\int_0^t V(B_s)ds\right)f(B_t)\right], \qquad t \in \mathbb{R}_+, \quad x \in \mathbb{R}^n.$$

We have

$$\begin{aligned}
\tilde{T}_{t+s} f(x) &= \mathbb{E}_x\left[\exp\left(-\int_0^{t+s} V(B_u)du\right)f(B_{t+s})\right] \\
&= \mathbb{E}_x\left[\exp\left(-\int_0^t V(B_u)du\right)\exp\left(-\int_t^{t+s} V(B_u)du\right)f(B_{t+s})\right] \\
&= \mathbb{E}_x\left[\mathbb{E}\left[\exp\left(-\int_0^{t+s} V(B_u)du\right)f(B_{t+s})\Big|\mathcal{F}_t\right]\right] \\
&= \mathbb{E}_x\left[\exp\left(-\int_0^t V(B_u)du\right)\mathbb{E}\left[\exp\left(-\int_t^{t+s} V(B_u)du\right)f(B_{t+s})\Big|\mathcal{F}_t\right]\right] \\
&= \mathbb{E}_x\left[\exp\left(-\int_0^t V(B_u)du\right)\mathbb{E}\left[\exp\left(-\int_0^s V(B_u)du\right)f(B_s)\Big|B_0 = x\right]_{x=B_t}\right] \\
&= \mathbb{E}_x\left[\exp\left(-\int_0^t V(B_u)du\right)\tilde{T}_s f(B_t)\right] \\
&= \tilde{T}_t\tilde{T}_s f(x),
\end{aligned}$$

hence $(\tilde{T}_t)_{t\in\mathbb{R}_+}$ has the semigroup property. Next we have

$$\begin{aligned}
\frac{\tilde{T}_t f(x) - f(x)}{t} &= \frac{1}{t}\left(\mathbb{E}_x\left[\exp\left(-\int_0^t V(B_u)du\right)f(B_t)\right] - f(x)\right) \\
&= \frac{1}{t}(\mathbb{E}_x[f(B_t)] - f(x)) + \frac{1}{t}\mathbb{E}_x\left[\exp\left(-\int_0^t V(B_u)du\right)f(B_t)\right] + o(t),
\end{aligned}$$

hence

$$\frac{d\tilde{T}_t}{dt}|_{t=0}f(x) = \frac{1}{2}\Delta f(x) - V(x)f(x), \qquad x \in \mathbb{R}, \tag{5.9}$$

and u given by (5.8) satisfies

$$\begin{aligned}\frac{\partial u}{\partial t}(t,x) &= \frac{d\tilde{T}_t}{dt}f(x)\\ &= \frac{d\tilde{T}_t}{dt}|_{t=0}\tilde{T}_t f(x)\\ &= \left(\frac{1}{2}\Delta - V(x)\right)\tilde{T}_t f(x)\\ &= \frac{1}{2}\Delta u(t,x) - V(x)u(t,x).\end{aligned}$$

□

Moreover, (5.9) also yields

$$\begin{aligned}\int_{\mathbb{R}^n} f(y)p_t(x,y)dy &= f(x) + \frac{1}{2}\int_0^t \int_{\mathbb{R}^n} \Delta_x f(y)p_s(x,y)dyds\\ &= f(x) + \frac{1}{2}\int_0^t \int_{\mathbb{R}^n} f(y)\Delta_x p_s(x,y)dyds,\end{aligned}$$

for all sufficiently regular functions f on $\mathbb{R}^n$, where $p_t(x,y)$ is the Gaussian density kernel. Hence we get, after differentiation with respect to t,

$$\frac{\partial p_t}{\partial t}(x,y) = \frac{1}{2}\Delta_x p_t(x,y). \tag{5.10}$$

From (5.10) we recover the harmonicity of h_y on $\mathbb{R}^n\backslash\{y\}$:

$$\begin{aligned}\Delta_x h_y(x) &= \Delta_x \int_0^\infty p_t(x,y)dt\\ &= \int_0^\infty \Delta_x p_t(x,y)dt\\ &= 2\int_0^\infty \frac{\partial p_t}{\partial t}(x,y)dt\\ &= 2\lim_{t\to\infty} p_t(x,y) - 2\lim_{t\to 0} p_t(x,y)\\ &= 0,\end{aligned}$$

provided $x \neq y$. The backward Kolmogorov partial differential equation

$$\begin{cases} -\dfrac{\partial u}{\partial t}(t,x) = \dfrac{1}{2}\Delta u(t,x) - V(x)u(t,x),\\ \\ u(T,x) = f(x),\end{cases} \tag{5.11}$$

can be similarly solved as follows.

Proposition 5.9. *Assume that* $f, V \in \mathcal{C}_b(\mathbb{R}^n)$ *and* V *is non-negative. Then the solution of* (5.11) *is given by*

$$u(t,x) = \mathbb{E}\left[\exp\left(-\int_t^T V(B_s)ds\right) f(B_T)\Big| B_t = x\right], \qquad (5.12)$$

$t \in \mathbb{R}_+$, $x \in \mathbb{R}^n$.

Proof. Letting $u(t,x)$ be defined by (5.12) we have

$$\begin{aligned}
&\exp\left(-\int_0^t V(B_s)ds\right) u(t,B_t) \\
&= \exp\left(-\int_0^t V(B_s)ds\right) \mathbb{E}\left[\exp\left(-\int_t^T V(B_s)ds\right) f(B_T)\Big|\mathcal{F}_t\right] \\
&= \mathbb{E}\left[\exp\left(-\int_0^T V(B_s)ds\right) f(B_T)\Big|\mathcal{F}_t\right],
\end{aligned}$$

$t \in \mathbb{R}_+$, $x \in \mathbb{R}^n$, which is a martingale by construction. Applying Itô's formula to this process we get

$$\begin{aligned}
&\exp\left(-\int_0^t V(B_s)ds\right) u(t,B_t) \\
&= u(0,B_0) + \int_0^t \exp\left(-\int_0^s V(B_\tau)d\tau\right) \langle \nabla_x u(s,B_s), dB_s\rangle \\
&\quad + \frac{1}{2}\int_0^t \exp\left(-\int_0^s V(B_\tau)d\tau\right) \Delta_x u(s,B_s)ds \\
&\quad - \int_0^t V(B_s)\exp\left(-\int_0^s V(B_\tau)d\tau\right) u(s,B_s)ds \\
&\quad + \int_0^t \exp\left(-\int_0^s V(B_\tau)d\tau\right) \frac{\partial u}{\partial s} u(s,B_s)ds.
\end{aligned}$$

The martingale property shows that the absolutely continuous finite variation terms vanish (see e.g. Corollary II-1 of Protter [Pro05]), hence

$$\frac{1}{2}\Delta_x u(s,B_s) - V(B_s)u(s,B_s) + \frac{\partial u}{\partial s}(s,B_s) = 0, \qquad s \in \mathbb{R}_+,$$

which leads to (5.11). □

5.5 Martin Boundary

Our aim is now to provide a probabilistic interpretation of the Martin boundary in discrete time. Namely we use the Martin boundary theory to study the way a Markov chain with transition operator P leaves the space E, in particular when E is a union

$$E = \bigcup_{n=0}^{\infty} E_n,$$

of transient sets E_n, $n \in \mathbb{N}$. We assume that E is a metric space with distance δ and that the Cauchy completion of E coincides with its Alexandrov compactification $(E, \hat{x})$.

For simplicity we will assume that the transition operator P is self-adjoint with respect to a reference measure m. Let now G denote the potential

$$Gf(x) := \sum_{n=0}^{\infty} P^n f(x), \qquad x \in E.$$

with kernel $g(\cdot, \cdot)$, satisfying

$$Gf(x) = \int_E f(y) g(x, y) m(dy), \qquad x \in E,$$

for a given reference measure m. Fix $x_0 \in E_1$. For f in the space $\mathcal{C}_c(E)$ of compactly supported function on E, define the kernel

$$k_{x_0}(x, z) = \frac{g(x, z)}{g(x, x_0)}, \qquad x, z \in E,$$

and the operator

$$K_{x_0} f(x) := \frac{Gf(x)}{g(x, x_0)} = \int_E k_{x_0}(x, z) f(z) m(dz), \qquad x \in E.$$

Consider a sequence $(f_n)_{n\in\mathbb{N}}$ dense in $\mathcal{C}_c(E)$ and the metric defined by

$$d(x, y) := \sum_{n=1}^{\infty} \zeta_n |K_{x_0} f_n(x) - K_{x_0} f_n(y)|,$$

where $(\zeta_n)_{n\in\mathbb{N}}$ is a sequence of non-negative numbers such that

$$\sum_{n=1}^{\infty} \zeta_n \|K_{x_0} f_n\|_\infty < \infty.$$

The Martin space $\hat{E}$ for X started with distribution rm is constructed as the Cauchy completion of $(E, \delta + d)$. Then $K_{x_0} f$, $f \in \mathcal{C}_c(E)$, can be extended by continuity to $\hat{E}$ since for all $\varepsilon > 0$ there exists $n \in \mathbb{N}$ such that for all $x, y \in E$,

$$\begin{aligned}
&|K_{x_0} f(x) - K_{x_0} f(y)| \\
&\leq |K_{x_0} f(x) - K_{x_0} f_n(x)| + |K_{x_0} f_n(x) - K_{x_0} f_n(y)| + |K_{x_0} f_n(y) - K_{x_0} f(y)| \\
&\leq \varepsilon + \zeta_n d(x, y),
\end{aligned}$$

and, from Proposition 2.3 of Revuz [Rev75], the sequence $(K_{x_0} f_n)_{n \in \mathbb{N}}$ is dense in $\{K_{x_0} f \ : \ f \in \mathcal{C}_c(E)\}$.

If $x \in \Delta E$, a sequence $(x_n)_{n \in \mathbb{N}} \subset E$ converges to x if and only if it converges to point at infinity $\hat{x}$ for the metric δ and $(K_{x_0} f(x_n))_{n \in \mathbb{N}}$ converges to $K_{x_0} f(x)$ for every $f \in \mathcal{C}_c(E)$. Finally we have the following result, for which we refer to [Rev75].

Theorem 5.10. *The sequence $(X_n)_{n \in \mathbb{N}}$ converges P_{x_0}-a.s. in $\hat{E}$ and the law of X_∞ under P_{x_0} is carried by ΔE.*

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Introduction to Random Walks on Noncommutative Spaces

Philippe Biane

Abstract We introduce several examples of random walks on noncommutative spaces and study some of their probabilistic properties. We emphasize connections between classical potential theory and group representations.

1 Introduction

Whereas random walks form one of the most investigated class of stochastic processes, their noncommutative analogues have been studied only recently. In these lectures I will present some results on random walks which take their values in noncommutative spaces. The notion of a noncommutative space has emerged progressively from the development of quantum physics, see e.g. [C]. The key idea is to consider not the space itself but the set of real, or complex functions on it. For a usual space, this forms an algebra, which is commutative by nature. A noncommutative space is given by a noncommutative (usually complex) algebra which is to be thought of as the algebra of complex functions on the space. We shall explain this idea in more details in section 2, and in particular define noncommutative probability spaces. Once noncommutative spaces have been defined in this way it is easy to define random variables, and stochastic processes taking their values in these spaces. Rather than starting an abstract theory, these lectures will consist mainly in a collection of examples, which I think show that this notion is interesting and worth studying. We shall begin with the most simple stochastic process namely the Bernoulli random walk. We shall show how to quantize it in order to construct the quantum Bernoulli random walk. Simple as it is this

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noncommutative stochastic process exhibits quite deep properties, related to group representation and potential theory. Actually interpreting it as a random walk with values in a noncommutative space, the dual of $SU(2)$, we will be lead to define random walks with values in duals of compact groups. The study of such random walks in the case of special unitary groups uncovers connections with potential theory, in particular with the Martin boundary. We will investigate more on these connections. From the Bernoulli random walk we can take limit objects, as in the central limit theorem. One of these objects is a noncommutative Brownian motion which we construct as a family of operators on a Fock space and interpret then as a continuous time stochastic process with independent increments, with values in the dual of the Heisenberg group. We then extend this construction to more general noncompact locally compact groups. Finally we will also start to consider quantum groups in the last section.

The next section consists in preliminaries about C^* and von Neumann algebras and noncommutative spaces.

2 Noncommutative Spaces and Random Variables

2.1 What are Noncommutative Spaces?

The random walks that we are going to study take their values in noncommutative spaces, so we should start by making this notion more precise. In many parts of mathematics, one studies spaces through the set of functions defined on them. There can be many kind of functions, e.g. measurable, integrable, continuous, bounded, differentiable, and so on. Each property of the functions reflects a property of the space on which they are defined. Sometimes, in probability theory for example, one is even not interested at all in the space, but only in the functions themselves, the random variables. Also very often the set of complex functions considered determines completely the underlying space. This is the case for example for compact topological spaces, determined by their algebra of continuous functions, or differentiable manifolds which are determined by their smooth functions. The common feature shared by these situations is that all these spaces of complex valued functions are commutative algebras. It has been realized, since the beginning of quantum mechanics that one can obtain a better description of nature by relaxing this commutativity hypothesis. Henceforth we shall consider a non commutative space as given by a complex algebra, which plays the role of space of functions on the space. We will see many examples throughout these lectures. Some algebras may come equipped with a supplementary structure, for example an antilinear involution, a norm, a preferred linear form, a topology, etc... Actually most of the times these algebras will be algebras of operators on some complex Hilbert space H, and the involution will be given by the adjoint operation. We shall decribe the kind of algebras we will consider, mainly C^* and von Neumann algebras. We will use the language and some basic results in the theory of these objects, but we will need no deep knowledge of them. We will only assume that the reader is familiar with the spectral theorem for selfadjoint operators on a Hilbert space. We refer for example to the treatises [D1], [D2] or [T] for more details.

2.2 C^* Algebras

A C^* algebra is a normed $*$-algebra which is isometric with a subalgebra of the algebra $B(H)$ of all bounded operators on some complex Hilbert space H, stable under taking the adjoint, and closed for the operator norm topology. Elements in a C^*-algebra of the form aa^* for some $a \in A$ are called positive. Positive elements are exactly the selfadjoint positive operators which belong to the algebra.

Let X be a locally compact topological space, then the algebra of complex continuous functions on X, vanishing at infinity, is a C^*-algebra, and the famous Gelfand-Naimark theorem states that any commutative C^*-algebra is isomorphic to such an algebra. The topological space is compact if and only if the algebra has a unit, and there is a one to one correspondence between the points of the space and the characters of the algebra, that is, the continuous algebra homomorphisms with values in the complex numbers, or equivalently with the maximal closed ideals, therefore the space is unique up to homeomorphism and can be recovered from the algebra. It is usually denoted by $spec(A)$ if A is the C^*-algebra. Thus we should think of a C^*-algebra as providing the algebra of continuous functions on some noncommutative space. Note that C^* algebras are closed under continuous functional calculus, namely if a is a self-adjoint element in a C^* algebra, and f a continuous functions on its spectrum, then the operator $f(a)$ also belongs to the algebra C. This can be easily seen by approximating uniformly f by polynomials on the spectrum of a.

If $A \subset B(H)$ is a C^*-algebra, then the multiplier algebra $M(A)$ of A is the set of all operators x such that $xA \subset A$ and $Ax \subset A$. It is a C^* algebra with a unit, containing A. It coincides with A if and only if A has a unit. If A is abelian, then $M(A)$ is just the algebra of all bounded continuous functions on $spec(A)$. In the noncommutative situation, it corresponds to the Stone-Cech compactification of the topological space underlying the algebra.

Continuous positive linear functionals on a C^* algebra play the role of positive bounded measures. Here positivity for a functional means that it is positive on positive elements. Again in the commutative case, by Riesz' theorem, such linear functionals correspond to finite positive Borel measures on the underlying topological space. Positive linear functionals of norm one are called states, and correspond to probability measures in the commutative case. A large supply of states is given by unit vectors in the Hilbert space on which the C^* algebra acts. Indeed any such vector ψ defines a state by the formula

$$\omega_\psi(a) = \langle a\psi, \psi\rangle \qquad a \in A$$

Given a self adjoint element a in a C^* algebra A, and a state σ on A, there exists a unique measure on $\mathbb{R}$, with compact support, such that

$$\sigma(f(a)) = \int f(x)d\mu(x) \qquad \text{for all continuous } f \text{ on } \mathbb{R}.$$

The support of this measure is included in the spectrum of a. The GNS construction assigns to every C^* algebra, with a continuous positive linear functional σ, a representation of the algebra on a Hilbert space. A linear functional is called tracial if for any $a, b \in A$ one has $\tau(ab) = \tau(ba)$.

Each continuous map between topological spaces $f : X \to Y$ gives rise to a continuous algebra morphism $\Phi_f : C_0(Y) \to C_0(X); h \mapsto h \circ f$, and conversely any such algebra morphism comes from a continuous map, therefore one can think of a homomorphism between C^* algebras as a continuous map between the underlying noncommutative spaces (with the direction of the arrows reversed). One must note however that there may exist very few morphisms between two C^* algebras. For example there does not exist any nonzero homomorphism from the finite dimensional C^* algebra $M_n(\mathbb{C})$ to $M_m(\mathbb{C})$ if $n > m$. Indeed this is a purely algebraic fact, since $M_n(\mathbb{C})$ is a simple algebra, if a homomorphism from $M_n(\mathbb{C})$ is not injective, then it must be 0.

2.3 von Neumann Algebras

Let S be a subset of $B(H)$, then its commutant S' is the set of bounded operators which commute with every element of S. A von Neumann algebra is a subalgebra of $B(H)$ which is closed under under taking the adjoint, and is equal to its bicommutant, i.e. the commutant of its commutant. By the von Neumann bicommutant theorem the von Neumann algebras are the $*$-subalgebra of $B(H)$, containing the identity operator, and closed for the strong topology. Since the strong topology is weaker than the operator norm topology any von Neumann algebra is also a unital C^* algebra, although generally too large to be interesting as such.

A von Neumann algebra is closed under Borel functional calculus, namely if $a \in M$ is self-adjoint and f is a bounded Borel function on the spectrum of a, then $f(a)$ belongs to M, and again, the same is true for $f(a_1, \ldots, a_n)$ where $a_1, \ldots, a_n$ are commuting selfadjoint operators in the von Neumann algebra, and f is a bounded Borel function defined on the product of their spectra.

The nuance between C^* algebras and von Neumann algebras can be grasped by looking at the commutative case. Indeed commutative von Neumann algebras correspond to measure spaces, more precisely any commutative von Neumann algebra is isomorphic to the algebra $L^\infty(X, m)$ where X is a measure space and m a positive measure (the algebra actually depends only on the class of the measure). This statement can be seen as a reformulation of the spectral theorem for commuting self-adjoint operators on a Hilbert space. Therefore it is natural to think of von Neumann algebras as "algebras of noncommutative random variables". A normal state on a von Neumann algebra is a positive linear form which is continuous for the σ-weak topology and takes the value 1 on the unit. It corresponds, in the commutative case, to a probability measure, which is absolutely continuous with respect to the measure m. We shall sometimes call a von Neumann algebra, with a normal state, a "non commutative probability space".

A weight on a von Neumann algebra is a map φ from the cone of positive elements of the von Neumann algebra to $[0, +\infty]$, which is additive, and homogeneous, i.e. $\varphi(\lambda x) = \lambda\varphi(x)$ for x positive and real $\lambda > 0$. A weight is called normal if $\sup_{i\in I} \varphi(x_i) = \varphi(\sup(x_i)_{i\in I})$ for every bounded increasing net $(x_i)_{i\in I}$. Coming back to the commutative case, weights are positive, possibly unbounded measures, in the measure class of m. A weight μ is called finite if $\mu(1) < \infty$, in this case μ is a multiple of a state.

Given a selfadjoint element, $a \in M$ and a normal state σ on M, we denote by μ_a the distribution of a, namely the measure such that

$$\sigma(f(a)) = \int f(x)d\mu_a(x)$$

for all bounded Borel functions on $spec(a)$. More generally if $a_1, \ldots, a_n$ is a family of commuting self-adjoint operators in M, their joint distribution is the unique probability measure $\mu_{a_1,\ldots,a_n}$ on $\mathbb{R}^n$ such that

$$\sigma(f(a_1, \ldots, a_n)) = \int f(x)d\mu_{a_1,\ldots,a_n}(x)$$

for all bounded Borel function f on $\mathbb{R}^n$.

Let $N \subset M$ be a von Neumann subalgebra, and σ a state on M, then a conditional expectation of M onto N is a norm one projection $\sigma(.|N)$ such that $\sigma(a|N) = a$ for all $a \in N$, $\sigma(abc|N) = a\sigma(b|N)c$ for all $a, c \in N, b \in M$, and $\sigma(\sigma(b|N)) = \sigma(b)$ for all $b \in M$. Given M, N and σ, such a map need not exist, but it always exists, and is unique, if σ is tracial.

We will consider spatial tensor products of von Neumann algebras. If $A \subset B(H)$ and $B \subset B(K)$ are two von Neumann algebras, their algebraic tensor product acts on the Hilbert space $H \otimes K$, and the spatial tensor product of A and B is defined as the von Neumann algebra generated by this tensor product. Given an infinite family of von Neumann algebras $(A_i; i \in I)$ equipped with normal states ω_i it is possible to construct an infinite tensor product $\otimes_i(A_i, \omega_i)$ which is a von Neumann algebra with a state $\otimes_i \omega_i$. One considers operators of the form $\otimes_{i\in I} a_i$ where $a_i \in A_i$ and $a_i \neq Id$ only for a finite number of $i \in I$. These generate an algebra, which is the algebraic tensor product of the A_i. One can define a positive linear functional on this algebraic tensor product by $\omega(\otimes_{i\in I} a_i) = \prod \omega_i(a_i)$. The GNS construction then yields a Hilbert space H, with a pure state on $B(H)$, and the von Neumann algebra tensor product is the von Neumann algebra in $B(H)$ generated by this algebraic tensor product.

2.4 Random Variables, Stochastic Processes with Values in some Noncommutative Space

Given a von Neumann algebra M equipped with a normal state σ, and a C^* algebra C, a random variable with values in C (or, more appropriately, in the noncommutative space underlying C), is a norm continuous morphism from C to M. The distribution of the random variable $\varphi : C \to M$ is the state on C given by $\sigma \circ \varphi$. If the algebra C is commutative, then it corresponds to some topological space, and the state $\sigma \circ \varphi$ to a probability measure on this space. When $C = C_0(\mathbb{R})$ there exists a self-adjoint element $a \in M$ such that $\varphi(f) = f(a)$ for all $f \in C$, and we are back to the situation in the preceding section, where the distribution of a was defined. We will call the state $\sigma \circ \varphi$ the distribution of the random variable φ. More generally a family of random variables with values in some noncommutative space, indexed by some set, is a stochastic process.

If A and B are two C^*-algebras, a positive map $\Phi : A \to B$ is a linear map such that $\Phi(a)$ is positive for each positive $a \in A$. When A and B are commutative, thus $A = C_0(X)$ and $B = C_0(Y)$, such a linear map can be realized as a measure kernel $k(y, dx)$ where for each $y \in Y$ one has a finite positive measure $k(y, dx)$ on X. If A and B are unital, and $\Phi(I) = I$ then this kernel is a Markov kernel, i.e. all measures are probability measures. Thus we see that the generalization of a Markov kernel to the non-commutative context can be given by the notion of positive maps. It turns out however that this notion is slightly too general to be useful and it is necessary to restrict oneself to a particular class called completely positive maps.

Definition 2.1. linear map between two C^* algebras A and B is called completely positive if, for all $n \geq 0$, the map $\Phi \otimes Id : A \otimes M_n(\mathbb{C}) \to B \otimes M_n(\mathbb{C})$ is positive. It is called unit preserving if furthermore $\Phi(Id) = Id$.

We shall consider semigroups of unit preserving, completely positive maps on a C^* algebra C. These will be indexed by a set of times which will be either the nonnegative integers (discrete times) or the positive real line (continuous time). Thus a discrete time semigroup of unit preserving, completely positive maps on a C^* algebra C will be a family $(\Phi_n : C \to C)_{n\geq 0}$ of completely positive maps, such that $\Phi_n \circ \Phi_m = \Phi_{n+m}$. In continuous time we will have a family $(\Phi_t)_{t\in\mathbb{R}_+}$ which satisfies $\Phi_t \circ \Phi_s = \Phi_{t+s}$. In the discrete time setting one has $\Phi_n = (\Phi_1)^n$ and the semigroup is deduced from the value at time 1. We shall denote generally the time set by T when we do not specify whether we are in discrete or continuous time.

Definition 2.2. Let C be a C^* algebra, then a dilation of a semigroup $(\Phi_t)_{t\in T}$ of completely positive maps on C is given by a von Neumann algebra M, with a normal state ω, an increasing family of von Neumann subalgebras $M_t; t \in T$, with conditional expectations $\omega(.|M_t)$, and a family of morphisms $j_t : C \to (M, \omega)$ such that for any $t \in T$ and $a \in C$, one has $j_t(a) \in M_t$ and for all $s < t$

$$\omega(j_t(a)|M_s) = j_s(\Phi_{t-s}(a)) \tag{2.1}$$

A dilation of a completely positive semigroup is the analogue in noncommutative probability of a Markov process, and the equation (2.1) expresses the Markov property of the process: the conditional expectation of the future on the past is a function of the present.

Given a completely positive semigroup and an initial state, a dilation always exists [S].

Consider a completely positive semigroup on a C^* algebra C, and let $B \subset C$ be a commutative C^* subalgebra, thus isomorphic to $C_0(X)$ for some locally compact topological space X. If the image algebras $j_t(B); t \in T$ generate a commutative von Neumann algebra $\mathcal{N} \subset M$, then there exists a probability space $(\Omega, \mathcal{F}, P)$ such that $(\mathcal{N}, \omega) \sim L^\infty(\Omega, \mathcal{F}, P)$, and random variables $X_t : \Omega \to X$, corresponding to the morphisms j_t restricted to B, which form a classical stochastic process. If furthermore the C^* algebra B is invariant by the completely positive semigroup, then this semigroup defines a Markov semigroup of transition probabilities on the space X, and the stochastic process $(X_t)_{t\in T}$ is a Markov process with these probability transitions. This remark will be at the basis of many constructions of classical stochastic processes starting from quantum ones.

Once a dilation of a completely positive semigroup is given, one can compute, for times $t_1 < \cdots < t_n$, and $a_1, \ldots, a_n \in C$,

$$\omega(j_{t_1}(a_1)\ldots j_{t_n}(a_n)) = \sigma(\Phi_{t_1}(a_1(\Phi_{t_2-t_1}(a_2(\ldots\Phi_{t_n-t_{n-1}}(a_n))\ldots)$$

where $\sigma = \omega \circ j_0$ is the initial state on C (the distribution of the process at time 0). Observe however that when the algebras $j_t(C); t \in T$ do not commute, this condition does not specifiy the values of

$$\omega(j_{t_1}(a_1)\ldots j_{t_n}(a_n))$$

when the times $t_1, \ldots, t_n$ are not ordered. We will say that two dilations $j^{(1)}, \omega_1$ and $j^{(2)}, \omega_2$, are equivalent if one has

$$\omega_1(j^{(1)}_{t_1}(a_1)\ldots j^{(1)}_{t_n}(a_n)) = \omega_2(j^{(2)}_{t_1}(a_1)\ldots j^{(2)}_{t_n}(a_n))$$

where $t_1, \dots, t_n$ is an arbitrary sequence of times (i.e. not necessarily increasing) and $a_1, \dots, a_n \in C$. Thus if C is a commutative algebra, then all commutative dilations with the same initial distribution are equivalent, but for a given semigroup of completely positive maps there may exist a lot of non equivalent dilations. Actually we shall encounter in these lectures some natural noncommutative dilations of Markov semigroups on classical spaces! An important source of such dilations comes from restrictions: if $B \subset C$ is a subalgebra and the completely positive semigroup leaves B invariant, then the restriction of $(j_t)_{t\in T}$ to the subalgebra B is a dilation of the restriction of the completely positive semigroup.

3 Quantum Bernoulli Random Walks

3.1 Quantization of the Bernoulli Random Walk

Our first example of a quantum random walk will be the quantization of the simple (or Bernoulli) random walk. This is just the random walk whose independent increments have values ± 1. In order to quantize it we will replace the set of increments $\{\pm 1\}$ by its quantum analogue, namely the space of two by two complex matrices, with its structure of C^*-algebra. The subset of hermitian operators is a four dimensional real subspace, generated by the identity matrix I as well as the three matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The matrices $\sigma_x, \sigma_y, \sigma_z$ are the Pauli matrices. They satisfy the commutation relations

$$[\sigma_x, \sigma_y] = 2i\sigma_z; \quad [\sigma_y, \sigma_z] = 2i\sigma_x; \quad [\sigma_z, \sigma_x] = 2i\sigma_y. \tag{3.1}$$

The group $SU(2)$ acts by the automorphisms $A \to UAU^*$ on this C^*-algebra. We observe that this group is much larger than the group of symmetries of the two points space (which consists just of a two elements group). This action leaves the space generated by I invariant, and acts by rotations on the real three dimensional space generated by the Pauli matrices. Indeed the inner product on the space of hermitian matrices $\langle A, B\rangle = Tr(AB)$ is invariant by unitary conjugation.

A state ω on $M_2(\mathbb{C})$ is given by a positive hermitian matrix S with trace 1, by the formula

$$\omega(A) = Tr(AS).$$

The most general such matrix can be written as

$$S = \frac{1}{2}\begin{pmatrix} 1+u & v+iw \\ v-iw & 1-u \end{pmatrix}$$

where $(u, v, w) \in \mathbb{R}^3$ satisfies $u^2 + v^2 + w^2 \leq 1$. The extreme points on the unit sphere (sometimes called the "Bloch sphere" in the physics litterature), correspond to pure states, when S is a projection on a one dimensional subspace. Any hermitian operator has a two-point spectrum, hence in a state ω its distribution is a probability measure on $\mathbb{R}$ supported by at most two points. In particular, for each of the Pauli matrices, its distribution in the state ω is a probability measure on $\{\pm 1\}$, given by

$$P(\sigma_x = 1) = \frac{1+v}{2} \quad P(\sigma_y = 1) = \frac{1+w}{2} \quad P(\sigma_z = 1) = \frac{1+u}{2} \tag{3.2}$$

Mimicking the construction of a random walk, we use the infinite product algebra $(M_2(\mathbb{C}), \omega)^{\otimes \mathbb{N}}$ (recall the construction of section 2.3). For each Pauli matrix we build the matrices

$$x_n = I^{\otimes(n-1)} \otimes \sigma_x \otimes I^{\otimes\infty} \quad y_n = I^{\otimes(n-1)} \otimes \sigma_y \otimes I^{\otimes\infty}, \quad z_n = I^{\otimes(n-1)} \otimes \sigma_z \otimes I^{\otimes\infty}$$

which represent the increments of the process. It is easy to see that, for example, the operators x_n, for $n \geq 1$, form a commuting family of operators, which is distributed, in the state ω^∞, as a sequence of independent Bernoulli random variables.

Then we put

$$X_n = \sum_{i=1}^n x_i; \quad Y_n = \sum_{i=1}^n y_i \quad Z_n = \sum_{i=1}^n z_i.$$

This gives us three families of operators $(X_n)_{n\geq 1}; (Y_n)_{n\geq 1}$ and $(Z_n)_{n\geq 1}$ on this space.

We observe that each of these three families consists in commuting operators, hence has a joint distribution. It is not difficult to check that this distribution is that of a Bernoulli random walk, whose increments have distribution given by the probability distributions on $\{\pm 1\}$ of formula (3.2). The three families of operators, however do not commute. In fact using the commutation relations (3.1) one sees that for n, m positive integers,

$$[x_n, y_m] = 2iz_m \delta_{nm}$$

and

$$[X_n, Y_m] = 2iZ_{n\wedge m} \tag{3.3}$$

as well as the similar relations obtained by cyclic permutation of X, Y, Z. We will call the family of triples of operators $(X_n, Y_n, Z_n); n \geq 1$ a quantum Bernoulli random walk. We shall later interpret this noncommutative process as a random walk with values in some noncommutative space, however for the moment we will study some of its properties related to the automorphisms of the algebra $M_2(\mathbb{C})$.

3.2 The Spin Process

Because of the rotation invariance of the commutation relations (3.1), we see that for any unitary matrix U we can define conjugated variables

$$\begin{aligned} x_n^U &= I^{\otimes(n-1)} \otimes U\sigma_x U^* \otimes I^{\otimes\infty} \\ y_n^U &= I^{\otimes(n-1)} \otimes U\sigma_y U^* \otimes I^{\otimes\infty} \\ z_n^U &= I^{\otimes(n-1)} \otimes U\sigma_z U^* \otimes I^{\otimes\infty} \end{aligned}$$

and

$$X_n^U = \sum_{i=1}^n x_i^U; \quad Y_n^U = \sum_{i=1}^n y_i^U \quad Z_n^U = \sum_{i=1}^n z_i^U$$

then this new stochastic process is obtained from the original quantum Bernoulli random walk by a rotation matrix. It follows by a simple computation, using the commutation relations, that $X_n^2 + Y_n^2 + Z_n^2$ is invariant under conjugation, namely one has

$$X_n^2 + Y_n^2 + Z_n^2 = (X_n^U)^2 + (Y_n^U)^2 + (Z_n^U)^2$$

for any unitary matrix U.

Lemma 3.1. *For all $m, n \geq 1$ one has*

$$[X_n^2 + Y_n^2 + Z_n^2, X_m^2 + Y_m^2 + Z_m^2] = 0$$

Actually we shall prove that $[X_n, X_m^2 + Y_m^2 + Z_m^2] = 0$ if $m \leq n$. This follows from the computation

$$[X_n, Y_m^2] = [X_n, Y_m]Y_m + Y_m[X_n, Y_m] = 2i(Z_mY_m + Y_mZ_m)$$

$$[X_n, Z_m^2] = [X_n, Z_m]Z_m + Z_m[X_n, Y_m] = -2i(Z_mY_m + Y_mZ_m)$$

Using invariance of the commutation relations by cyclic permutation of X, Y, Z we also have $[Y_n, X_m^2 + Y_m^2 + Z_m^2] = [Z_n, X_m^2 + Y_m^2 + Z_m^2] = 0$, and the result follows. □

We deduce from this that the family of operators $(X_n^2 + Y_n^2 + Z_n^2); n \geq 1$ is commutative, and therefore defines a classical process. We shall compute its distribution now. For this we introduce the operators $S_n = \sqrt{X_n^2 + Y_n^2 + Z_n^2 + I}$. By the preceding Lemma, the family $(S_n)_{n\geq 0}$ is a commuting family of operators, therefore one can consider their joint distribution.

Theorem 3.2. *Let us take for ω the tracial state, then the operators $(S_n; n \geq 1)$ form a Markov chain, with values in the positive integers, such that $P(S_1 = 2) = 1$, and transition probabilities*

$$p(k, k+1) = \frac{k+1}{2k}; \quad p(k, k-1) = \frac{k-1}{2k}.$$

In order to prove the theorem, it is enough to consider the process up to a finite time n. So we shall restrict considerations to a finite product $M_2(\mathbb{C})^{\otimes n}$ acting on $(\mathbb{C}^2)^{\otimes n}$. We remark that the state $\omega^{\otimes n}$ on $(\mathbb{C}^2)^{\otimes n}$ is the unique tracial state, and it gives, to every orthogonal projection on a subspace V, the value $\frac{\dim(V)}{2^n}$. We shall find a basis of this space consisting of joint eigenvectors of the operators $(S_k; 1 \le k \le n)$. For this we analyze the action of the operators $A_n^+ := \frac{1}{2}(X_n - iY_n)$ and $A_n^- = \frac{1}{2}(X_n + iY_n)$. One has

$$A_n^+ = \sum_{j=1}^n I^{\otimes(j-1)} \otimes \alpha^+ \otimes I^{\otimes n-j} \qquad A_n^- = \sum_{j=1}^n I^{\otimes(j-1)} \otimes \alpha^- \otimes I^{\otimes n-j}$$

where

$$\alpha^+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad \alpha^- = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

Let us call e_0, e_1 the canonical basis of $\mathbb{C}^2$. An orthonormal basis of $(\mathbb{C}^2)^{\otimes n}$ is given by the vectors $e_U; U \subset \{1, 2, \ldots, n\}$ where $e_U = e_{i_1} \otimes \ldots \otimes e_{i_n}$, $i_k = 1$ if $k \in U$ and $i_k = 0$ if $k \notin U$. In terms of this basis the action of A_n^+ and A_n^- is given by

$$\begin{aligned} A_n^+ e_U &= \textstyle\sum_{k \notin U} e_{U \cup \{k\}} \\ A_n^- e_U &= \textstyle\sum_{k \in U} e_{U \setminus \{k\}} \\ Z_n e_U &= (n - 2|U|) e_U \end{aligned}$$

Let us consider the vector $e_\emptyset = e_0^{\otimes n}$ and its images by the powers of A_n^-, normalized to have norm one. These are the vectors

$$\varepsilon_n^j = \sqrt{\frac{j!(n-j)!}{n!}} \sum_{U \subset \{1,2,\ldots,n\}; |U| = j} e_U \qquad j = 0, 1, \ldots, n$$

and these vectors are orthogonal. The action of the operators A_n^+, A_n^-, Z_n on these vectors is given by

$$\begin{aligned} A_n^+ \varepsilon_n^j &= \sqrt{(j+1)(n-j)} \varepsilon_n^{j+1} \\ A_n^- \varepsilon_n^j &= \sqrt{j(n-j+1)} \varepsilon_n^{j-1} \\ Z_n \varepsilon_n^j &= (n-2j) \varepsilon_n^j \\ S_n \varepsilon_n^j &= (n+1) \varepsilon_n^j \end{aligned}$$

In particular we see that these vectors belong to the eigenspace of S_n of eigenvalue $n+1$. We shall generalize this computation to find the common eigenspaces of the operators $S_1, S_2, \ldots, S_n$.

Lemma 3.3. *Let $J = (j_1, \ldots, j_n)$ be a sequence of integers such that*

- *i)* $j_1 = 2$
- *ii)* $j_i \ge 1$ *for all* $i \le n$
- *iii)* $|j_{i+1} - j_i| = 1$ *for all* $i \le n-1$

then there exists a subspace H_J of $(\mathbb{C}^2)^{\otimes n}$ of dimension $j_n = l+1$, which is an eigenspace of $S_1, \ldots, S_n$, with respective eigenvalues $j_1, \ldots, j_n$, and an orthonormal basis $(\phi_0, \ldots, \phi_l)$ such that

$$\begin{aligned} A_n^+ \phi_j &= \sqrt{(j+1)(l-j)}\phi_{j+1} \\ A_n^- \phi_j &= \sqrt{j(l-j+1)}\phi_{j-1} \\ Z_n \phi_j &= (l-2j)\phi_j \end{aligned}$$

Furthermore, the spaces H_J are orthogonal and $(\mathbb{C}^2)^{\otimes n} = \oplus_J H_J$.

Proof of the lemma. We shall use induction on n. The lemma is true for $n = 1$, using $\phi_0 = e_0; \phi_1 = e_1$. Assume the lemma holds for n, and let $J = (j_1, \ldots, j_n)$ be a sequence satisfying the conditions $i), ii), iii)$, of the lemma. We shall decompose the space $H_J \otimes \mathbb{C}^2$ as a direct sum of two subspaces. Let the vectors ψ_j and η_j be defined by

$$\psi_j = \sqrt{\frac{l-j+1}{l+1}}\phi_j \otimes e_0 + \sqrt{\frac{j}{l+1}}\phi_{j-1} \otimes e_1 \quad j = 0, \ldots, l+1$$

and

$$\eta_j = \sqrt{\frac{j+1}{l+1}}\phi_{j+1} \otimes e_0 - \sqrt{\frac{l-j}{l+1}}\phi_j \otimes e_1 \quad j = 0, \ldots, l-1$$

It is easy to check that these vectors form an orthonormal basis of the tensor product $H_J \otimes \mathbb{C}^2$, and a simple computation using

$$X_{n+1} = X_n + I^{\otimes n} \otimes \sigma_x, Y_{n+1} = Y_n + I^{\otimes n} \otimes \sigma_y, Z_{n+1} = Z_n + I^{\otimes n} \otimes \sigma_z$$

shows that these vectors have the right behaviour under these operators. □

We can now prove theorem 3.2, indeed for any sequence satisfying the hypotheses of lemma 3.3 one has

$$P(S_1 = j_1, \ldots, S_n = j_n) = \frac{j_n}{2^n} = \frac{j_1}{2}\frac{j_2}{2j_1} \cdots \frac{j_n}{2j_{n-1}}$$

where the right hand side is given by the distribution of the Markov chain of theorem 3.2. □

We shall give another, more conceptual, proof of the former result in section 5, using the representation theory of the group $SU(2)$ and Clebsch-Gordan formulas. For this we shall interpret the quantum Bernoulli random walk as a Markov process with values in a noncommutative space, but we need first to give some definitions pertaining to bialgebras and group algebras, which we do in the next section.

4 Bialgebras and Group Algebras

4.1 Coproducts

Let X be a finite set, and $\mathcal{F}(X)$ be the algebra of complex functions on X. A composition law on X is a map $X \times X \to X$. This gives rise to a unit preserving algebra morphism $\Delta : \mathcal{F}(X) \to \mathcal{F}(X \times X)$, where $\mathcal{F}(X \times X)$ is the algebra of functions on $X \times X$, and one has a natural isomorphism $\mathcal{F}(X \times X) \sim \mathcal{F}(X) \otimes \mathcal{F}(X)$. Conversely, such an algebra morphism $\Delta : \mathcal{F}(X) \to \mathcal{F}(X) \otimes \mathcal{F}(X)$ comes from a composition law, and many properties of the composition law can be read on it. For example, associativity translates into coassociativity of the coproduct which means that

$$(\Delta \otimes I) \circ \Delta = (I \otimes \Delta) \circ \Delta$$

whereas commutativity gives cocommutativity for the coproduct, which means that

$$v \circ \Delta = \Delta$$

where $v : \mathcal{F}(X) \otimes \mathcal{F}(X) \to \mathcal{F}(X) \otimes \mathcal{F}(X)$ is the flip automorphism $v(a \otimes b) = b \otimes a$. In order to obtain an analogue of a composition law in the noncommutative context, one can define a coproduct for any algebra A as a morphism $\Delta : A \to A \otimes A$, however in general the algebraic tensor product is too small for obtaining interesting examples. Think for example to the case $A = C_b(X)$, X a locally compact space, and see that $A \otimes A \subset C_b(X \times X)$ is a small subspace. We shall therefore consider coproducts which take values in a suitable completion of the algebraic tensor product. An algebra endowed with a coassociative coproduct is called a bialgebra. If the algebra is a C^* (resp. a von Neumann) algebra and the tensor product is the minimal C^* product (resp. the von Neumann algebra tensor product), then one has a C^* (resp. a von Neumann) bialgebra.

Some further properties of a coproduct are the existence of the dual notion of the unit element and the inverse, which are respectively called a counit, $\varepsilon : A \to \mathbb{C}$ and an antipode, $i : \Delta \to \Delta$.

A Hopf algebra is a bialgebra with a unit and an antipode, satisfying some compatibility conditions. I refer for example to [K] for an exposition of Hopf algebras and quantum groups.

4.2 Some Algebras Associated to a Compact Group

We shall investigate in more details the notions above in the case of the group algebra of a compact group, which we assume for simplicity to be separable. Recall that every representation of a compact group can be made unitary, and can be reduced to an orthogonal direct sum of irreducible representations. The right regular representation of a compact group G is the representation of G on $L^2(G, m)$ (where m is a Haar measure on G) by right translations $\rho_g f(h) = f(hg^{-1})$ and the left regular representation acts by left translations $\lambda_g f(h) = f(gh)$. A fundamental theorem is the Peter-Weyl theorem. It states that every irreducible representation of G arises in the decomposition of the left (or right) regular representation, actually one has an orthogonal direct sum

$$L^2(G) = \oplus_{\chi \in \hat{G}} E_\chi$$

where $\hat{G}$ is the (countable) set of equivalence classes of irreducible representations of G, and for $\chi \in \hat{G}$, E_χ is the space of coefficients of the representation i.e. the vector space generated by functions on G of the form

$$f(g) = \langle \chi(g)u, v \rangle$$

where u, v are vectors in the representation space of χ ($\langle ., . \rangle$ being an invariant hermitian product on the space). The space E_χ is finite dimensional, its dimension being $\dim(\chi)^2$, and it is an algebra for the convolution product on G, isomorphic to the matrix algebra $M_n(\mathbb{C})$ with $n = \dim(\chi)$. We shall denote this space M_χ when we want to emphasize its algebra structure.

We shall describe several algebras associated to G. The first one is the convolution algebra $\mathcal{A}^0(G)$ generated by the coefficients of the finite dimensional representations. As a vector space it is the algebraic direct sum $\mathcal{A}^0(G) = \oplus_\chi M_\chi \sim \oplus_\chi M_{\dim(\chi)}(\mathbb{C})$. There are larger algebras such as $L^1(G)$ the space of integrable functions (with respect to the Haar measure on G), and $C^*(G)$ the C^* algebra generated by $L^1(G)$. This algebra consists of sequences $(m_\chi; \chi \in \hat{G})$ such that $m_\chi \in M_\chi; |m_\chi| \to 0$ as $\chi \to \infty$.

The multiplier algebra of $C^*(G)$ coincides with the von Neumann algebra $\mathcal{A}(G)$, which is generated (topologically) by the left translation operators $\lambda_g; g \in G$, it consists of sequences $(m_\chi; \chi \in \hat{G})$ such that $\sup_\chi |m_\chi| < \infty$. In both cases, the norm in these algebras is $\sup_\chi |m_\chi|$. Note that the left and right translation operators λ_g and ρ_g are unitary, and the right translation operators generate the commutant of $\mathcal{A}(G)$.

When the group G is abelian, there is a natural isomorphism, given by Fourier transform, between the algebra $\mathcal{A}(G)$ and $L^\infty(\hat{G})$ where here $\hat{G}$ is the group of characters of G (this is consistent with our earlier notation since then all irreducible representations of G are one dimensional and are thus characters). This group of characters is a discrete abelian group, and its Haar measure is the counting measure.

In the general case, the algebra $L^\infty(\hat{G})$ is isomorphic with the center of $\mathcal{A}(G)$, since a bounded function on $\hat{G}$ can be identified with a sequence $(m_\chi)_{\chi \in \hat{G}}$ of scalar operators.

Any closed subgroup of G generates a von Neumann subalgebra $\mathcal{A}(H)$ furthermore the coproduct Δ restricts to this subalgebra and defines a coproduct $\Delta : \mathcal{A}(H) \to A(H) \otimes A(H)$. If the subgroup is abelian, then this subalgebra is commutative and is isomorphic to the algebra $L^\infty(\hat{H})$, Finally we shall also use the algebra $\hat{\mathcal{A}}(G) = \prod_\chi M_\chi$ which consists in unbounded operators on $L^2(G)$, with common dense domain $\oplus_\chi E_\chi$ (algebraic direct sum), affiliated with the von Neumann algebra $\mathcal{A}(G)$. One has natural inclusions

$$\mathcal{A}^0(G) \subset C^*(G) \subset M(C^*(G)) = \mathcal{A}(G) \subset \hat{\mathcal{A}}(G)$$

The algebra $\hat{\mathcal{A}}(G) \otimes \hat{\mathcal{A}}(G)$ is an algebra of operators on the algebraic direct sum $\oplus_{\chi,\chi'} E_\chi \otimes E_{\chi'}$ and we denote by $\hat{\mathcal{A}}(G)\hat{\otimes}\hat{\mathcal{A}}(G)$ its completion for simple convergence on $\oplus_{\chi,\chi'} E_\chi \otimes E_{\chi'}$. One has

$$\hat{\mathcal{A}}(G) \otimes \hat{\mathcal{A}}(G) = \prod_\chi M_\chi \otimes \prod_\chi M_\chi \subset \hat{\mathcal{A}}(G)\hat{\otimes}\hat{\mathcal{A}}(G) \sim \prod_{\chi,\chi'} M_\chi \otimes M_{\chi'}$$

The $*$ algebra structure extends obviously to $\hat{\mathcal{A}}(G)$, and an element is positive if and only if its components are positive.

4.3 The Coproduct

The coproduct formula $\Delta : \lambda_g \to \lambda_g \otimes \lambda_g$ extends by linearity and continuity to the von Neumann algebra $\mathcal{A}(G)$ if we use the von Neumann algebra tensor product. It defines a structure of cocommutative von Neumann bialgebra on $\mathcal{A}(G)$. One can also define an extension of the coproduct

$$\hat{\Delta} : \hat{\mathcal{A}}(G) \to \hat{\mathcal{A}}(G)\hat{\otimes}\hat{\mathcal{A}}(G).$$

Indeed it is easy to check that for any $\chi \in \hat{G}$, and $a \in M_\chi$, the operator $\Delta(a)$ is nonzero on the space $E_{\chi'} \otimes E_{\chi''}$ if and only if χ has a non zero multiplicity in the decomposition of the tensor product representation $E_{\chi'} \otimes E_{\chi''}$. It follows that for any sequence $(a_\chi)_{\chi\in\hat{G}} \in \prod_{\chi\in\hat{G}} M_\chi$ the sum $\sum_{\chi\in\hat{G}} \Delta(a_\chi)$ is a finite sum in each component $E_\chi \otimes E_{\chi'}$ therefore it defines an element in $\hat{\mathcal{A}}(G)\hat{\otimes}\hat{\mathcal{A}}(G) \sim \prod_{\chi,\chi'} M_\chi \otimes M_{\chi'}$.

One can define the convolution of two finite weights μ and ν by the formula

$$\mu * \nu = (\mu \otimes \nu) \circ \Delta$$

since the coproduct is cocommutative and coassociative, one checks that this is an associative and commutative operation.

4.4 The Case of Lie Groups

For compact Lie groups there is another algebra of interest, which is the envelopping algebra of the Lie algebra. Recall that the Lie algebra of a Lie group is composed of right invariant vector fields on the group. As such it acts on the L^2 space as a family of unbounded operators. Therefore the Lie algebra is a subspace of the "big" algebra $\hat{\mathcal{A}}(G)$, and the algebra generated by this subspace is naturally isomorphic to the envelopping Lie algebra (for simply connected groups). The elements of the Lie algebra have the following behaviour with respect to the extended coproduct on $\hat{\mathcal{A}}(G)$

$$\Delta(X) = X \otimes I + I \otimes X$$

This can be seen by taking derivatives with respect to s in the equation

$$\Delta(e^{sX}) = e^{sX} \otimes e^{sX}$$

where $e^{sX}; s \in \mathbb{R}$ is the one parameter subgroup generated by X.

4.5 States and Weights

A normal state ν on $\mathcal{A}(G)$ is determined by its value on the generators λ_g, thus by the function $\phi_\nu(g) = \nu(\lambda_g)$. It is a classical result that a function ϕ on G corresponds to a state on $C^*(G)$, and to a normal state on $\mathcal{A}(G)$, if and only if it is a continuous positive definite function on the group, satisfying $\phi(e) = 1$.

Every normal weight on $\mathcal{A}(G)$ is given by a sequence of weights $(\nu_\chi)_{\chi \in \hat{G}}$ on each of the subalgebras M_χ, therefore for a weight ν on $\mathcal{A}(G)$ there exists a sequence of positive elements $f_\chi \in M_\chi$ such that $\nu_\chi(a) = Tr(af_\chi)$ for all $a \in M_\chi$. Conversely any such sequence f_χ defines a normal weight, thus normal weights on $\mathcal{A}(G)$ correspond to positive elements in $\hat{\mathcal{A}}(G)$.

5 Random Walk on the Dual of $SU(2)$

5.1 The Dual of $SU(2)$ as a Noncommutative Space

We shall now interpret the process constructed in section 3 as a random walk on a noncommutative space. For this we consider the group $SU(2)$ of unitary 2×2 matrices with determinant 1. It is well known that the irreducible representations of this group are finite dimensional, moreover, for each integer $n \geq 1$ there exists, up to equivalence, exactly one irreducible representation of dimension n, therefore one has

$$\mathcal{A}(SU(2)) = \oplus_{n=1}^{\infty} M_n(\mathbb{C})$$

as a von Neumann algebra direct sum and similarly the C^* algebra of $SU(2)$ can be identified with the algebra of sequences $(M_n)_{n\geq 1}$ where M_n is an $n \times n$ matrix and one has $\|M_n\| \to 0$ as $n \to \infty$. We shall interpret this C^*-algebra as the space of "functions" vanishing at infinity on some noncommutative space. The associated von Neumann algebra corresponds to the space of "bounded functions" on our noncommutative space. In order to get a better picture of this space it is desirable to have a geometric understanding of its structure. For this we first note that this space has a continuous group of symmetries, since the group $SU(2)$ acts on the algebra by inner automorphisms. Since the elements $\pm I$ act trivially, this is really an action of the quotient $SU(2)/\{\pm I\}$ which is isomorphic with the group $SO(3)$, therefore this space has a three dimensional rotational symmetry. We can understand this symmetry by looking at some special elements in the larger algebra $\hat{\mathcal{A}}(SU(2))$, which correspond to "unbounded functions". Let us consider the self-adjoint elements corresponding to the Pauli matrices, viewed as elements of the Lie algebra of $SU(2)$ (or rather the complexified Lie algebra). These define unbounded operators on $L^2(SU(2))$, which we shall denote X, Y, Z, and which lie in $\hat{\mathcal{A}}(SU(2))$. A good way to think about these three functions is as three "coordinates" on our space, corresponding to three orthogonal directions. Each of these elements has a spectrum which is exactly the set of integers (which you can view as the group dual to the one parameter group generated by one of these Lie algebra elements). Moreover this is true also of any linear combination $xX+yY+zZ$ with $x^2+y^2+z^2=1$. This means that if you are in this space and try to measure your position, you can measure, as in quantum mechanics, one coordinate in some direction (x, y, z) using the operator $xX+yY+zZ$, and you will always find an integer. Thus the space has some discrete feature, in that you always get integer numbers for your coordinates, but also a continuous rotational symmetry which comes from the action of $SU(2)$ by automorphisms of the algebra. This is obviously impossible to obtain in a classical space. Of course since the operators in different directions do not commute, you cannot measure your position in different directions of space simultaneously. What you can do nevertheless is measure simultaneoulsy one coordinate in space, and your distance to the origin. This last measurement is done using the operator $D = \sqrt{I+X^2+Y^2+Z^2} - I$ which is in the center of the algebra $\hat{\mathcal{A}}(SU(2))$, and therefore can be measured simultaneously with any other operator. Its eigenvalues are the nonnegative integers $0, 1, 2 \ldots$, and its spectral projections are the identity elements of the algebras $M_n(\mathbb{C})$, more precisely, one has in $\hat{\mathcal{A}}(SU(2))$

$$D = \sum_{n=1}^{\infty} (n-1) I_{M_n(\mathbb{C})}$$

We thus see that the subalgebra $M_n(\mathbb{C})$ is a kind of "noncommutative sphere of radius $n-1$", and moreover by looking at the eigenvalues of the operators $xX + yY + zZ$ in the corresponding representation, we see

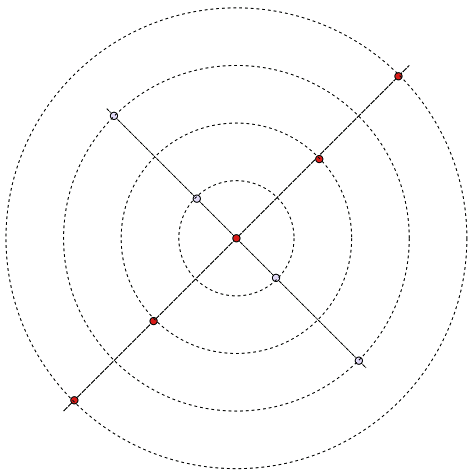

Fig. 1 Noncommutative space underlying $\mathcal{A}(SU(2))$.

that on any "radius" of this sphere, corresponding to a direction of space, the coordinate on this radius can only take the n values $n-1, n-3, n-5, \ldots, -n+1$.

If we rescale the noncommutative sphere of large radius to have radius 1, it looks more and more like a classical sphere, see e.g. [Rie] for a precise statement.

5.2 Construction of the Random Walk

Let ω be a state on $M_2(\mathbb{C})$, which we can also consider as a state on $\mathcal{A}(SU(2))$ by the projection $\mathcal{A}(SU(2)) \to M_2(\mathbb{C})$. Let us consider the infinite tensor product algebra, with respect to the product state $\nu = \omega^{\otimes\infty}$ on $\mathcal{N} = \otimes_1^\infty \mathcal{A}(SU(2)))$.

Let $T : \mathcal{N} \to \mathcal{N}$ be defined by $\Delta \otimes s$ where $s : \mathcal{A}(SU(2))^{[2,\infty[} \to \mathcal{A}(SU(2))^{[3,\infty[}$ is the obvious shift isomorphism. Let $j_n : \mathcal{A}(SU(2)) \to \mathcal{N}$ be the morphisms defined by by $j_n = T^n \circ i$ where $i(a) = a \otimes I^\infty$ is the GNS representation of $\mathcal{A}(SU(2))$ associated with ω, acting on the first factor. Note that one has actually $\mathcal{N} = \otimes_1^\infty M_2(\mathbb{C})$ and $i(a) = \rho_2(a) \otimes I^\infty$ where ρ_2 is a two dimensional irreducible representation. The morphisms j_n can be extended to the large algebra $\hat{\mathcal{A}}(SU(2))$ and for V in the Lie algebra, using the formula for the coproduct one checks that

$$j_n(V) = \sum_{i=1}^{n} I^{\otimes(i-1)} \otimes V \otimes I^{\otimes\infty}$$

Thus the quantum Bernoulli random walk is obtained by taking the operators $(j_n(X), j_n(Y), j_n(Z))$ where X, Y, Z are the Lie algebra elements corresponding to the Pauli matrices. For $n \geq 0$, we let $\mathcal{N}_n$ be the algebra generated by the first n factors in the tensor product. There exists a conditional expectation $\nu(.|\mathcal{N}_n)$ with respect to the state ν onto such a subalgebra, it is given simply by $I \otimes \omega^\infty$ on the factorization $\mathcal{N} = \mathcal{A}(SU(2))^{\otimes n} \otimes \mathcal{A}(SU(2))^{\otimes [n+1,\infty[}$.

The family of morphisms $(j_n)_{n\geq 1}$ form a noncommutative process wih values in the dual of $SU(2)$. The following proposition is left to the reader, as an exercise in manipulation of coproducts.

Proposition 5.1. *The family of morphisms $j_n; n \geq 1$, together with the family of algebras $\mathcal{N}, \mathcal{N}_n; n \geq 1$, and the conditional expectations $\nu(.|\mathcal{N}_n)$, form a dilation of the completely positive map $\mathcal{A}(SU(2)) \to \mathcal{A}(SU(2))$ given by $\Phi_\omega = (I \otimes \omega) \circ \Delta$.*

Let us now consider the three one-parameter subgroups generated by the Pauli matrices, they consist respectively of the matrices

$$\begin{pmatrix} \cos\theta & i\sin\theta \\ i\sin\theta & \cos\theta \end{pmatrix} \quad \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \quad \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix} \qquad \theta \in [0, 2\pi[$$

Each of these subgroups generates a commutative von Neumann subalgebra of $\mathcal{A}(SU(2))$, which is isomorphic with the group von Neumann algebra of the group $U(1)$ of complex numbers of modulus 1. Such a von Neumann algebra is isomorphic, by Pontryagin duality, to the algebra of bounded functions on the dual group, therefore the restriction of the dilation to this subalgebra provides a random walk on this dual group, which is isomorphic to $\mathbb{Z}$. Thus we recover, from the abstract considerations on duals of compact groups, our concrete Bernoulli random walks. In terms of our noncommutative space, we can observe a particle undergoing this random walk along any fixed direction of space, and what we see is a Bernoulli random walk (recall that the coordinate in some fixed direction of space can only take integer values).

We now turn to the spin process which can be interpreted in terms of the restriction of the dilation $(j_n)_{n\geq 1}$ to the center of the group algebra $\mathcal{A}(G)$. This center consists of operators of the form $(m_\chi; \chi \in \hat{G})$ where each m_χ is a scalar operator in M_χ, it is a commutative algebra, isomorphic with the algebra of bounded functions on $\hat{G}$ (recall that we have assumed that $\hat{G}$ is countable). Equivalently it is the algebra generated by the operator D i.e. the algebra of operators of the form $f(D)$ where f is a bounded complex function on the nonnegative integers. It is also easy to compute the restriction of the completely positive map Φ_ω to this center. It is given by the Clebsch-Gordan formula which computes the decomposition into irreducible of a tensor product of representations of the group $SU(2)$. What we need is the formula (where ρ_n is the n-dimensional irreducible representation)

$$\rho_2 \otimes \rho_n = \rho_{n-1} \oplus \rho_{n+1}$$

which tells us that the Markov chain can jump from n to either $n-1$ or $n+1$, furthermore the transition probabilities are proportional to the dimensions of the targets, since we are in the trace state. We see that the restriction of j_n to this algebra thus corresponds to the spin process.

Finally there are other commutative algebras which are invariant under the completely positive map. They are generated by the center of $\mathcal{A}(SU(2))$ and by a one parameter subgroup. Each such algebra is a maximal abelian subalgebra of $\mathcal{A}(SU(2))$, and its spectrum can be identified with the set of pairs (m, n) of integers such that $n \geq 1$ and $m \in \{n-1, n-3, \ldots -n+1\}$. One can compute the associated Markov semigroup, using the Clebsch Gordan formulas for products of coefficient functions of the group $SU(2)$. However the images of such an algebra by the morphisms $(j_n)_{n\geq 1}$ do not commute. Thus in this way we get a noncommutative dilation of a purely commutative semigroup. We will come back to this Markov chain when we study Pitman's theorem and quantum groups.

6 Random Walks on Duals of Compact Groups

It is easy to generalize the construction of the preceding section by replacing the group $SU(2)$ by an arbitrary compact group G. We will do a construction parallel to the usual construction of a random walk on a group. Let ϕ_0 and ϕ be continuous positive definite functions on G, with $\phi_0(e) = \phi(e) = 1$, thus these functions correspond to normal states ν_0 and ν on $\mathcal{A}(G)$. The state ν_0 will play the role of initial condition of our Markov chain, whereas the state ν represents the distribution of the increments. To the state ν is associated a completely positive map

$$\Phi_\nu : \mathcal{A}(G) \to \mathcal{A}(G) \qquad \Phi_\nu = (I \otimes \nu) \circ \Delta.$$

The completely positive map generates a semigroup $\Phi_\nu^n; n \geq 1$. We now build the infinite tensor product $\mathcal{N} = \mathcal{A}(G)^\infty$ with respect to the state $\nu_0 \otimes \nu^{\otimes\infty}$, and obtain a noncommutative probability space $(\mathcal{N}, \omega)$. Let $T : \mathcal{N} \to \mathcal{N}$ defined by $\Delta \otimes s$ where $s : \mathcal{A}(G)^{[1,\infty[} \to \mathcal{A}(G)^{[2,\infty[}$ is the obvious isomorphism. Let $j_n : \mathcal{A}(G) \to \mathcal{N}$ be the morphisms defined by induction $j_n = T^n \circ i$ where $i(a) = a \otimes I^\infty$ is the inclusion of $\mathcal{A}(G)$ into the first factor (strictly speaking this is an inclusion only if the state ν_0 is faithful).

Let us translate the above construction in the case of an abelian group, in terms of the dual group $\hat{G}$. The states ν and ν_0 correspond to probability measures on $\hat{G}$, the probability space is now the product of an infinite number of copies of $\hat{G}$, with the product probability $\nu_0 \otimes \nu^{\otimes\infty}$, and the maps j_n correspond to functions $X_n : \hat{G}^\infty \to G$ given by $X_n(g_0, g_1, \ldots, g_k, \ldots) = g_0 g_1 \ldots g_{n-1}$. We thus recover the usual construction of a random walk.

For $n \geq 0$, we let $\mathcal{N}_n$ be the algebra generated by the first $n+1$ factors in the tensor product. There exists a conditional expectation $\omega(.|\mathcal{N}_n)$ with respect to the state ω onto such a subalgebra, it is given simply by $I \otimes \nu^\infty$ on the factorization $\mathcal{N} = \mathcal{A}(G)^{\otimes(n+1)} \otimes \mathcal{A}(G)^{\otimes\infty}$.

Proposition 6.1. *The morphisms $(j_n)_{n\geq 0}$, together with the von Neumann algebras $\mathcal{N}, \mathcal{N}_n, n \geq 0$ and the state ω, form a dilation of the completely positive semigroup $(\Phi_\nu^n)_{n\geq 1}$, with initial distribution ν_0.*

The proof of this proposition follows exactly the case of $SU(2)$ treated in the preceding section.

Let H be a closed commutative subgroup of G, then its dual group $\hat{H}$ is a countable discrete abelian group. The von Neumann subalgebra $\mathcal{A}(H)$ generated by H in $\mathcal{A}(G)$ is isomorphic to $L^\infty(\hat{H})$, and the restriction of the positive definite function ϕ to H is the Fourier transform of a probability measure μ on $\hat{H}$. The coproduct Δ restricts to a coproduct on the subalgebra generated by H, thus the images of $\mathcal{A}(H)$ by the morphisms j_n generate commuting subalgebras of $\mathcal{N}$. These restrictions thus give a random walk on the dual group $\hat{H}$, whose independent increments are distributed according to μ.

We now consider another commutative algebra, namely the center $\mathcal{Z}(G)$ of $\mathcal{A}(G)$. Recall that this center is isomorphic with the space $L^\infty(\hat{G})$ of bounded functions on the set of equivalence classes of irreducible representations of G. As a von Neumann algebra of operators on $L^2(G)$, it is generated by the convolution operators by integrable central functions (recall that a function f on G is central if it satisfies $f(ghg^{-1}) = f(h)$ for all $h, g \in G$).

Proposition 6.2. *The algebras $j_n(\mathcal{Z}(G)); n \geq 1$ commute.*

Proof. Let $a, b \in \mathcal{Z}(G)$ and let $k \leq l$ we have to prove that $j_k(a)$ and $j_l(b)$ commute. Let $a' = i(a), b' = i(b)$, and note that a' and b' belong to the center of $\mathcal{N}$. One has

$$\begin{aligned} j_k(a)j_l(b) &= T^k(a')T^k(T^{l-k}(b')) \\ &= T^k(a'T^{l-k}(b')) \\ &= T^k(T^{l-k}(b')a') \\ &= T^l(b')T^k(a') \\ &= j_l(b)j_k(a) \end{aligned}$$

□

Furthermore one has.

Proposition 6.3. *If the function ϕ is central then $\Phi_\nu(\mathcal{Z}(G)) \subset \mathcal{Z}(G)$.*

Proof. Indeed if ψ is central function, belonging to $\mathcal{A}^0(G)$, then $\Phi_\nu(\psi) = \phi\psi$ is a central function on the group, and thus defines an element of $\mathcal{Z}(G)$. □

We deduce from the preceding propositions that, in the case when the increments correspond to a central state, the restriction of the dilation $(j_n)_{n\geq 0}$ to the center of the algebra $\mathcal{A}(G)$ defines a Markov process on $\hat{G}$, whose transition operator is given by the restriction of Φ_ν to the center $\mathcal{Z}(G)$. We shall now give a more concrete form of the transition probabilites of this Markov chain.

Proposition 6.4. *For χ an irreducible character of G, let*

$$\phi\chi = \sum_{\chi' \in \hat{G}} h_\phi(\chi', \chi)\chi'$$

be the expansion of the positive definite central function $\phi\chi$ into a combination characters, then the probability transitions of the Markov chain obtained from the restriction of $(j_n)_{n\geq 1}$ to the center are given by

$$p_\phi(\chi', \chi) = \frac{dim(\chi)}{dim(\chi')} h_\phi(\chi', \chi)$$

Proof. For $\chi \in \hat{G}$, the convolution operator associated with the function $\dim(\chi)\chi$ is the minimal projection of $\mathcal{Z}(G)$ associated with χ. In other words it corresponds to the indicator function 1_χ in the isomorphism of $L^\infty(\hat{G})$ with $\mathcal{Z}(G)$. The transition operator for the restriction of the dilation to the center is the restriction to this center of Φ_ω. On the other hand, the transition probabilities $p_\phi(\chi, \chi')$ are related to these indicator functions by $\Phi_\omega(1_{\chi'}) = \sum_\chi p_\phi(\chi', \chi)1_\chi$. The conclusion follows immediately. □

7 The Case of $SU(n)$

7.1 Some Facts About the Group $SU(n)$

We shall investigate the quantum random walk defined in the preceding section when the group G is the group $SU(n)$ of unitary matrices with determinant 1. First we recall some basic facts about this group and its representations. Let $\mathbf{T} \subset SU(n)$ be the subgroup of diagonal matrices, which is a maximal torus. The group of characters of $\mathbf{T}$ is an $n-1$ dimensional lattice, generated by the elements (the notation e is here to suggest the exponential function)

$$e(e_i)(\begin{pmatrix} u_1 & & 0 \\ & \ddots & \\ 0 & & u_n \end{pmatrix}) = u_j$$

These elements satisfy the relation (written in additive notation) $e_1 + e_2 + \ldots + e_n = 0$, which corresponds to the relation $e(e_1)e(e_2)\ldots e(e_n) = 1$ for the characters. We denote by $\mathbf{P}$ this group, and by $\mathbf{P}_+$ the subset of positive weights, i.e.

$$\mathbf{P}_+ = \{m_1 e_1 + \ldots + m_{n-1}e_{n-1} | m_1 \geq m_2 \geq \ldots \geq m_{n-1}\}$$

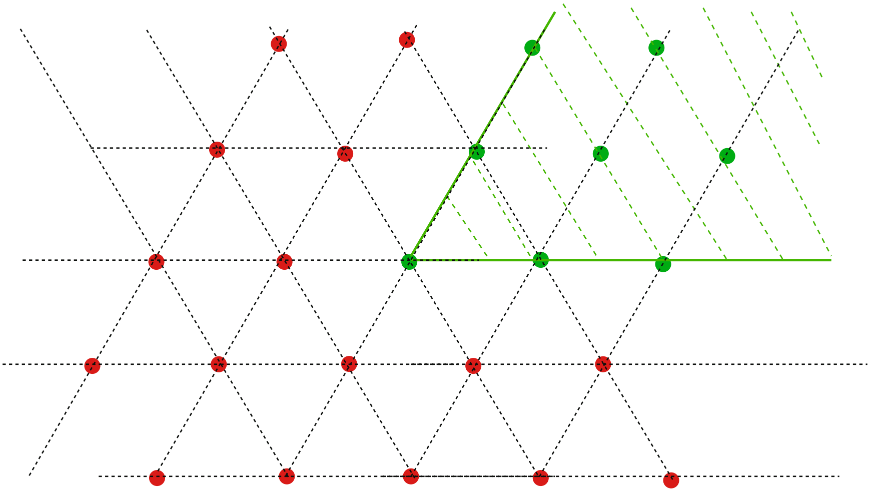

Fig. 2

We shall also need the set

$$\mathbf{P}_{++} = \{m_1 e_1 + \ldots + m_{n-1} e_{n-1} | m_1 > m_2 > \ldots > m_{n-1}\}$$

and note that the two sets are in bijection by

$$\mathbf{P}_{++} = \mathbf{P}_{+} + \rho \tag{7.1}$$

where $\rho = (n-1)e_1 + (n-2)e_2 + \ldots + e_{n-1}$ is the half sum of positive roots. The symmetric group acts on this character group by permutation of the e_i.

Below is a picture of $\mathbf{P}$ and $\mathbf{P}_+$ for the group $SU(3)$. Thus $\mathbf{P}$ consists of the points in a triangular lattice in the plane, and $\mathbf{P}_+$ is the intersection of this triangular lattice with a cone, fundamental domain for the action of the symmetric group S_3. The subset $\mathbf{P}_{++}$ consists in points of $\mathbf{P}_+$ which are in the interior of the cone.

Recall from the representation theory of the group $SU(n)$ (see e.g. [BtD], [GW], or [Z]) that the equivalence classes of irreducible representations of $SU(n)$ are in one to one correspondence with the elements of $\mathbf{P}_+$, which are called "highest weights". For each $x \in \mathbf{P}$ let $e(x)$ be the associated character of $\mathbf{T}$, then the character of the representation with highest weight $x \in \mathbf{P}_+$ given, for $u \in \mathbf{T}$, by Weyl's character formula

$$\chi_x(u) = \frac{\sum_{\sigma \in S_n} \epsilon(\sigma) e(\sigma(x+\rho))(u)}{\sum_{\sigma \in S_n} \epsilon(\sigma) e(\sigma(\rho))(u)} \tag{7.2}$$

In particular the defining representation of $SU(n)$ has character $e(e_1) + \ldots + e(e_n)$ corresponding to the highest weight e_1. The normalized positive definite

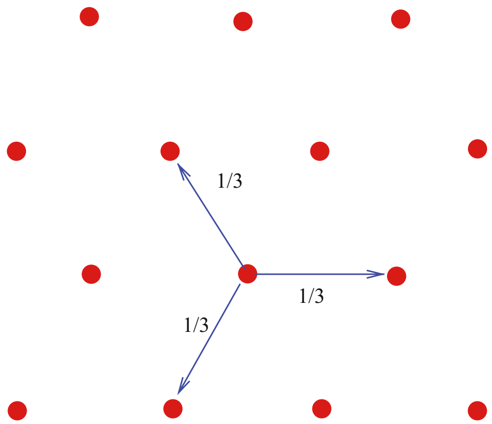

Fig. 3 The random walk on the dual of the maximal torus for SU(3).

function on $SU(n)$ corresponding to this character is $\phi(g) = \frac{1}{n}Tr(g)$. We shall investigate the quantum random walk associated with this positive definite function.

7.2 Two Classical Markov Chains

We shall obtain two classical Markov chains by restricting the Markov chain associated with ϕ to suitable subalgebras of $C^*(SU(n))$. The first subalgebra is that generated by the maximal torus $\mathbf{T}$. This algebra is isomorphic to the algebra of functions vanishing at infinity on the dual group $\mathbf{P}$. It is easy to see that the restriction to the torus of the quantum random walk $(j_n)_{n\geq 0}$, constructed using ϕ, is a random walk on the lattice $\mathbf{P}$ with increments distributed as $\frac{1}{n}(\delta_{e_1} + \ldots + \delta_{e_n})$. Its one step transition probabilities are given by

$$p_1(x,y) = \frac{1}{n} \quad \text{if } y \in \{x+e_1, \ldots, x+e_n\}$$
$$p_1(x,y) = 0 \quad \text{if not}$$

We give the picture for the case of the group $SU(3)$.

The second subalgebra is the center of $C^*(SU(n))$. By the preceding section, it can be identified with the space of functions vanishing at infinity on $\mathbf{P}_+$. We shall rather use the identification of the set of irreducible representations with $\mathbf{P}_{++}$ given by (7.1). As we saw in section 6 the restriction of the dilation $(j_n)_{n\geq 0}$ gives a classical Markov chain on the spectrum of the center, therefore we obtain in this way a Markov chain on $\mathbf{P}_{++}$, the generator of the Markov chain being given by the restriction of the generator of the quantum Markov chain on $\mathcal{A}(SU(2))$.

We shall now derive a relation between these two Markov chains (the one obtained from the maximal torus, and the one from the center). The set of highest weights, $\mathbf{P}_{++}$ is the intersection of $\mathbf{P}$ with the Weyl chamber, which is the cone

$$\mathbf{C} = \{x_1 e_1 + \ldots + x_{n-1} e_{n-1} | x_1 > x_2 > \ldots > x_{n-1}\}$$

We consider now the random walk on $\mathbf{P}$ killed at the exit of this cone. Thus the transition probabilites of this killed random walk are given by

$$\begin{aligned} p^0(x,y) &= \tfrac{1}{n} \quad \text{if } y \in \mathbf{P}_{++} \cap \{x+e_1, \ldots, x+e_n\} \\ p^0(x,y) &= 0 \quad \text{if not.} \end{aligned}$$

The sum $\sum_y p^0(x,y)$ is < 1 for points near the boundary, corresponding to the fact that the random walk has a nonzero probability of being killed.

Let $x \in \mathbf{P}_{++}$ and consider the irreducible representation ξ_x of $SU(n)$, with highest weight $x - \rho$. We can use Weyl's character formula (7.2) for decomposing the representation $\xi_x \otimes \xi_n$ (where ξ_n is the defining representation of $SU(n)$).

We remark that $\frac{1}{n} \sum_{j=1}^n e(e_j) = \frac{1}{n!} \sum_{\sigma \in S_n} e(\sigma(e_1))$. One has

$$\begin{aligned} \chi_n \chi_{x-\rho} &= \frac{1}{n}(e(e_1) + \ldots + e(e_n)) \frac{\sum_{\sigma \in S_n} \epsilon(\sigma) e(\sigma(x))}{\sum_{\sigma \in S_n} \epsilon(\sigma) e(\sigma(\rho))} \\ &= \frac{\sum_{\tau \in S_n} \sum_{\sigma \in S_n} \epsilon(\sigma) e(\sigma(x) + \tau(e_1))(u)}{n! \sum_{\sigma \in S_n} \epsilon(\sigma) e(\sigma(\rho))} \\ &= \frac{1}{n} \frac{\sum_{j=1}^n \sum_{\sigma \in S_n} \epsilon(\sigma) e(\sigma(x + e_j))}{\sum_{\sigma \in S_n} \epsilon(\sigma) e(\sigma(\rho))} \\ &= \frac{1}{n} \sum_{y \in \{x+e_1, x+e_2, \ldots, x+e_n\} \cap \mathbf{P}_{++}} \chi_{y-\rho} \end{aligned}$$

since if $y = x + e_j$ belongs to $\mathbf{P}_+ \setminus \mathbf{P}_{++}$ then it is fixed by some reflexion in S_n and thus the sum $\sum_{\sigma \in S_n} \epsilon(\sigma) e(\sigma(x + e_j))$ vanishes.

For $x \in \mathbf{P}_{++}$, let us denote $h(x)$ the dimension of the representation with highest weight $x - \rho$. We conclude from the preceding computation and Proposition 6.4, that the transition probabilities for the Markov chain on $\mathbf{P}_{++}$ are

$$q(x,y) = \frac{h(y)}{h(x)} p^0(x,y) \qquad x, y, \in \mathbf{P}_{++} \tag{7.3}$$

Since the transition operator is unit preserving, it follows in particular that the function h is a positive harmonic function with respect to the transition kernel p^0, i.e. satisfies

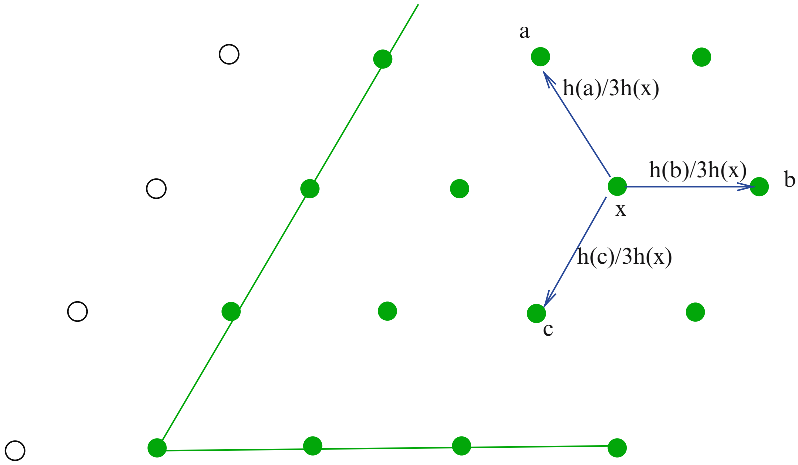

Fig. 4

$$h(x) = \sum_y h(y)p^0(x, y) \quad \text{for all } x \in \mathbf{P}_{++},$$

Again we draw the picture in the case of $SU(3)$.

Let us recall that, given transition (sub)probabilities $p(x, y)$ for a Markov chain, and a positive harmonic function h for p, i.e. a function such that

$$h(x) = \sum_y h(y)p(x, y) \qquad \text{for all } x$$

one calls the Markov chain with transition probabilities $\frac{h(y)}{h(x)}p(x, y)$ the Doob conditioning, or h-transform, of the Markov chain with transition probabilities p.

We can summarize the preceding discussion in the following proposition.

Proposition 7.1. *The Markov chain obtained by restriction to the center is related to the random walk on the dual of the maximal torus by a killing at the exit of the Weyl chamber followed by a Doob conditioning using the dimension function on the set of highest weights.*

For more information on Doob's conditioning, I refer to the books by Kemeny, Knapp and Snell [KKS], or Revuz [R].

One could ask whether this relation, between the Markov chains on the dual of the torus and on the center, holds for more general groups and positive definite functions. It turns out that the fundamental concept in this direction is that of a minuscule weight, see [B3] for more details.

8 Choquet-Deny Theorem for Duals of Compact Groups

8.1 The Choquet-Deny Theorem in an Abelian Group

As we have seen in the preceding section, the fact that the dimension function is a positive harmonic function on the Weyl chamber plays an important role in understanding the quantum random walk on the dual of $SU(n)$. A natural question arises, is this positive harmonic function unique? We shall answer this question, which is purely a question of "classical" potential theory using the theory of quantum random walks. Actually we shall do this by extending a well known result of Choquet and Deny [CD] on harmonic measures for locally compact abelian goups. The Choquet-Deny theorem describes completely the solutions of the convolution equation

$$\mu * \phi = \phi \tag{8.1}$$

on a locally compact abelian group G, where μ is a positive finite measure, and ϕ is an unknown positive measure. One assumes that the subgroup generated by the support of μ is the whole group. In order to state the Choquet-Deny theorem, one needs to define the exponentials on the group G. These are the continuous functions f on G, with values in $]0, +\infty[$, which are multiplicative, i.e. satisfy

$$f(gh) = f(g)f(h)$$

for all $g, h \in G$. An exponential $e : G \to]0, +\infty[$ is called μ-harmonic if one has $\int_G e(-x)\mu(dx) = 1$. The set of μ-harmonic exponentials is a Borel subset of the set of all continuous functions on G, which we denote by $\mathcal{E}_\mu$. Let ϕ be a positive measure on G of the form $\phi(dx) = e(x)dx$ where dx is the Haar measure on G and e is a μ-harmonic exponential, then one has for all positive measurable functions f

$$\begin{aligned}
\int_G f(x)\phi * \mu(dx) &= \int_G \int_G f(x+y)\phi(dx)\mu(dy) \\
&= \int_G \int_G f(x+y)e(x)dx\mu(dy) \\
&= \int_G \int_G f(x)e(x-y)dx\mu(dy) \\
&= \int_G f(x)e(x)dx \int_G e(-y)\mu(dy) \\
&= \int_G f(x)\phi(dx)
\end{aligned}$$

therefore the measure ϕ is μ-harmonic. i.e. satisfies the equation (8.1). The Choquet-Deny theorem states that every solution is a convex combination of solutions of this kind.

Theorem 8.1 (Choquet-Deny). *Assume that the subgroup generated by the support of the measure μ is G, then every positive measure ϕ, solution of the convolution equation (8.1), is absolutely continuous with respect ot the Haar measure on G, and its density has a unique representation as an integral*

$$\frac{d\phi(x)}{dx} = \int_{\mathcal{E}_\mu} e(x) d\nu_\phi(e)$$

where ν_ϕ is some finite positive measure on $\mathcal{E}_\mu$.

This result contains in particular the determination of all positive harmonic functions for the transition operator associated with the measure μ, indeed if h is such a positive μ-harmonic function, then the measure $h(-x)dx$ is a μ-harmonic measure.

Note that a locally compact abelian group corresponds to a commutative and cocommutative Hopf C^*-algebra. What we shall do next is to extend this theorem to (a class of) cocommutative Hopf C^*-algebras. This will allow us to answer the question about the uniqueness of the positive harmonic function. Before we state our analogue of the Choquet-Deny theorem on the dual of a compact group, we will first clarify some points about states and weights.

8.2 Some Further Properties of Duals of Compact Groups

Let G be a compact group and $\mathcal{A}(G)$ be its von Neumann algebra. This von Neumann algebra has a structure of cocommutative Hopf-von Neumann algebra for the coproduct Δ, counit ε and antipode i given respectively by continuous linear extension of

$$\Delta(\lambda_g) = \lambda_g \otimes \lambda_g \quad \varepsilon(\lambda_g) = \delta_{e,g} \quad i(\lambda_g) = \lambda_{g^{-1}}.$$

We have seen in section 4.3 that the convolution of two finite normal weights μ and ν on $\mathcal{A}(G)$ is defined by the formula $\mu * \nu = (\mu \otimes \nu) \circ \Delta$. Assume now that μ is a positive finite weight and ϕ is positive, then we can write ϕ as a sum of finite weights $\phi = \sum_\chi \phi_\chi$ with respect to the restrictions of ϕ to the subalgebras M_χ. The sum $\sum_\chi \nu * \phi_\chi$ is then a sum of positive finite weights and thus it defines a (not necessarily normal) weight on $\mathcal{A}(G)$. We can therefore consider the equation (8.1) where this time μ and ϕ are positive normal weights, with μ finite.

Next we define the notion of exponential. The following definition is a straighforward extension of the definition in the case of abelian groups.

Definition 8.2. A *group-like element* is a non zero element f of $\hat{\mathcal{A}}(G)$, such that

$$\Delta(f) = f \otimes f.$$

If this element is positive, then we call it an *exponential.*

If μ is a finite weight, f is an exponential and $\mu(i(f)) = 1$ then we call f a μ-harmonic exponential.

Let f, g, h be positive elements in $\hat{\mathcal{A}}(G)$ then one has the identity

$$tr(f \otimes g\Delta(h)) = tr(i(h) \otimes g\Delta(i(f))) \tag{8.2}$$

which is easily checked on coefficient functions. Let $g \in \hat{\mathcal{A}}(G)$ be associated to μ, i.e. $\mu(.) = tr(g.)$, then it follows from 8.2 that for all h

$$\begin{aligned}\phi * \mu(h) &= tr(f \otimes g\Delta(h))\\ &= tr(i(h) \otimes g\Delta(i(f)))\\ &= tr(i(h)i(f))tr(gi(f))\\ &= \phi(h)\end{aligned}$$

Thus if f is a μ-harmonic exponential, and ϕ is the weight associated with f, then ϕ satisfies the equation (8.1).

8.3 The Analogue of the Choquet-Deny Theorem

We shall assume that the state ν satisfies a non degeneracy condition which is the analogue, in the noncommutative setting, of the requirement that the support of the measure generates the whole group. This condition states that for every finite weight ρ on $\mathcal{A}(G)$ which is supported by some algebra M_χ for $\chi \in \hat{G}$, there exists an integer $n \geq 1$ and a constant $c > 0$ such that $c\nu^{*n} \geq \rho$.

Theorem 8.3. *Let ϕ be a ν-harmonic weight, then there exists a unique finite positive measure on the set of ν-harmonic exponentials such that*

$$\phi = \int_{\mathcal{E}_\mu} e\, dm_\phi(e)$$

Sketch of proof. We let $\mathcal{S}_\nu$ be the convex cone of normal weights satisfying

$$\phi * \nu \leq \phi$$

This cone is a closed subset of $\hat{\mathcal{A}}$, and we can use Choquet's integral representation theorem to conclude that any element of this cone can be written as the barycenter of a measure supported on the set of its extremal rays. Now one can analyze the extremal rays of this set, and see that such an extremal ray consists in multiples of an exponential. The uniqueness argument comes from the existence of an algebra of functions on the cone, which separates points, see [B4] for details.

8.4 Examples

For a finite group, the set of exponentials is reduced to the identity.

If the state ν is tracial, then there exists only one ν-harmonic exponential, namely the identity. In the case of the group $SU(n)$, the exponentials are in one to one correspondence with the positive elements in $SL(n, \mathbb{C})$.

From these results we deduce that the positive harmonic function h of Proposition 7.1 was unique. Indeed in order to prove that a function h is the unique (up to a multiplicative constant) positive harmonic function for a transition kernel p, it is enough to check that all the positive harmonic functions for the relativized kernel $\frac{h(y)}{h(x)}p(x,y)$ are constant, which is what the Choquet-Deny theorem tells us.

9 The Martin Compactification of the Dual of $SU(2)$

In the preceding section we have seen that the classical Choquet-Deny theorem about solutions of convolution equations has an analogue in duals of compact groups. This allows one to give an explicit description of all μ-harmonic positive functions for a finite positive measure μ on a commutative group. By the Choquet-Deny theorem the positive μ-harmonic functions admit a unique integral representation in terms of minimal μ-harmonic functions, and these minimal harmonic functions can be identified with exponentials. The next natural question in this line of ideas is to describe the Martin compactification associated to a random walk with values in $\mathbb{Z}^n$. This Martin compactification provides a way to attach a boundary to the space $\mathbb{Z}^n$ in order to obtain a compact space, where the boundary is naturally identified with the set of minimal μ-harmonic functions. The Martin compactification of $\mathbb{Z}^n$ was computed by Ney and Spitzer in a classical paper [NS], where they showed that it consists in adding a sphere at infinity, and identifying this sphere with the set of minimal harmonic functions with the help of the Gauss map. In this section we will describe the Martin compactification of some quantum random walks with values in the dual of $SU(2)$. We will first recall some basic facts about classical Martin boundaries, then describe Ney and Spitzer's theorem, before going to the case of the dual of $SU(2)$.

9.1 The Martin Compactification for Markov Chains

Consider a Markov chain on a countable state space E. The Markov chain has transition subprobabilities $p(x,y), x,y \in E$, i.e. we have $\sum_y p(x,y) \leq 1$, so that the kernel is submarkovian and the process may die in a finite time. There is an associated transition operator given by

$$Pf(x) = \sum_{y\in E} p(x,y)f(y)$$

and the iterated operator is given by n-step transition probabilities

$$P^n f(x) = \sum_{E} p_n(x,y)f(y)$$

We assume that the associated Markov chain is transient, so that the potential

$$U = \sum_{n=0}^{\infty} P^n$$

is finite, i.e. the function

$$u(x, y) = \sum_{n=0}^{\infty} p_n(x, y) < \infty$$

Let us choose an initial distribution $r(dx)$ such that the function $rU(y) = \sum_E u(x, y)r(dx)$ is everywhere > 0. The Martin kernel is defined by

$$k(x, y) = \frac{u(x, y)}{rU(y)}$$

It follows from the Harnack inequalities that the functions $k(x, .)$ form a uniformly continuous family on E. The Martin compactification of the Markov chain is the smallest compact topological space $\bar{E}_u$, which contains E as a dense subset, and such that these functions extend continuously to the boundary $\partial E_u = \bar{E}_u \setminus E$. This space exists because the functions $k(x, .)$ separate the points of E and because of the uniform continuity. For any $\xi \in \partial E_u$ the function $x \mapsto k(x, \xi)$ is a p-harmonic function. Recall that a positive p-harmonic function f on E is called minimal if for every positive p-harmonic function g satisfying $g \leq Cf$ for some $C > 0$, one has actually $g = cf$ for some constant c. One can prove that any minimal p-harmonic function f, which is r-integrable, is a multiple of $k(., \xi)$ for some $\xi \in \partial E_u$. The subset ∂E_m of $\xi \in \partial E_u$ such that $k(., \xi)$ is minimal is a Borel subset, and one can prove that any positive p-harmonic function f, which is r-integrable, admits a representation

$$f = \int_{\partial E_u} k(., \xi) dm_f(\xi)$$

with a unique positive measure m_f.

9.2 The Martin Compactification of $\mathbb{Z}^d$

When the Markov chain is a random walk on $\mathbb{Z}^d$, with increments distributed as μ, a (sub)probability measure on $\mathbb{Z}^d$, we have seen that every positive μ-harmonic function admits an integral representation in terms of exponentials. When the increments of the random walk are integrable, Ney and Spitzer have determined explicitly the Martin compactification of $\mathbb{Z}^d$, which we shall now describe. Let $\phi : \mathbb{R}^d \to [0, +\infty]$ be the function

$$\phi(x) = \sum_{y \in \mathbb{Z}^d} e^{\langle x, y \rangle} \mu(dy)$$

We assume that it is finite in a neighbourhood of the set

$$\mathcal{E}_\mu = \{x|\phi(x) = 1\}$$

Then the set $\mathcal{E}_\mu$ is the boundary of the convex set $\{x|\phi(x) \leq 1\}$ and it is either reduced to a point or homeomorphic to a sphere. In the latter case the homeomorphism can be expressed thanks to the Gauss map as

$$\frac{\nabla\phi}{\|\nabla\phi\|}$$

Since ϕ is convex this is a homeomorphism from $\mathcal{E}_\mu$ onto the unit sphere. Ney and Spitzer proved that the Martin compactification is homeomorphic to the usual compactification of $\mathbb{Z}^d$ by a sphere at infinity, where the identification between the sphere and the set of minimal μ-harmonic functions is provided by the map above.

9.3 Noncommutative Compactifications

Before we investigate the problem of finding an analogue of the Ney-Spitzer theorem for the dual of $SU(2)$ let us translate in the noncommutative language the notion of a compactification of a topological space. So let X be a topological space, and $\bar{X}$ a compact space such that $X \subset \bar{X}$ is a dense open subset, and $\partial\bar{X} = \bar{X} \setminus X$ is the boundary, then $C(\bar{X})$ is can be identified with a subalgebra of $C_b(X)$, the algebra of all bounded continuous functions on X, and one has an exact sequence

$$0 \to C_0(X) \to C(\bar{X}) \to C(\partial X) \to 0$$

where the first map is the continuous extension, to $\bar{X}$, by 0 on the boundary, of a function on X, and the second map is the restriction to a closed subset. A compactification of $C_0(X)$ is thus given by a certain commutative C^*-subalgebra of the multiplier algebra of $C_0(X)$, containing $C_0(X)$. In the case of the Martin compactification this subalgebra is just the algebra generated by $C_0(X)$ and by the functions $y \mapsto k(x,y)$. The vector space generated by functions of the form $y \mapsto k(x,y)$ can be identified with the image of the Martin kernel, considered as an integral operator $f \mapsto \sum_{x\in E} f(x)k(x,y)$. It is this interpretation of the Martin kernel that has a natural noncommutative analogue.

9.4 The Martin Kernel for the Quantum Random Walk

We consider a central quantum random walk, therefore we have a positive definite central function ϕ on $SU(2)$ such that $\phi(e) \leq 1$, and the associated state ν on $\mathcal{A}(SU(2))$. We have seen that it has an associated transition kernel given by the completely positive map $\Phi_\nu = (I \otimes \nu) \circ \Delta$. This map acts as $\lambda_g \mapsto \phi(g)\lambda_g$ on the generators λ_g of the von Neumann algebra $\mathcal{A}(SU(2))$. We know that if $\phi(e) = 1$ then there exists only one ϕ-harmonic weight, namely the one given by the function 1. In this case we expect that the Martin boundary will be given by a one point compactification, which consists just in adding a unit to the algebra, so in order to avoid this case, we shall assume here that $\phi(e) < 1$.

We can consider the associated potential which is equal to $U = \sum_{n=0}^{\infty} \Phi_\nu^n$, and which acts by multiplication by the function $\sum_{n=0}^{\infty} \phi^n = \frac{1}{1-\phi}$. We shall consider the action of the potential on the space of coefficients i.e. the direct sum $\oplus_\chi M_\chi$ where each element of this space can be identified with a polynomial function on $SU(2)$ acting by convolution, i.e. by the operator $\int_{SU(2)} p(g)\lambda_g dg$. Then the Martin kernel will be defined, by analogy with the case of classical Markov chains, by

$$p \mapsto \frac{\int_{SU(2)} \frac{p(g)}{1-\phi(g)} \lambda_g dg}{\int_{SU(2)} \frac{1}{1-\phi(g)} \lambda_g dg}$$

Note that the operator $\int_{SU(2)} \frac{1}{1-\phi(g)} \lambda_g dg$ lies in the center of $\mathcal{A}(SU(2))$, therefore there is no ambiguity in the quotient of the preceding formula.

9.5 Pseudodifferential Operators of Order Zero and the Martin Compactification

In order to find the Martin compactification of the quantum random walk, we shall identify the C^*-algebra generated by $C^*(SU(2))$ and by the image of the Martin kernel, and show that it gives rise to a three terms exact sequence. We will first exhibit a certain exact sequence

$$0 \to C^*(SU(2)) \to \mathcal{M} \to C(S^2) \to 0 \tag{9.1}$$

where $\mathcal{M}$ is our sought for Martin compactification, and $C(S^2)$ is the algebra of continuous functions on the two dimensional sphere S^2. For this we consider the three operators in $\hat{\mathcal{A}}(SU(2))$ associated with Pauli matrices, which we call X, Y, Z, and the Casimir operator $C = X^2+Y^2+Z^2+I$ which acts by $(n+1)^2$ on the space of coefficients of the n-dimensional representation of $SU(2)$, and build three operators

$$x = XC^{-1/2}, y = YC^{-1/2}, z = ZC^{-1/2}$$

Clearly these operators are self-adjoint and bounded. Using the commutation relations (3.1) one can see that $[x, y],\ [x, z],\ [y, z]$ and $x^2 + y^2 + z^2 - I$ are compact operators on $L^2(SU(2))$. It follows that there exists a map from the algebra generated by x, y, z to the algebra of polynomial function on the sphere, sending x, y, z to the three coordinate functions, and this map vanishes on the compact operators. Actually this map extends by continuity to the C^* algebra generated by x, y and z and yields the exact sequence (9.1). One can interpret also the algebra $\mathcal{M}$ as the algebra of right invariant pseudo differential operators of order zero on $SU(2)$, then the map $\mathcal{M} \to C(S^2)$ of (9.1) is the principal symbol map (see [B5]). Once we have introduced the exact sequence above, we can state the theorem which is the analogue, for central states on the dual of $SU(2)$, of the Ney-Spitzer theorem.

Theorem 9.1. *The C^* algebra generated by the image of the Martin kernel is the algebra $\mathcal{M}$. The Martin kernel yields a section $K : C(S^2) \to \mathcal{M}$.*

The proof of the theorem relies on a detailed analysis of the Clebsch-Gordan formulas, see [B5].

Recently the problem of the Martin or Poisson boundary have been considered for quantum groups, see [Col], [I], [INT]

10 Central Limit Theorems for the Bernoulli Random Walk

Just as in the classical case there exists central limit theorems for the Bernoulli random walk, however the noncommutativity here plays an important role, and according to whether the state we chose is central or not the limit is quite different.

10.1 The Case of a Central State

We consider the triple of processes $(X_n, Y_n, Z_n)_{n\geq 1}$ constructed in section (3.1). We use the tracial state to contruct the product, $M_2(\mathbb{C})^{\otimes\infty}$ which is thus endowed with the tracial state $\sigma = (\frac{1}{2}Tr)^{\otimes\infty}$. We renormalize the three processes according to

$$X_t^{(\lambda)} = \frac{X_{[\lambda t]}}{\sqrt{\lambda}}, \qquad Y_t^{(\lambda)} = \frac{Y_{[\lambda t]}}{\sqrt{\lambda}}, \qquad Z_t^{(\lambda)} = \frac{Z_{[\lambda t]}}{\sqrt{\lambda}}$$

where $[x]$ is the integer part of x. This triple of processes converges when $\lambda \to \infty$, in the sense of moments, towards a three dimensional Bownian motion.

Theorem 10.1. *Let $(X_t, Y_t, Z_t)_{t\geq 0}$ be a three dimensional Brownian motion, then for any polynomial in $3n$ noncommuting indeterminates P, and all times $t_1, \ldots, t_n$, one has*

$$\lim_{\lambda\to\infty} \sigma(P(X_{t_1}^{(\lambda)}, Y_{t_1}^{(\lambda)}, Z_{t_1}^{(\lambda)}, \ldots, X_{t_n}^{(\lambda)}, Y_{t_n}^{(\lambda)}, Z_{t_n}^{(\lambda)})) =$$

$$E[P(X_{t_1}, Y_{t_1}, Z_{t_1}, \ldots, X_{t_n}, Y_{t_n}, Z_{t_n})]$$

Let us sketch the proof of this result. It is enough to prove the result for monomials. First we see that for any real coefficients x, y, z the process $xX_t^{(\lambda)} + yY_t^{(\lambda)} + zZ_t^{(\lambda)}$ converges towards real Brownian motion. By polarization this implies that for any monomial in X, Y, Z the sum over all monomials with the same total partial degrees in X, Y, Z converges towards the required limit. Consider two monomials of the form $M_1X_t^{(\lambda)}Y_s^{(\lambda)}M_2$ and $M_1Y_s^{(\lambda)}X_t^{(\lambda)}M_2$, their difference is, thanks to the commutation relations, $M_1Z_{s\wedge t}^{(\lambda)}M_2/\sqrt{\lambda}$. This is a monomial of smaller degree, with a factor $1/\sqrt{\lambda}$. We conclude, by induction on degrees of monomials, that the difference betwen the expectations of the two monomials $M_1X_t^{(\lambda)}Y_s^{(\lambda)}M_2$ and $M_1Y_s^{(\lambda)}X_t^{(\lambda)}M_2$ converges to 0 as $\lambda \to \infty$. It follows that the expectations of all monomials with the same partial degrees in variables converge to the same limit. □

We observe that the spin process, normalized by $S_{[\lambda t]}/\sqrt{\lambda}$ converges in distribution to a three dimensional Bessel process as $\lambda \to \infty$.

10.2 The Case of a Pure State

Now we consider the quantum Bernoulli random walk with the pure state given by the vector e_0. We shall consider the convergence of the moments of the triple of processes

$$(X_t^{(\lambda)}, Y_t^{(\lambda)}, Z_t^{(\lambda)}) = (\frac{X_{[\lambda t]}}{\sqrt{\lambda}}, \frac{Y_{[\lambda t]}}{\sqrt{\lambda}}, \frac{Z_{[\lambda t]}}{\lambda}); t \geq 0.$$

We shall prove that there exists operators $(X_t, Y_t, Z_t)_{t\geq 0}$ on some Hilbert space H with a vector $\Omega \in H$, such that for every polynomial in noncommuting indeterminates $P(X_{t_1}, Y_{t_1}, Z_{t_1}, \ldots, X_{t_n}, Y_{t_n}, Z_{t_n})$ one has

$$\lim_{n\to\infty}\langle P(X_{t_1}^{(\lambda)}, Y_{t_1}^{(\lambda)}, Z_{t_1}^{(\lambda)}, \ldots, X_{t_n}^{(\lambda)}, Y_{t_n}^{(\lambda)}, Z_{t_n}^{(\lambda)})e_0^\infty, e_0^\infty\rangle) =$$

$$\langle P(X_{t_1}, Y_{t_1}, Z_{t_1}, \ldots, X_{t_n}, Y_{t_n}, Z_{t_n})\Omega, \Omega\rangle$$

For this we shall first investigate the case where $n = 1, t_1 = 1$, thus we have just three operators $(\frac{X_n}{\sqrt{n}}, \frac{Y_n}{\sqrt{n}}, \frac{Z_n}{n})$ and let $n \to \infty$. Let H be a Hilbert space with a countable orthonormal basis $\varepsilon_0, \ldots, \varepsilon_n, \ldots$, and let us define operators, with domain the algebraic sum $\oplus_{i=0}^n \mathbb{C}\varepsilon_i$, by the formula

$$\begin{aligned} a^+(\varepsilon_i) &= \sqrt{j+1}\,\varepsilon_{j+1} \\ a^-(\varepsilon_j) &= \sqrt{j}\,\varepsilon_{i-1} \end{aligned} \qquad (10.1)$$

Theorem 10.2. *For any polynomial in three noncommutative indeterminates one has*

$$\lim_{n\to\infty}\langle P(\frac{X_n}{\sqrt{n}},\frac{Y_n}{\sqrt{n}},\frac{Z_n}{n})e_0^{\otimes n},e_0^{\otimes n}\rangle = \langle P(a^+ + a^-,\frac{1}{i}(a^+ - a^-),I)\varepsilon_0,\varepsilon_0\rangle$$

The proof is immediate by inspection of the formula (3.2) and comparison with (10.1). □

Observe that one has the adjointness relations

$$\langle a^+u,v\rangle = \langle u,a^-v\rangle$$

for all u,v in the domain. It follows that the operators $a^+ + a^-$ and $\frac{1}{i}(a^+ - a^-)$ are unbounded symmetric operators on H, and thus are closable. We will see below that they have self-adjoint extensions. They satisfy the commutation relation

$$[a^+,a^-] = -I$$

on their common domain, spanned by the vectors ε_i.

The operators a^+, a^- thus obtained are well known under the name of creation and annihilation operators for the quantum harmonic oscillator. One can give a natural model for these operators using a gaussian random variable. For this, remark that the distribution of the operator $a^+ + a^-$ is gaussian. This follows easily from the fact that each X_n follows a standard binomial distribution, and the convergence of this binomial distribution to the gaussian distribution, by the de Moivre-Laplace theorem. This property of the operator $a^+ + a^-$, and the fact that ε_0 is a cyclic vector for $a^+ + a^-$, i.e. the vectors $(a^+ + a^-)^n\varepsilon_0$ span a dense subspace of H, allows us to identify the space H in a natural way with the L^2 space of a gaussian random variable. The vectors ε_n can be obtained from the vectors $(a^+ + a^-)^n$ by the Gram-Schmidt orthogonalization procedure. It is well known that, for a gaussian variable X, the polynomials obtained by the Gram-Schmidt orthonormalization process from the sequence X^n are the Hermite polynomials. Thus when we identify the space H with the L^2 space of the gaussian measure on $\mathbb{R}$ the vectors ε_n become identified with the Hermite polynomials. Then the operator a^- is identified with $\frac{d}{dx}$ and the operator a^+ with $x - \frac{d}{dx}$.

The product a^+a^- has eigenvalues $0,1,2,\dots$ corresponding to the the respective eigenvectors $\varepsilon_0,\varepsilon_1,\dots$. It is known as the number operator in quantum field theory.

We will in the next section systematize the construction above and show how to deduce the limit of the renormalized quantum random walk to a quantum Brownian motion.

10.3 Fock Spaces

Let H be a complex Hilbert space. For each integer n the symmetric group S_n acts on $H^{\otimes n}$ by permutation of the factors in the tensor product.

Definition 10.3. We denote $H^{\circ n}$ the subspace of $H^{\otimes n}$ formed by vectors invariant under the action of S_n.

If $h_1, \ldots, h_n \in H$ then we let

$$h_1 \circ \ldots \circ h_n = \frac{1}{\sqrt{n!}} \sum_{\sigma \in S_n} h_{\sigma(1)} \otimes \ldots \otimes h_{\sigma(n)}$$

which is a multiple of the orthogonal projection of $h_1 \otimes \ldots \otimes h_n$ on $H^{\circ n}$. One has

$$\langle h_1 \ldots \circ h_n, h'_1 \circ \ldots \circ h'_n \rangle = \sum_{\sigma \in S_n} \prod_{i=1}^{n} \langle h_i, h'_{\sigma(i)} \rangle$$

The Fock space built on H is the Hilbert space direct sum

$$\Gamma(H) = \oplus_{n=0}^{\infty} H^{\circ n}$$

where $H^{\circ 0}$ is a one dimensional Hilbert space spanned by a unit vector Ω, called the vacuum vector of the Fock space. The algebraic direct sum $\oplus_{alg,n=0}^{\infty} H^{\circ n}$, denoted by $\Gamma_0(H)$, is a dense subspace of $\Gamma(H)$.

For every $h \in H$ we define the exponential vector associated with h by

$$\xi(h) = \sum_{n=0}^{\infty} \frac{h^{\circ n}}{n!}$$

one has

$$\langle \xi(h), \xi(h') \rangle = e^{\langle h,k \rangle}$$

furthermore the vectors $\xi(h); h \in H$ form a linearly free subset, generating algebraically a dense subspace of $\Gamma(H)$.

If the space H is written as the orthogonal direct sum of two Hilbert subspaces $H = H_1 \oplus H_2$, then there is a canonical isomorphism

$$\Gamma(H) \sim \Gamma(H_1) \otimes \Gamma(H_2) \tag{10.2}$$

which can be obtained, for example, by identifying the exponential vector $\xi(v_1+v_2) \in \Gamma(H)$, where $v_1 \in H_1$ and $v_2 \in H_2$, with the vector $\xi(v_1) \otimes \xi(v_2) \in \Gamma(H_1) \otimes \Gamma(H_2)$.

Let $h \in H$, we define two operators on the domain $\Gamma_0(H)$ by

$$a_h^+(h_1 \circ \ldots \circ h_n) = h \circ h_1 \circ \ldots \circ h_n$$
$$a_h^-(h_1 \circ \ldots \circ h_n) = \textstyle\sum_{i=1}^{n} \langle h_i, h \rangle h_1 \circ \ldots \circ \hat{h}_i \circ \ldots \circ h_n$$

Operators of the form a_h^+ are called creation operators while the a_h^- are called annihilation operators. When H is one dimensional, generated by a unit vector u there is a natural identification of $\Gamma(H)$ with the Hilbert space of the preceding section where the vector $u^{\circ n}$ is identified with $\sqrt{n!}\epsilon_n$. Then the operators a_u^+ and a_u^- coincide with a^+ and a^-.

Another operator of interest on $\Gamma(H)$ is the number operator Λ which has eigenvalue n on the subspace $H^{\circ n}$. If $(e_i)_{i\in I}$ is an orthonormal basis in H, then the number operator Λ has the expansion

$$\Lambda = \sum_i a_{e_1}^+ a_{e_i}^-.$$

One can see that the creation and annihilation operators satisfy the adjoint relation

$$\langle a_h^+ u, v\rangle = \langle u, a_h^- v\rangle \qquad h, u, v \in \Gamma_0(H)$$

as well as the commutation relation

$$[a_h^+, a_k^-] = -\langle h, k\rangle I$$

on the domain $\Gamma_0(H)$. In particular they are closable, and it is easy to see that the exponential vectors belong to the domain of their closure, with

$$a_h^+\xi(h') = \frac{d}{dt}\xi(h' + th)_{t=0} \quad a_h^-\xi(h') = \langle h', h\rangle\xi(h) \tag{10.3}$$

We shall see that the real part of the creation operator $P_h = a_h^+ + a_h^-$ has a self-adjoint extension, as well as its imaginary part Q_h. For this we consider the following Weyl operators, given on the vector space generated by exponential vectors by the formula

$$W_u\xi(h) = \xi(h+u)e^{-\langle h,u\rangle - \frac{1}{2}\langle u,u\rangle}$$

It is easy to check that

$$\langle W_u\xi(h), W_u\xi(h')\rangle = \langle \xi(h), \xi(h')\rangle \tag{10.4}$$

for all $u, v, h, h' \in H$, therefore the operators W_u extend to unitary operators on $\Gamma(H)$, furthermore

$$W_u W_v = W_{u+v}e^{-i\Im\langle u,v\rangle} \tag{10.5}$$

and for any $u \in H$ the operators $(W_{itu}; t \in \mathbb{R})$ form a one parameter group of unitary operators, whose generator is given by P_u on exponential vectors. Similarly, the operators $(W_{tu}; t \in \mathbb{R})$ form a one parameter group of unitary operators, whose generator is given by Q_u, and more generally for $\theta \in [0, 2\pi[$ the vectors $(W_{e^{i\theta}tu}; t \in \mathbb{R})$ form a one parameter group of unitary operators, whose generator is given by $\cos\theta Q_u + \sin\theta P_u$.

It follows from Stone's theorem that P_u, Q_u, and all their linear combinations, have a self adjoint extension. These operators satisfy the commutation relation

$$[P_u, Q_v] = -2i\Re\langle u, v\rangle.$$

We observe that if H splits as an orthogonal direct sum $H = H_1 \oplus H_2$ and $u \in H_1$, then the operator W_u admits a decomposition $W_u = W_u \otimes I$ in the decomposition (10.2).

Let now $K \subset H$ be a real Hilbert subspace such that $\Im\langle u, v\rangle = 0$ for all $u, v \in K$ (if K is maximal, it is called a Lagrangian subspace), then by (10.5) the unitary operators $W_{iu}; u \in K$ form a commutative family, and the generators $P_u, u \in K$ of the one parameter subgroups $(W_{itu}; t \in \mathbb{R})$ form a commuting family of self-adjoint operators with common dense domain $\Gamma_0(H)$. We can therefore investigate the joint distribution of these operators.

Proposition 10.4. *The operators P_u, for $u \in K$ form a gaussian family with covariance $\langle P_u, P_v\rangle = \langle u, v\rangle$.*

The operators Q_u, for $u \in K$ form a gaussian family with covariance $\langle Q_u, Q_v\rangle = \langle u, v\rangle$.

For the proof it is enough to prove that any linear combination of these operators has a gaussian distribution with the right variance, i.e. that P_u is a gaussian with variance $\langle u, u\rangle$. For this one computes the Fourier transform

$$\langle e^{iP_u}\Omega, \Omega\rangle = \langle e^{iP_u}\xi(0), \xi(0)\rangle = \langle \xi(u)e^{-\frac{1}{2}\langle u,u\rangle}, \xi(0)\rangle = e^{-\frac{1}{2}\langle u,u\rangle}$$

The proof for the operators Q_u is similar. □

We let now $H = L^2(\mathbb{R}_+)$, and take as Lagrangian subspace the subspace of real valued functions. Then the family $(P_t := P_{1_{[0,t]}}; t \geq 0)$ has the covariance $\langle P_t, P_s\rangle = s \wedge t$, and thus has the distribution of a real brownian motion. The same is true of the operators $Q_t := \frac{1}{i}(a^+_{1_{[0,t]}} - a^-_{1_{[0,t]}})$ which form another Brownian motion satisfying the commutation relations

$$[P_t, Q_t] = 2it$$

We shall call the pair $(P_t, Q_t)_{t\geq 0}$ of continuous time processes a noncommutative brownian motion.

We can now state the limit result we had in view in the beginning of this section.

Theorem 10.5. *For any polynomial P in noncommuting variables, one has*

$$\lim_{\lambda\to\infty}\langle (P(X^{(\lambda)}_{t_1}, Y^{(\lambda)}_{t_1}, Z^{(\lambda)}_{t_1}, \ldots, X^{(\lambda)}_{t_n}, Y^{(\lambda)}_{t_n}, Z^{(\lambda)}_{t_n})e_0^\infty, e_0^\infty\rangle) = \\ \langle P(P_{t_1}, Q_{t_1}, t_1.I, \ldots, P_{t_n}, Q_{t_n}, t_n.I))\Omega, \Omega\rangle]$$

The proof is an elaboration of the proof we gave for one time.

We shall see in the next section that, again, one can interpret this pair of processes as a noncommutative Markov process with values in a noncommutative space.

The noncommutative Brownian motion is the basis of a theory of noncommutative stochastic integration which has been developped by Hudson and Parthasarathy, see e.g. [Pa].

11 The Heisenberg Group and the Noncommutative Brownian Motion

The Heisenberg group is the set $\mathcal{H} = \mathbb{C} \times \mathbb{R}$ endowed with the group law

$$(z, w) \star (z', w') = (z + z', w + w' + \Im(z\bar{z}'))$$

This is a nilpotent group, its center being $\{0\} \times \mathbb{R}$, and the Lebesgue measure on $\mathbb{C} \times \mathbb{R}$ is a left and right Haar measure for this group.

The Weyl operators defined in the preceding section on a Fock space $\Gamma(\mathbb{C})$ define unitary representations of the group $\mathcal{H}$, by setting, for $\tau \in \mathbb{R}^*$,

$$\rho_\tau(z, w) = W_{z\tau^{1/2}} e^{i\tau w}$$

if $\tau > 0$ and

$$\rho_\tau(z, w) = W_{\bar{z}|\tau|^{1/2}} e^{i\tau w}$$

if $\tau < 0$.

Another family of representations is given by the one dimensional characters

$$\rho_\xi(z, w) = e^{i\Re(z\bar{\xi})}$$

for $\xi \in \mathbb{C}$.

All these representations are irreducible, are non equivalent and they exhaust the family of equivalence classes of irreducible representations of $\mathcal{H}$.

We consider the C^* algebra of $\mathcal{H}$, which is the C^*-algebra generated by the convolution algebra $L^1(\mathcal{H})$ on $L^2(\mathcal{H})$. This algebra is a sub C^*-algebra of $B(L^2(\mathcal{H}))$. Let us denote $z = q + ip$ then the Lie algebra of $\mathcal{H}$ is composed of the vector fields

$$\frac{\partial}{\partial w}; \quad \frac{\partial}{\partial q} + p\frac{\partial}{\partial w}; \quad \frac{\partial}{\partial p} - q\frac{\partial}{\partial w}.$$

We shall denote by iT, iQ, iP the unbounded operators on $L^2(\mathcal{H})$, affiliated to $C^*(\mathcal{H})$, which correspond to these vector fields. Thus P, Q, T are unbounded self-adjoint operators, which satisfy the commutation relation

$$[P, Q] = -2iT.$$

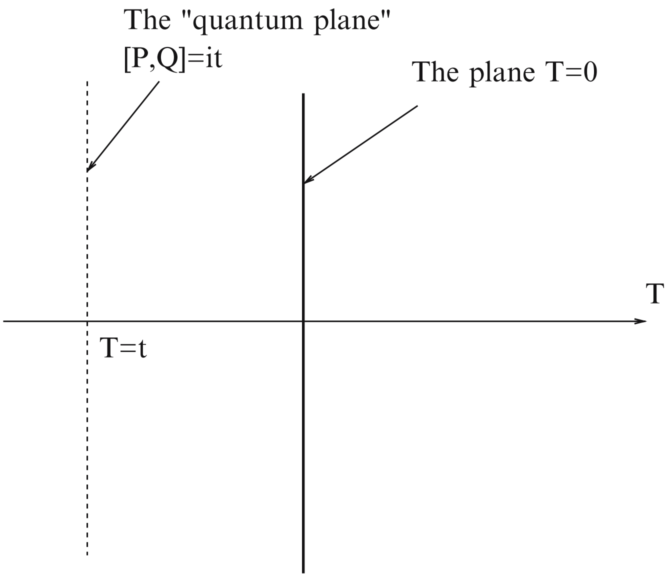

Fig. 5 The dual of the Heisenberg group.

As in the case of $SU(2)$ one can give a heuristic description of the noncommutative space dual to $\mathcal{H}$ using the generators of the Lie algebra of $\mathcal{H}$, which define three noncommuting unbounded self-adjoint operators P, Q, T. We think of these operators as coordinate functions on this dual space, satisfying the commutation relations

$$[P, Q] = -2iT \quad [P, T] = [Q, T] = 0.$$

Since the coordinate T belongs to the center, it allows to decompose the space into slices according to the values of this coordinate. When $T = 0$, the coordinates P and Q commute, and the corresponding slice is a usual plane, with two real coordinates. This corresponds to the one dimensional representations of the group. When $T = \tau$ a non zero real number, the two coordinates P, Q generate a von Neumann algebra isomorphic to $B(H)$, and corresponding to the irreducible representation sending T to τI. Note that in this representation the operator $P^2 + Q^2$ has a discrete spectrum $2|\tau|, 6|\tau|, 10|\tau|, \ldots$.

Let us consider, for $t \geq 0$, the functions on $\mathcal{H}$

$$\varphi_t^{\pm}(z, w) = \langle \rho_{\pm t}(z, w)\Omega, \Omega\rangle = e^{\pm itw - \frac{1}{2}tz\bar{z}}.$$

By construction, these functions are positive definite functions on $\mathcal{H}$, and form two multiplicative semigroups. To these functions correspond convolution semigroups of states, and semigroups of completely positive maps.

The semigroup of noncommutative brownian motion on the dual of $\mathcal{H}$ is the associated semigroup of completely positive maps on $C^*(\mathcal{H})$. Recall that this semigroup is obtained by composing the coproduct $\Delta : C^*(\mathcal{H}) \to M(C^*(\mathcal{H})) \otimes M(C^*(\mathcal{H}))$ (recall that $M(A)$ is the multiplier algebra of A) with the state associated with the function. Thus

$$\Phi_t^{\pm} = (\nu_{\varphi_t^{\pm}} \otimes I) \circ \Delta$$

or equivalently

$$\Phi_t^{\pm}(\lambda_g) = \varphi_t^{\pm}(g)\lambda_g \quad \text{for } g \in \mathcal{H}.$$

Let ν be a state on $C^*(\mathcal{H})$, and $\rho_\nu : C^*(\mathcal{H}) \to B(H_\nu)$ be the associated GNS representation. We consider the two families of homomorphisms

$$\begin{aligned} j_t^{\pm} &: C^*(\mathcal{H}) \to B(H_\nu \otimes \Gamma(L^2(\mathbb{R}_+))) \\ j_t^{\pm}(z,w) &= \rho_\nu(z,w) \otimes W_{z1_{[0,t]}} e^{\pm itw} \end{aligned}$$

We shall prove that these homomorphisms constitute dilations of some completely positive convolution semigroups on $C^*(\mathcal{H})$. For each time $t \geq 0$ we have a direct sum decomposition $L^2(\mathbb{R}_+) = L^2([0,t]) \oplus L^2([t,+\infty[)$ and a corresponding factorization

$$\Gamma(L^2(\mathbb{R}_+)) = \Gamma(L^2([0,t])) \otimes \Gamma(L^2([t,+\infty[))$$

Accordingly for each $t > 0$ there are subalgebras

$$W_t = B(\Gamma(L^2([0,t]))) \otimes I \subset B(\Gamma(L^2(\mathbb{R}_+)))$$

and linear maps

$$E_t := Id \otimes \langle .\Omega_{[t}, \Omega_{[t}\rangle : B(\Gamma(L^2(\mathbb{R}_+))) \to W_t$$

where $\Omega_{[t}$ is the vacuum vector of the space $\Gamma(L^2([0,t]))$.

Lemma 11.1. *For each $t \geq 0$ the map E_t is a conditional expectation with respect to the state $\langle .\Omega, \Omega\rangle$.*

Indeed if $a \in B(L^2(\mathbb{R}_+))$ has a decomposition $a = a_{t]} \otimes a_{[t}$ then one has

$$E_t(a) = a_{t]} \otimes \langle a_{[t}\Omega_{[t}, \Omega_{[t}\rangle$$

and for $b, c \in B(L^2([0,t]))$

$$\begin{aligned} \langle bac\mathcal{E}(u), \mathcal{E}(v)\rangle &= \langle bE_t(a)c\mathcal{E}(u1_{[0,t]}), \mathcal{E}(v1_{1[0,t]})\rangle\langle a_{[t}\mathcal{E}(u1_{[t,+\infty[}), E(v1_{[t,+\infty[})\rangle \\ &= \langle bE_t(a)c\mathcal{E}(u), \mathcal{E}(v)\rangle \end{aligned}$$

One checks easily that the homomorphism $j_t^{\pm}$ sends $C^*(\mathcal{H})$ to W_t, furthermore we have

Proposition 11.2. *The maps* $(j_t^{\pm}, E_t, W_t)$ *form a dilation of the completely positive semigroup* $\Phi_t^{\pm}$*, with initial distribution* ν*.*

Proof. This is a bookkeeping exercise using the definition of the Weyl operators, one has to check that, for $t, s \geq 0$ and $u, v \in L^2(\mathbb{R}_+)$, one has

$$\langle j_{t+s}^{\pm}(z,w)\mathcal{E}(u1_{[0,t]}), \mathcal{E}(v1_{[0,t]})\rangle = e^{\pm isw - \frac{1}{2}s|z|^2} \langle j_t^{\pm}(z,w)\mathcal{E}(u1_{[0,t]}), \mathcal{E}(v1_{[0,t]})\rangle$$

□

For every one parameter subgroup of $\mathcal{H}$, there is a completely positive semigroup given by restriction of $(\Phi_t^{\pm})_{t\geq 0}$. For subgroups of the form $(xz, 0); u \in \mathbb{R}$, with $z \in \mathbb{C}^*$ isomorphic to $\mathbb{R}$, one sees that the semigroup is that of Brownian motion on the dual group. Thus we recover the Brownian motions (P_t, Q_t) of the preceding section by looking at $j_t(P)$ and $j_t(Q)$.

The restriction to the center $(0, w); w \in \mathbb{R}$ gives a semigroup of uniform translation on the real line.

11.1 The Quantum Bessel Process

Bessel processes are radial parts of Brownian motions. Here we shall exploit the action of the unitary group $U(1)$ on the Heisenberg group in order to find an abelian algebra which is left invariant by the semigroup and study the Markov process associated with the restriction of $\Phi_t^{\pm}$ to this subalgebra. Let $e^{i\theta}$ be a complex number with modulus 1, then there exists an automorphism a_θ of the Heisenberg group defined by

$$a_\theta(z, w) = (e^{i\theta}z, w)$$

and this automorphism extends to an automorphism of the C^* algebra.

Proposition 11.3. *The subalgebra of* $C^*(\mathcal{H})$ *composed of elements invariant under the above action of* $U(1)$ *is an abelian* C^* *algebra.*

The characters of this abelian C^*-algebra have been computed by A. Koranyi, they are given by the formula

$$\chi(f) = \int_{\mathcal{H}} \omega(g)f(g)dg$$

for $f \in L^1(\mathcal{H})$, invariant under the action of $U(1)$, where ω belongs to the set of functions

$$\{\omega_{\tau,m} | \tau \in \mathbb{R}^*, m \in \mathbb{N}\} \cup \{\omega_\mu | \mu \in \mathbb{R}_+\}$$

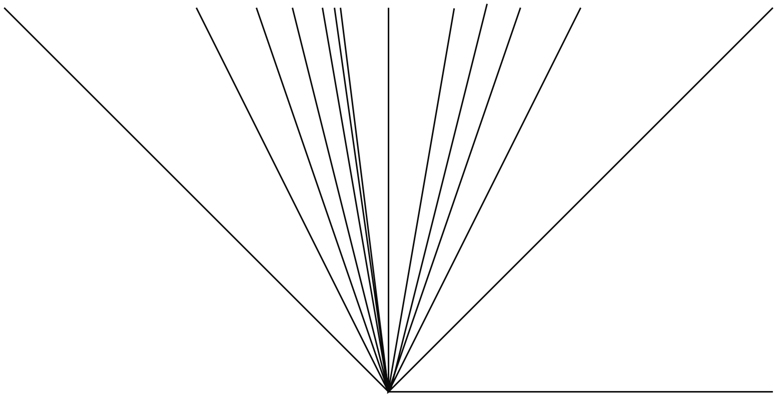

Fig. 6 The Heisenberg fan.

with

$$\omega_{\tau,m}(z,w) = me^{i\tau w - \frac{1}{2}|\tau||z|^2} L_m(|\tau||z|^2)$$

$$\omega_\mu(z,w) = j_0(\mu|z|^2)$$

Here L_m are the Laguerre polynomials defined by the generating series

$$\sum_{m=0}^{\infty} L_m(x)t^m = \frac{e^{-\frac{xt}{1-t}}}{1-t}$$

and j_0 is the usual Bessel function.

The spectrum of the algebra $C_R^*(\mathcal{H})$ can be identified with a closed subset of $\mathbb{R}^2$, which consists in the union of the halflines $\{(x, kx); x > 0\}$ for $k \in \mathbb{N}$, the halflines $(x, kx); x < 0$ for $k \in \mathbb{N}^*$, and the halfline $(0, y); y \geq 0$.

It is the spectrum of the unbounded operator $\frac{1}{2}(P^2 + Q^2 - T)$, and this algebra is the algebra of functions of this operator.

The picture gives a “fan” consisting of a union of halflines originating from 0 as depicted below.

We shall call noncommutatif Bessel semigroup the restriction of $\Phi_t^{\pm}$ to the abelian subalgebra $C_R^*(\mathcal{H})$. In order to compute this semigroup we need, for each character ω to decompose the functions $\omega\varphi_t$ into an integral of characters. The result is given by the following.

Proposition 11.4. *The noncommutative Bessel semigroup Φ_t^+ is given by the following kernel.*

If $x = (\sigma, -k\sigma)$ with $\sigma < 0$ and $\tau = \sigma + t$ then

$$q_t(x, dy) = \sum_{l=k}^{\infty} \frac{(l-1)!}{(k-1)!(l-k)!}(1 - \frac{\tau}{\sigma})^{l-k}(\frac{\tau}{\sigma})^k \delta_{(\tau,-l\tau)}(dy)$$

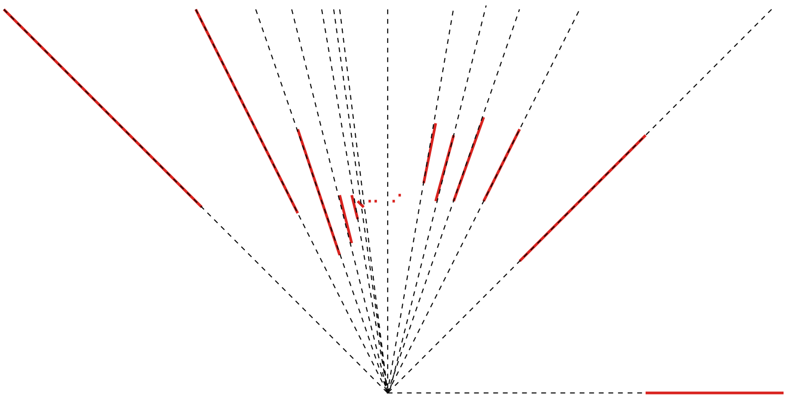

Fig. 7

If $x = (\sigma, -k\sigma)$ *with* $\sigma < 0$ *and* $0 = \sigma + t$, $(y = 0, r)$ *then*

$$q_t(x, dy) = \frac{(\frac{r}{t})^{k-1}}{(k-1)!} e^{-\frac{r}{t}} \delta_0 \otimes dr$$

If $x = (\sigma, -k\sigma)$ *with* $\sigma < 0$ *and* $\tau = \sigma + > 0$ *then*

$$q_t(x, dy) = \sum_{l=0}^{\infty} \frac{(l+k-1)!}{(k-1)!l!} (1 - \frac{\tau}{t})^{l+k} (\frac{\tau}{t})^k \delta_{(\tau, l\tau)}(dy)$$

If $x = (0, r)$ *then*

$$q_t(x, dy) = \frac{(\frac{r}{t})^{k-1}}{l!} e^{-\frac{t}{lt}} \delta_{t,lt}(dy)$$

If $x = (\sigma, k\sigma)$ *with* $\sigma > 0$ *and* $\tau = \sigma + t$

$$q_t(x, dy) = \sum_{l=0}^{l=k} \frac{(l-1)!}{(k-1)!(l-k)!} (1 - \frac{\sigma}{\tau})^{k-l} (\frac{\sigma}{\tau})^l \delta_{(\tau, l\tau)}(dy)$$

The computations can be found in [B6].

A typical trajectory of the process is depicted in the above picture. It starts from a point $(\sigma, -\sigma)$ with $\sigma < 0$. During the whole process the first coordinates follows a uniform translation to the right. The trajectory starts on the line $y = -x$, and with an intensity $\frac{dt}{-\sigma+t}$, then jumps to the line $(y = -2x)$, which it follows before jumping to the next line $(y = -3x)$ with an intensity $\frac{2dt}{-\sigma+t}$, and so on, until it reaches after infinitely many jumps the line $x = 0$, then the process on the right half plane does the jumps from the line $(y = kx)$ to $(y = (k-1)x)$, until it finally reaches the line $y = 0$ where it stays forever. One can actually construct this process from a birth and death process known as the Yule process, and the embedding of this process into the Heisenberg fan yields a construction of the space-time boundary of this process, see [B6].

12 Dilations for Noncompact Groups

12.1 The General Case

We shall now extend the preceding construction to the case of arbitrary locally compact groups. Let G be a locally compact group, with right Haar measure m, and consider its convolution algebra $L^1(G)$. We endow this algebra with the norm $\|f\| = \sup \|\rho(f)\|$ where the supremum is over all unitary representations ρ of the group G, extended to the algebra $L^1(G)$. This yields the full C^*-algebra of G, denoted $C^*(G)$. When the group G is amenable, for example if G is compact or for the Heisenberg group which we have met before, this coincides with the completion of the action of the group on $L^2(G)$, which is called the reduced C^*-algebra of G. When the group is nonamenable, $C_r^*(G)$ is strictly smaller than $C^*(G)$. A continuous positive definite function on G, such that $\varphi(e) = 1$ defines a state as well as a completely positive contraction on $C^*(G)$, whose restriction to $L^1(G)$ is given by $f \mapsto f\varphi$. Let now ψ be a continuous, conditionally negative definite function on G, with $\psi(e) = 0$. Recall that this means that for all $t \geq 0$ the function $e^{-t\psi}$ is a positive definite function on G, or equivalently, by Schönberg's theorem, that for all $z_1, \ldots, z_n \in \mathbb{C}$ with $\sum_i z_i = 0$, and $g_1, \ldots, g_n \in G$ one has

$$\sum_{ij} z_i \bar{z}_j \psi(g_j^{-1} g_i) \leq 0.$$

There is an associated semigroup of completely positive contractions on $C^*(G)$. We shall now, following Parthasarathy and Schmidt [PS], construct a dilation of this semigroup. Let ν be a state on $C^*(G)$ which will be the initial state. The GNS construction yields a unitary representation π of G on a Hilbert space H_π, and $\eta \in H_\pi$ such that $\nu(x) = \langle \pi(x)\eta, \eta \rangle$ for $x \in C^*(G)$. A variant of the GNS construction associates to the function ψ a unitary representation of G in a Hilbert space H_ψ, and a cocycle $v : G \to H_\psi$ for this representation. Thus v is a continuous function which satisfies

$$v(gh) = gv(h) + v(g)$$

and

$$\langle v(g), v(h) \rangle = -\psi(h^{-1}g) + \psi(g) + \psi(h^{-1}) - \psi(e) \tag{12.1}$$

for all $g, h \in G$. Conversely, any function ψ satisfying the above equation for some representation and cocycle v is conditionally negative definite. Indeed one has

$$\sum_{ij} z_i \bar{z}_j \psi(g_j^{-1} g_i) = -\|\sum_j z_j v(g_j)\|^2 \leq 0$$

if $\sum_j z_j = 0$.

Let $\Gamma = \Gamma(L^2(\mathbb{R}_+) \otimes H_\psi)$, and let $\mathcal{W} = B(H_\pi \otimes \Gamma) \sim B(H_\pi) \otimes B(\Gamma)$. Let ω be the pure state on $\mathcal{W}$ associated with the vector $\eta \otimes \Omega$. One can define the subalgebras $\mathcal{W}_t = B(H_\pi \otimes \Gamma_t) \otimes Id$ associated with the orthogonal decomposition $L^2(\mathbb{R}_+) \otimes H_\psi = (L^2([0,t]) \otimes H_\psi) \oplus (L^2([t,+\infty[) \otimes H_\psi)$, and the conditional expectations $E_t : \mathcal{W} \to \mathcal{W}_t$ with respect to the state ω. One defines a unitary representation of G on exponential vectors by

$$V^t(g)(\mathcal{E}(u)) = e^{t\psi(g)+\langle 1_{[0,t]}\otimes v_t(g),u\rangle}\mathcal{E}(U^t(g)(u) + 1_{[0,t]} \otimes v_t(g))$$

One thus gets a representation of G on $H_\pi \otimes \Gamma$ by taking the tensor product of V^t with the representation π, and this yields a family of morphisms $j_t : C^*(G) \to \mathcal{W}$.

Proposition 12.1. *The family $(j_t, \mathcal{W}, \mathcal{W}_t, E_t, \omega)$ forms a dilation of the completely positive semigroup, with initial distribution ν.*

The proof is a bookkeeping exercise. This construction has been extended by Schürmann to a class of bialgebras, see [Sc], allowing him in particular to give a nice construction of the Azéma martingales.

12.2 Free Groups

Let now F_n be a free group on n generators $g_1, \ldots, g_n$. Each element of F_n can be written in a unique way as a reduced word $w = g_{i_1}^{\varepsilon_1} \ldots g_{i_k}^{\varepsilon_k}$, where one has $\varepsilon_j = \pm 1$ for all j and $i_1 \neq i_2 \neq i_3 \ldots i_{k-1} \neq i_k$. For such an element one defines its length $l(w) = k$. This is the smallest integer k such that w can be expressed as a product of k elements in the set $\{g_1, g_1^{-1}, g_2, \ldots, g_n, g_n^{-1}\}$.

Proposition 12.2. *(Haagerup [H]) The function l is conditionally negative definite on F_n.*

Proof. Consider the Cayley graph of F_n built on the generators. Thus this graph has as vertices the elements of F_n and its edges are the pairs $\{g, h\}$ such that $h^{-1}g$ is a generator or the inverse of a generator. This Cayley graph is a regular tree in which each vertex has $2n$ neighbours. For any $g \in F_n$ one can consider the unique shortest path in the graph between Id and g. Let E_n be the set of edges of the Cayley graph, endowed with the counting measure, then one defines $v(g) \in L^2(E_n)$ to be the indicator function of this shortest path from Id to g in the Cayley graph. Thus $v(g)(e) = 1$ if and only if the edge e is on the shortest path from Id to g. One can easily check, using the properties of trees that for any $h, h \in F_n$ one has

$$l(g) + l(h) - l(h^{-1}g) = 2\langle v(g), v(h)\rangle_{L^2(F_n)}$$

indeed this scalar product counts the number of common edges in the shortest paths from Id to g and h. This implies, by (12.1) that l is conditionally negative definite. □

It follows from the previous proposition that there exists, on the full C^* algebra of F_n, a semigroup of unit preserving completely positive maps, given by the formula

$$\Phi_t(\lambda_g) = e^{-tl(g)}\lambda_g$$

The theory of the previous section allows us to construct a dilation of this semigroup. As before we shall be interested in the restriction of this completely positive semigroup to commutative subalgebras. The first one will be the subalgebra of the subgroup generated by one of the generators. Let g_i be this generator, then this subgroup is isomorphic to $\mathbb{Z}$ by $k \mapsto g_i^k$, therefore its dual is isomorphic to the group of complex numbers of modulus 1. The restriction gives us a Markov semigroup on the group of complex numbers of modulus 1. This semigroup is easy to characterize, it sends the function $e^{ik\theta}$ on the unit circle to the function $e^{-|k|+ik\theta}$. In other words this is the integral operator on the unit circle given by the Poisson kernel

$$P_t(\theta, \theta') = \frac{1 - e^{-2t}}{1 - 2e^{-t}\cos(\theta - \theta') + e^{-2t}}.$$

This is a convolution semigroup, as expected.

The other commutative algebra of interest is the algebra $\mathcal{R}(F_n)$ consisting of radial elements. It is generated by the elements $\chi_l = \sum_{l(g)=l} \lambda_g$ for $l = 0, 1, \ldots$, and it is immediate that the completely positive semigroup associated with the length function leaves this algebra invariant. Actually one has $\Phi_t(\chi_l) = e^{-tl}\chi_l$. These elements satisfy the relations

$$\begin{aligned}
\chi_0 &= I \\
\chi_1^2 &= \chi_2 + 2n\chi_0 \\
\chi_l\chi_l &= \chi_{l+1} + (2n-1)\chi_{l-1} \qquad l \geq 2
\end{aligned}$$

From this we conclude that $\mathcal{R}(F_n)$ is the commutative von Neumann algebra generated by the self-adjoint element χ_1, and its spectrum is the spectrum of χ_1. In order to compute the norm of χ_l we need just to consider the trivial representation of F_n in which all g_i are mapped to the identity, and we get $\|\chi_l\| = 2n(2n-1)^{l-1}$ for $l \geq 1$, the number of elements of length l in F_n. Any character $\varphi : \mathcal{R}(F_n) \to \mathbb{C}$ is determined by its values on χ_1. For such a character φ, with $\varphi(\chi_1) = x$, one has

$$\varphi(\chi_0) = 1; \ \varphi(\chi_2) = x^2 - 2n; \quad \varphi(\chi_{l+1}) = x\varphi(\chi_l) - (2n-1)\varphi(\chi_{l-1}) \text{ for } l \geq 2$$

from which one infers that

$$\varphi(\chi_l) = \frac{\lambda_1^{l+1} - \lambda_2^{l+1}}{\lambda_1 - \lambda_2} - \frac{\lambda_1^{l-1} - \lambda_2^{l-1}}{\lambda_1 - \lambda_2} \qquad \text{for } l \geq 1 \tag{12.2}$$

where λ_1, λ_2 are the two roots of the equation $\lambda^2 - x\lambda + 2n - 1 = 0$.

We verify that the character φ_x defined by the formula above is real and bounded if and only if $x \in [-2n, 2n]$. The spectrum of the algebra $\mathcal{R}(F_n)$ thus coincides with the interval $[-2n, 2n]$, and the element χ_l corresponds to a polynomial function $P_l(\chi_1) = \chi_l$, where the polynomials are determined by the recursion

$$P_0 = 1, \quad P_1(x) = x, \quad xP_l(x) = P_{l+1}(x) + (2n-1)P_{l-1}.$$

This three term recursion relation is characteristic of a sequence of orthogonal polynomials. The orthogonalizing measure is the distribution of χ_1 in the noncommutative probability space $(\mathcal{A}(F_n), \delta_e)$ where δ_e is the pure state, in the left regular representation of F_n, corresponding to the identity. Thus $\delta_e(\lambda_g) = 1$ if $g = e$ and $\delta_e(\lambda_g) = 0$ if not. This measure is known as the Kesten measure (see [Ke]) and has the density

$$dm_n(x) = \frac{2n}{2n-1} 4\pi \frac{\sqrt{4(2n-1) - x^2}}{4n^2 - x^2}$$

on the interval $[-2\sqrt{2n-1}, 2\sqrt{2n-1}]$. The discrepancy between the interval $[-2n, 2n]$ which is the spectrum of χ_1 and the support of the measure m_n comes from the fact that F_n is a nonamenable group and therefore some of its unitary representations are not weakly contained in the regular representation.

The semigroup of the restriction of $(\Phi_t)_{t\geq 0}$ to the subalgebra $\mathcal{R}(F_n)$ sends the polynomial function $P_l(x)$ on the interval $[-2n, 2n]$ to the function $e^{-tl}P_l(x)$. We can compute the transition probabilities $p_t(x, dy)$ by finding the integral representation

$$e^{-tl}P_l(x) = \int_{[-2n,2n]} p_t(x, dy) P_l(y)$$

for each $x \in [-2n, 2n]$.

If x belongs to the support of the Kesten measure, then since the polynomials $P_l; l \geq 0$ form an orthogonal basis of the L^2 space of the Kesten measure, and $\|P_l\|_2^2 = 2n(2n-1)^l$ one obtains p_t through the orthogonal expansion

$$p_t(x, dy) = e^{-t} dm_n(y) + \sum_{l=1}^{\infty} e^{-tl} \frac{1}{2n(2n-1)^{l-1}} P_l(x) P_l(y) dm_n(y)$$

When x is outside this support, then by (12.2) the sequence $P_l(x)$ is unbounded and has exponential growth of rate $\xi = \frac{x + \sqrt{x^2 - 4(2n-1)}}{2}$ and the character value $e^{-tl}P_l(x)$ has the asymptotic behaviour $e^{-tl}\xi^l$ as $l \to \infty$, and if $e^{-t}\xi > 2\sqrt{2n-1}$, then let $x(t) = e^{-t}\xi + (2n-1)e^t/\xi$. The function $e^{-tl}P_l(x)$ can be written as is a linear combination of $P_l(x(t))$, which picks up the dominant term as $l \to \infty$ and the $P_l(y)$ for y in the interval $[-2\sqrt{2n-1}, 2\sqrt{2n-1}]$. More precisely the quantity

$$Q_l^t(x) = e^{-tl}P_l(x) - \frac{e^{-t}\xi - (2n-1)e^t/\xi}{e^{-t}\xi - e^t/\xi}\frac{\xi - (2n-1)/\xi}{\xi - 1/\xi}P_l(x(t))$$

decreases exponentially as $l \to \infty$, and thus one has

$$p_t(x, dy) = c_t\delta_{x(t)} + \sum_{l=1}^{\infty} e^{-tl}\frac{1}{2n(2n-1)^{l-1}}(P_l(x) - c_tP_l(x(t)))P_l(y)dm_n(y)$$

with $c_t = \frac{e^{-t}\xi-(2n-1)e^t/\xi}{e^{-t}\xi-e^t/\xi}\frac{\xi-(2n-1)/\xi}{\xi-1/\xi}$. If $\xi(t) < 2\sqrt{2n-1}$ then there is a similar decomposition, but the term c_t is 0.

Thus the process starting form a point $x \in [-2n, 2n] \setminus [-2\sqrt{2n-1}, 2\sqrt{2n-1}]$ performs a translation towards the central interval, and at some point jumps into it, and after that performs a certain pure jump process inside the interval $[-2\sqrt{2n-1}, 2\sqrt{2n-1}]$ where it remains forever.

13 Pitman's Theorem and the Quantum Group $SU_q(2)$

13.1 Pitman's Theorem

Let $(B_t)_{t\geq 0}$ be a real Brownian motion, with $B_0 = 0$, and let

$$S_t = \sup_{0\leq s\leq t} B_s$$

then Pitman's theorem states that the stochastic process

$$R_t = 2S_t - B_t; \qquad t \geq 0$$

is a three dimensional Bessel process, i.e. is distributed as the norm of a three dimensional Brownian motion. There is a discrete version of Pitman's theorem, actually it is this discrete version that Pitman proved in his original paper [Pi]. We start from a symmetric Bernoulli random walk $X_n = x_1 + \ldots + x_n$ where the x_i are i.i.d. with $P(x_i) = \pm 1 = 1/2$, and build the processes $S_n = \max_{1\leq k\leq n} X_k$, and $T_n = 2S_n - X_n$. Pitman proved in [Pi] that $(T_n)_{n\geq 0}$ is a Markov chain on the nonegative integers, with probability transitions

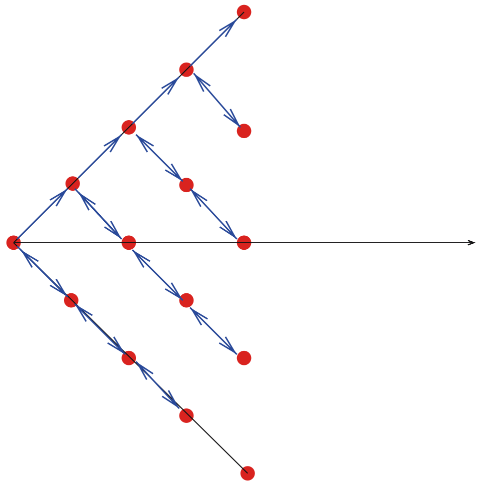

Fig. 8

$$p(k,k+1) = \frac{k+2}{2(k+1)} \quad p(k,k-1) = \frac{k}{2(k+1)}$$

and the theorem about Brownian motion can be obtained by taking the usual approximation of Brownian motion by random walks. We see that this Markov chain is, up to a shift of 1 in the variable, exactly the one that we obtained in Theorem 3.2 when considering the spin process. This is not a coincidence as we shall see, actually we will understand this connection by introducing quantum groups in the picture. Before that, let us give the proof of Pitman's theorem We consider the stochastic process $((S_n, X_n); n \geq 1)$, with values in $\{(s,k) \in \mathbb{N} \times \mathbb{Z} \,|\, s \geq k\}$. It is easy to see that this stochastic process is a Markov chain, with transition probabilities

$$\begin{aligned} p((s,k),(s,k+1)) &= \tfrac{1}{2}, \quad p((s,k),(s,k-1)) = \tfrac{1}{2} \qquad \text{for } s > k \\ p((s,s),(s+1,s+1)) &= \tfrac{1}{2}, \quad p((s,s),(s,s-1)) = \tfrac{1}{2} \end{aligned}$$

from which we can deduce the probability transitions of the Markov chain $((T_n, X_n); n \geq 1)$, with values in $\{(t,k) \in \mathbb{N}^* \times \mathbb{Z} \,|\, k \in (-t, -t+2, \ldots, t-2, t)\}$,

$$\begin{aligned} p((t,k),(t-1,k+1)) &= \tfrac{1}{2}, \quad p((t,k),(t+1,k-1)) = \tfrac{1}{2} \quad \text{ if } t > k \quad (13.1) \\ p((t,t),(t+1,t+1)) &= \tfrac{1}{2}, \quad p((t,t),(t+1,t-1)) = \tfrac{1}{2} \end{aligned}$$

The transition probabilities are depicted in this picture.

One checks then, by induction on n, that the conditional distribution of X_n, knowing $T_1, \ldots, T_n$, is the uniform distribution on the set $\{-T_n, -T_n + 2, \ldots, T_n - 2, T_n\}$. Then it follows that $(T_n; n \geq 0)$ is a Markov chain with the right transition probabilities.

13.2 A Markov Chain Associated with the Quantum Bernoulli Random Walk

In section 5.2 we have seen that the quantum Bernoulli random walk gives rise in a natural way to two Markov chains, one being the classical Bernoulli random walk, and the other being the spin process. These two processes were obtained in the preceding section as coordinates of a certain two-dimensional Markov chain given by the transition probabilities (13.1). We can also consider a two-dimensional Markov chain having these two processes as marginals, by considering the Markov chain of the end of section 5.2. Recall that this Markov chain was obtained by restricting the generator of the quantum Bernoulli random walk to the commutative subalgebra $\mathcal{P}(SU(2)) \subset \mathcal{A}(SU(2))$ generated by the center $\mathcal{Z}(SU(2))$ and by a one parameter subgroup. The spectrum of this algebra can be identified with the set

$$\hat{P} = \{(r,k) \in \mathbb{N} \times \mathbb{Z} \,|\, k \in \{-r, -r+2, \ldots, r-2, r\}\}$$

Indeed this algebra is generated by the pair of commuting self-adjoint operators X, D in the sense that it consists in bounded functions of the pair (X, D). The joint spectrum of these operators can be computed from the explicit description of the irreducible representations of $SU(2)$, and coincides with $\hat{P}$. The probability transitions can be obtained by using the Clebsch-Gordan formula, or equivalently by the computation in the proof of Lemma 3.3. One finds

$$\begin{aligned}
p((r,k),(r+1,k+1)) &= \frac{r+k+2}{2(r+1)} \\
p((r,k),(r+1,k-1)) &= \frac{r-k+2}{2(r+1)} \\
p((r,k),(r-1,k+1)) &= \frac{r-k}{2(r+1)} \\
p((r,k),(r-1,k-1)) &= \frac{r+k}{2(r+1)}.
\end{aligned}$$

These transition probabilities are on this picture

Thus, although this Markov chain has the same one-dimensional marginal as the one of the preceding section, they do not coincide. We will see that in order to recover the transitions (13.1) we will have to introduce quantum groups.

13.3 The Quantum Group $SU_q(2)$

The Hopf algebra $\mathcal{A}(SU(2))$ can be deformed by introducing a real parameter q. The algebraic construction proceeds with the introduction of three

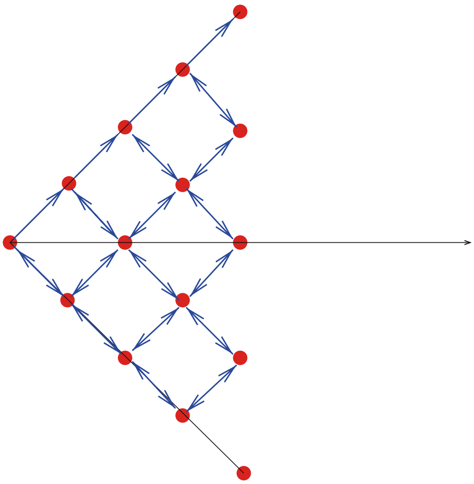

Fig. 9

generators t, e, f which are required to satisfy the relations

$$tet^{-1} = q^2 e, \quad tft^{-1} = q^{-2} f, \quad ef - fe = \frac{t - t^{-1}}{q - q^{-1}}$$

and a coproduct which is given by

$$\Delta(t) = t \otimes t, \quad \Delta(e) = e \otimes t^{-1} + 1 \otimes e, \quad \Delta(f) = f \otimes 1 + t \otimes f$$

Formally putting $t = q^h$ and letting q converge to 1 one finds in the limit the defining relations for the envelopping algebra of the Lie algebra of $SU(2)$, as well as the coproduct.

One can prove that the irreducible finite dimensional representations of this algebra are deformations of those of $SU(2)$, indeed for each integer $r \geq 0$ there exists two representation in V_{r+1}^{+} and V_{r+1}^{-}, with bases $v_k^{r\pm}; k \in \{-r, -r+2, \ldots, r-2, r\}$, given by

$$\begin{aligned} tv_j^{r\pm} &= \pm q^j v_j^{r\pm} \\ ev_j^{r\pm} &= \pm\sqrt{\left[\frac{r-j}{2}\right]_q \left[\frac{r+j+2}{2}\right]_q} v_{j+2}^{r\pm} \\ fv_j^{r\pm} &= \sqrt{\left[\frac{r-j+2}{2}\right]_q \left[\frac{r+j}{2}\right]_q} v_{j-2}^{r\pm}. \end{aligned}$$

with $[n]_q = \frac{q^n - q^{-n}}{q - q^{-1}}$. Using the coproduct one can define the tensor product of two representations, and this tensor product obeys the same rules as the one for representations of $SU(2)$ i.e. one has

$$V^{\epsilon_1}_{r_1+1} \otimes V^{\epsilon_2}_{r_2+1} = \bigoplus_{r=|r_2-r_1|,|r_2-r_1|+2,\dots,r_1+r_2} V^{\epsilon_1\epsilon_2}_{r+1}.$$

We will now restrict our attention to representations of the kind V_l^+, and consider the von Neumann-Hopf algebra $\mathcal{A}^+(SU_q(2)) = \oplus_{r\geq 0} End[V^+_{r+1}]$, which is isomorphic, as an algebra, to $\mathcal{A}(SU(2))$, but whose coproduct is deformed. The subalgebra $\mathcal{P}(SU_q(2))$ generated by t and by the center remains unchanged in the deformation. We consider the tracial state $\frac{1}{2}Tr$ on the two-dimensional component, and consider the associated random walk. As in the case of $SU(2)$, the restriction of the associated Markov transtion operator to the commutative algebra $\mathcal{P}(SU_q(2))$ defines a Markov chain on the spectrum of this algebra, whose transition probabilities can be computed, using the deformed Clebsch Gordan formulas, as in Klimyk et Vilenkin [KV], formulas (6) et (9), §14.4.3, to give

$$p((r,k),(r+1,k+1)) = q^{(r-k)/2}\frac{\left[\frac{r+k+2}{2}\right]_q}{[r+1]_q} = \frac{q^{r+1}-q^{-k-1}}{2(q^{r+1}-q^{-r-1})} \tag{13.2}$$

$$p((r,k),(r+1,k-1)) = q^{-(r+k)/2}\frac{\left[\frac{r-k+2}{2}\right]_q}{2[r+1]_q} = \frac{q^{-k+1}-q^{-r-1}}{2(q^{r+1}-q^{-r-1})}$$

$$p((r,k),(r-1,k+1)) = q^{-(r+k+2)/2}\frac{\left[\frac{r-k}{2}\right]_q}{2[r+1]_q} = \frac{q^{-k-1}-q^{-r-1}}{2(q^{r+1}-q^{-r-1})}$$

$$p((r,k),(r-1,k-1)) = q^{(r-k+2)/2}\frac{\left[\frac{r+k}{2}\right]_q}{2[r+1]_q} = \frac{q^{r+1}-q^{-k+1}}{2(q^{r+1}-q^{-r-1})}$$

Letting q tend to 0, one checks that (13.2) converges to (13.1), and thus we get Pitman's theorem as an outcome of the $q \to 0$ limit of the quantum Bernoulli random walk, see [B7] for details.

This observation is at the basis of a vast generalization of Pitman's theorem, see e.g. [BBO].

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Interactions between Quantum Probability and Operator Space Theory

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Abstract We give a brief aspect of interactions between quantum probability and operator space theory by emphasizing the usefulness of noncommutative Khintchine type inequalities in the latter theory. After a short introduction to operator spaces, we present various Khintchine type inequalities in the noncommutative setting, including those for Rademacher variables, Voiculescu's semicircular systems and Shlyakhtenko's generalized circular systems. As an illustration of quantum probabilistic methods in operator spaces, we prove Junge's complete embedding of Pisier's OH space into a noncommutative L_1, for which Khintchine inequalities for the generalized circular systems are a key ingredient.

1 Introduction

It is well-known that probabilistic methods are important methods in Banach space theory. As operator spaces are quantized Banach spaces, one would naturally expect that quantum probability should play a non negligible role in the young operator space theory. This is indeed the case. In fact, quantum probability and operator space theory are intimately related and there exist many interactions between them. For instance, the recent remarkable development of noncommutative martingale inequalities is directly influenced and motivated by operator space theory. In particular, the establishment of the noncommutative Doob maximal inequality by Junge [J1] is inspired by Pisier's theory of vector-valued noncommutative L_p-spaces. On the other hand, the noncommutative Burkholder/Rosenthal inequalities can be used

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to determine the linear structure of symmetric subspaces of noncommutative L_p-spaces (see [JX]). The recent works of Pisier/Shlyakhtenko [PS] on the operator space Grothendieck inequality and of Junge [J2] on the complete embedding of OH into a noncommutative L_1 are two more beautiful examples of illustration of these interactions. Certain Khintchine type inequalities are key ingredients in both works.

It is clear today that quantum probability is of increasing importance in operator space theory. We will try to convince the reader of this in this course by presenting a very brief aspect of interactions between the two theories. Our presentation is around Khintchine type inequalities. In consequence, noncommutative L_p-spaces are at the heart of these lectures.

This course can be divided into three parts. The first one gives a brief introduction to operator space theory. We start with a short discussion on completely positive maps between C*-algebras in order to prepare the introduction to operator spaces and completely bounded maps. Our introduction to operator spaces begins with concrete operator spaces, i.e., those which are closed subspaces of $B(H)$ and the Haagerup-Paulsen-Wittstock factorization theorem for completely bounded maps, which should be understood together with its predecessor, Stinespring's factorization theorem for completely positive maps. We then pass to Ruan's fundamental characterization of abstract operator spaces. It is Ruan's theorem that allows us to do basic operations on operator spaces such that duality, quotient and interpolation. Meanwhile, some important examples of operator spaces are given, including column space C, row space R and Pisier's operator Hilbert space OH. This first part ends with an outline of Pisier's vector-valued noncommutative L_p-spaces. We concentrate here only on Schatten classes.

The second part is of quantum probabilistic character. The main object of this part is various noncommutative Khintchine inequalities. It becomes clear nowadays that Khintchine type inequalities are of paramount importance in operator space theory and more generally in noncommutative analysis. The inequalities we present are those for Rademacher variables, free group generators, Voiculescu's semicircular systems and Shlyakhtenko's generalized circular systems. The proofs of these inequalities in noncommutative L_p-spaces are often quite technical and tricky. But what will be needed in the third part concerns only the case $p = 1$, which is often easier. We should point out that the von Neumann algebra generated by a generalized circular system is of type III, which turns our presentation of noncommutative L_p-spaces somehow more complicated. This is, unfortunately, unavoidable in view of the complete embedding of OH into a noncommutative L_1 presented later.

The short third part is devoted to Junge's complete embedding of OH into a noncommutative L_1. We first present OH as a quotient of a subspace of $C \oplus R$ (a theorem of Pisier), which is given by the graph of a closed densely defined operator on ℓ_2. We then prove that any such graph embeds completely isomorphically into a noncommutative L_1-space.

2 Completely Positive Maps

This section gives a brief discussion on completely positive maps between C*-algebras. Our references for operator algebras are [KR] and [T]. Let us fix some notations used throughout this course:

- $B(H)$ denotes the space of all bounded linear operators on a complex Hilbert space H.
- A often denotes a C*-algebra; so A can be regarded as a C*-subalgebra of $B(H)$ for some H. A_+ denotes the positive cone of A.
- M denotes a von Neumann algebra and M_* the predual of M.
- $\mathbb{M}_n$ denotes the algebra of complex $n \times n$ matrices; so $\mathbb{M}_n$ can be identified with $B(\ell_2^n)$.
- $\mathbb{M}_n(A)$ denotes the algebra of $n \times n$ matrices with entries in A. This is again a C*-algebra. If $A \subset B(H)$, then $\mathbb{M}_n(A)$ is a C*-subalgebra of $\mathbb{M}_n(B(H)) \simeq B(\ell_2^n(H))$.
- ℓ_p denotes the ℓ_p-space of complex sequences (x_k) such that $(\sum_k |x_k|^p)^{1/p} < \infty$, $1 \le p \le \infty$ (with the usual modification for $p = \infty$). The n-dimensional version of ℓ_p is denoted by ℓ_p^n.

Definition 2.1. Let $u : A \to B$ be a linear map between two C*-algebras.

i) u is called *positive* if $u(A_+) \subset B_+$.
ii) u is called *completely positive* (c.p. for short) if u_n is positive for every $n \ge 1$, where $u_n = \mathrm{id}_{\mathbb{M}_n} \otimes u : \mathbb{M}_n(A) \to \mathbb{M}_n(B)$ is defined by $u_n((x_{ij})) = (u(x_{ij}))$.

Remark 2.2. It is easy to check that a positive map $u : A \to B$ is automatically continuous. If in addition A is unital, then $\|u\| = \|u(1)\|$ (see [Pa]).

Examples:

1) **Homomorphisms.** Every homomorphism $\pi : A \to B$ is c.p.. By *homomorphism* we mean a linear map satisfying: $\pi(xy) = \pi(x)\pi(y)$ and $\pi(x^*) = \pi(x)^*$ for all $x, y \in A$. Recall that a homomorphism π is necessarily contractive, i.e., $\|u\| \le 1$. If in addition π is injective, then π is isometric.
2) **Multiplications.** Let $a \in A$ and define $C_a : A \to A$ by $C_a(x) = a^*xa$. Then C_a is c.p. and $\|C_a\| = \|a^*a\| = \|a\|^2$. More generally, if H and K are two Hilbert spaces and $a : K \to H$ a bounded operator, then $C_a : B(H) \to B(K)$ defined by $C_a(x) = a^*xa$, is c.p..

The classical theorem of Stinespring states that any c.p. map is the composition of two maps of the previous types.

Theorem 2.3. (**Stinespring's factorization**)
Let A be a C-algebra and B a C*-subalgebra of $B(K)$. Let $u : A \to B$ be c.p.. Then there are a Hilbert space H, a representation $\pi : A \to B(H)$ (i.e., a homomorphism) and a bounded operator $a : H \to K$ such that*

$$u(x) = a^* \pi(x) a, \quad \forall\, x \in A.$$

Namely, $u = C_a \circ \pi$.

We refer to [T] for the proof of this theorem. We deduce immediately the following

Corollary 2.4. *If $u : A \to B$ is c.p., then*

$$\|u\|_{cb} \stackrel{\text{def}}{=} \sup_n \|u_n : \mathbb{M}_n(A) \to \mathbb{M}_n(B)\| < \infty.$$

Namely, u is completely bounded. Moreover, $\|u\|_{cb} = \|u\|$.

Exercises:

1) Prove that a positive map is automatically continuous.
2) Let A be a C*-algebra. Prove that $x = (x_{ij})_{i,j} \in \mathbb{M}_n(A)$ is positive iff x is a sum of matrices of the form $(a_i^* a_j)_{i,j}$ with $a_1, ..., a_n \in A$.
3) Let A and B be C*-algebras with B commutative. Prove that every positive map $\varphi : A \to B$ is automatically c.p..

3 Concrete Operator Spaces and Completely Bounded Maps

We consider in this section closed subspaces of $B(H)$ and completely bounded maps between them. The analogue for the present setting of the Stinespring factorization given in the previous section is the Haagerup-Paulsen-Wittstock factorization for completely bounded maps, which is fundamental in the theory. The references for this and next sections are [ER], [Pa] and [P3].

Definition 3.1. A (*concrete*) *operator space* is a closed subspace E of $B(H)$ for some Hilbert space H.

Let E be a Banach space, and let B_{E^*} denote the unit ball of the dual E^* of E. B_{E^*} becomes a compact topological space when equipped with the w*-topology. Then $E \subset C(B_{E^*})$ isometrically. More precisely, given $x \in E$ define $\widehat{x} : B_{E^*} \to \mathbb{C}$ by $\widehat{x}(\xi) = \xi(x)$. Then $x \mapsto \widehat{x}$ establishes an isometry from E into $C(B_{E^*})$. But now $C(B_{E^*})$ is a commutative C*-algebra, so $C(B_{E^*}) \subset B(H)$ for some H. In this way, any Banach space is an operator space. However, according to the preceding definition, an operator space E is given together with an embedding of E into a $B(H)$. More precisely, an operator space is a pair of a Banach space E and an embedding of E into some $B(H)$. On the other hand, $B(H)$ admits a natural matricial structure: $\mathbb{M}_n(B(H)) = B(\ell_2^n(H))$ for every $n \in \mathbb{N}$. This should be reflected in E too. In particular, the "admissible" morphisms in the category of operator spaces should respect this matricial structure.

Matricial Structure. Let $E \subset B(H)$ be an operator space. Then E inherits the matricial structure of $B(H)$ by virtue of the embedding $\mathbb{M}_n(E) \subset \mathbb{M}_n(B(H))$. More precisely, let $\mathbb{M}_n(E)$ be the space of $n \times n$ matrices with entries in E. Then $\mathbb{M}_n(E)$ is equipped with the norm induced by that of $B(\ell_2^n(H))$.

Definition 3.2. Let $E \subset B(H)$ and $F \subset B(K)$ be two operator spaces. Let $u : E \to F$ be a linear map.

i) u is called *completely bounded* (c.b. for short) if
$$\|u\|_{cb} = \sup_{n \geq 1} \|u_n\| < \infty,$$
where $u_n = \mathrm{id}_{\mathbb{M}_n} \otimes u : \mathbb{M}_n(E) \to \mathbb{M}_n(F)$ is defined by $u_n((x_{ij})) = (u(x_{ij}))$. $CB(E, F)$ denotes the space of all c.b. maps from E to F.

ii) u is called a *complete isomorphism* if u is a c.b. bijection and u^{-1} is also c.b..

iii) u is called *completely isometric* if u_n is isometric for every n. If u is a bijection and both u and u^{-1} are completely isometric, u is called a *complete isometry* .

Examples:

1) **C*-algebras.** Let A be a C*-algebra. Then A is a C*-subalgebra of some $B(H)$; so A is an operator space. The resulting matricial structure on A is called the *natural operator space structure* of A. In particular, any von Neumann algebra has its natural operator space structure. Note that this natural operator space structure of A is independent, up to complete isometry, of particular representation of A as C*-subalgebra of $B(H)$ for a faithful representation is completely isometric.

2) **Minimal structure.** Let E be a Banach space. Then we have the isometric embedding $E \subset C(B_{E^*})$, which turns E an operator space, denoted by $\min(E)$. This operator space structure is called the *minimal structure* on E. The adjective "minimal" means that this structure induces the least matricial norms on $\mathbb{M}_n(E)$. Indeed, assume that E itself is an operator space and consider also the associated minimal operator space $\min(E)$. Then by Proposition 3.3 below, the identity map on E induces a complete contraction from E to $\min(E)$. Namely, for any n and any $x \in \mathbb{M}_n(E)$
$$\|x\|_{\mathbb{M}_n(\min(E))} \leq \|x\|_{\mathbb{M}_n(E)} \,.$$

3) **Maximal structure.** Similarly, we can introduce a maximal operator space structure on a Banach space E. Let Φ be the family of all pairs $\varphi = (u_\varphi, H_\varphi)$ with H_φ a Hilbert space and $u_\varphi : E \to B(H_\varphi)$ a contraction. Let $\mathcal{H}$ be the Hilbert space direct sum of the H_φ:

$$\mathcal{H} = \bigoplus_{\varphi\in\Phi} H_\varphi \,.$$

Then $B(\mathcal{H})$ contains as C*-subalgebra the C*-algebra direct sum of the $B(H_\varphi)$:

$$B(\mathcal{H}) \supset \bigoplus_{\varphi\in\Phi} B(H_\varphi)\,.$$

Define $J : E \to B(\mathcal{H})$ by $J(x) = \big(u_\varphi(x)\big)_{\varphi\in\Phi} \in \oplus_{\varphi\in\Phi} B(H_\varphi)$. It is clear that J is isometric. This yields an isometric embedding of E into $B(\mathcal{H})$. Identifying E and $J(E) \subset B(\mathcal{H})$, we turn E an operator space. This operator space structure is called the *maximal structure* of E and denoted by $\max(E)$. By definition, one sees that if E itself is an operator space, then the identity map $\mathrm{id}_E : \max(E) \to E$ is completely contractive.

4) **Column and row spaces.** Let (e_{ij}) denote the standard matrix units of $B(\ell_2)$. Define

$$C = \overline{\mathrm{span}}(e_{i1},\ i \geq 1) \quad \text{and} \quad R = \overline{\mathrm{span}}(e_{1j},\ j \geq 1).$$

Thus we get two operator spaces $C \subset B(\ell_2)$ and $R \subset B(\ell_2)$. Note that C (resp. R) is identified as the first column (resp. row) subspace of $B(\ell_2)$. The operator space structures of C and R are easily determined. Let $x \in \mathbb{M}_n(C), y \in \mathbb{M}_n(R)$ and write

$$x = \sum_i x_i \otimes e_{i1}, \quad y = \sum_i y_i \otimes e_{1i}, \quad x_i,\ y_i \in \mathbb{M}_n.$$

Then

$$\|x\|_{\mathbb{M}_n(C)} = \Big\|\sum_i x_i^* x_i\Big\|^{1/2}, \quad \|y\|_{\mathbb{M}_n(R)} = \Big\|\sum_i y_i y_i^*\Big\|^{1/2}.$$

The n-dimensional versions of C and R are denoted by C^n and R^n, respectively. As Banach spaces both C and R are isometric to ℓ_2 via the identification $e_{i1} \sim e_{1i} \sim e_i$, where (e_i) denotes the canonical basis of ℓ_2. We will see at the end of this section that they are not completely isomorphic.

Proposition 3.3. *Let $E \subset B(H)$ be an operator space and A a commutative C^*-algebra. Then any bounded map $u : E \to A$ is automatically c.b. and* $\|u\|_{cb} = \|u\|$.

Proof. Let us first consider the case where $A = \mathbb{C}$. Let $u : E \to \mathbb{C}$ be a continuous linear functional with $\|u\| \leq 1$. For any $n \in \mathbb{N}$ we must show that $u_n : \mathbb{M}_n(E) \to \mathbb{M}_n$ is a contraction. To this end let $x \in \mathbb{M}_n(E)$, and let $\alpha, \beta \in \ell_2^n$ (α and β being viewed as column matrices). Then

$$\begin{aligned} \big|\langle u_n(x)\alpha,\ \beta\rangle\big| &= \Big|\sum_{i,j=1}^n u(x_{ij})\alpha_j\bar{\beta}_i\Big| = \Big|u\Big(\sum_{i,j=1}^n x_{ij}\alpha_j\bar{\beta}_i\Big)\Big| \\ &\leq \Big\|\sum_{i,j=1}^n x_{ij}\alpha_j\bar{\beta}_i\Big\| = \big\|\beta^* x\alpha\big\| \leq \|\beta\|\,\|x\|\,\|\alpha\|. \end{aligned}$$

Taking the supremum over all x, α, β in the respective unit balls, we deduce that $\|u_n\| \leq 1$. Thus u is a complete contraction.

The general case can be easily reduced to the previous one. Indeed, since A is commutative, we can assume $A = C_0(\Omega)$ for some locally compact topological space Ω, where $C_0(\Omega)$ denotes the C*-algebra of all continuous functions on Ω which tend to zero at infinity. Then $\mathbb{M}_n(A) = C_0(\Omega; \mathbb{M}_n)$, the C*-algebra of continuous functions from Ω to $\mathbb{M}_n$ which vanish at infinity. The norm of an element $y = (y_{ij}) \in C_0(\Omega; \mathbb{M}_n)$ is given by

$$\|y\| = \sup_{\omega\in\Omega} \big\|\big(y_{ij}(\omega)\big)\big\|_{\mathbb{M}_n}.$$

Now let $u : E \to A$ be bounded. Then

$$\|u_n\| = \sup\big\{\big\|\big(u(x_{ij})(\omega)\big)\big\|_{\mathbb{M}_n}\ :\ \omega \in \Omega,\ x \in \mathbb{M}_n(E),\ \|x\| \leq 1\big\}.$$

It follows that

$$\|u\|_{cb} = \sup_{\omega\in\Omega} \|\delta_\omega \circ u\|_{cb},$$

where $\delta_\omega : C_0(\Omega) \to \mathbb{C}$ is the evaluation at ω: $\delta_\omega(f) = f(\omega)$. We are thus reduced to the one dimensional case. □

Prototypical Examples of c.b. Maps:

1) **Homomorphisms between C*-algebras**. These maps are c.b. for they are c.p.. Moreover, they are completely contractive. Note also that an injective homomorphism is completely isometric.
2) **Multiplications by bounded operators**. Given $a \in B(H)$ define

$$L_a : B(H) \to B(H),\ x \mapsto ax \quad \text{and} \quad R_a : B(H) \to B(H),\ x \mapsto xa.$$

Then L_a and R_a are c.b. and

$$\|L_a\|_{cb} = \|R_a\|_{cb} = \|a\|.$$

Thus if $E \subset B(H)$, then $L_a\big|_E$ and $R_a\big|_E$ are also c.b..

The following theorem asserts that any c.b. map is the composition of a homomorphism, a left multiplication and a right multiplication. This is the c.b. analogue of Stinespring's factorization. We refer to [ER] and [P3] for the proof.

Theorem 3.4. (**Haagerup-Paulsen-Wittstock factorization**) *Let $E \subset B(H)$ and $F \subset B(K)$ be two operator spaces. Let $u : E \to F$ be a c.b. map. Then there are a Hilbert space $\widetilde{H}$, a representation $\pi : B(H) \to B(\widetilde{H})$ and two bounded operators $a, b \in B(K, \widetilde{H})$ such that*

$$u(x) = b^* \pi(x) a, \quad \forall\, x \in E.$$

Namely, $u = L_{b^*} \circ R_a \circ \pi\big|_E$. Moreover,

$$\|u\|_{cb} = \inf \big\{ \|a\| \, \|b\| \big\},$$

where the infimum is taken over all factorizations of u as above.

Corollary 3.5. (**Hahn-Banach type extension**) *Every c.b. map $u : E \to B(K)$ admits a c.b. extension $\tilde{u} : B(H) \to B(K)$ such that $\|\tilde{u}\|_{cb} = \|u\|_{cb}$.*

Proof. Take a factorization $u = L_{b^*} \circ R_a \circ \pi\big|_E$ such that $\|u\|_{cb} = \|a\| \, \|b\|$. Then $\tilde{u} = L_{b^*} \circ R_a \circ \pi$ is the desired extension of u. □

Let $E \subset B(H)$ be an operator space. Then E inherits the order of $B(H)$, which allows us to define positive and completely positive maps on E. Thus a map $u : E \to B(K)$ is c.p. if u_n sends the positive part of $\mathbb{M}_n(E)$ into that of $\mathbb{M}_n(B(K))$ for every n.

Corollary 3.6. (**Decomposability of c.b. maps**) *Every c.b. map $u : E \to B(K)$ is decomposable in the sense that there are four c.p. maps u_k such that*

$$u = u_1 - u_2 + i(u_3 - u_4)$$

with $\|u_k\|_{cb} \le \|u\|_{cb}$.

Proof. Let $u = L_{b^*} \circ R_a \circ \pi\big|_E$ according to Theorem 3.4. Then the corollary immediately follows from the polarization identity with

$$u_k = \frac{1}{4}\, C_{a+i^k b} \circ \pi\big|_E\,, \quad 1 \le k \le 4,$$

where C_a is the multiplication by a from the right and by a^* from the left. □

Usually, we do not distinguish completely isometric operator spaces. The distance between two operator spaces is measured by the operator space analogue of the Banach-Mazur distance in the theory of Banach spaces. The Banach-Mazur distance of two Banach spaces E and F is

$$d(E,F) = \inf\big\{\|u^{-1}\|\,\|u\| \;:\; u : E \to F \text{ is an isomorphism}\big\}.$$

If E and F are isomorphic, $d(E,F) < \infty$; otherwise, $d(E,F) = \infty$.

Definition 3.7. Given two operator spaces E and F define

$$d_{cb}(E,F) = \inf\big\{\|u^{-1}\|_{cb}\,\|u\|_{cb} \;:\; u : E \to F \text{ is a complete isomorphism}\big\}.$$

Pisier [P1] proved that if $\dim E = \dim F = n$, then $d_{cb}(E,F) \le n$. We will see that the upper bound is attained for the pair (C^n, R^n). To this end, let us introduce a general definition.

Definition 3.8. An operator space E is called homogeneous if every bounded map on E is c.b. and $\|u\|_{cb} = \|u\|$. E is called Hilbertian if E is isometric to a Hilbert space.

It is easy to see that $\min(E)$ and $\max(E)$ are homogeneous. On the other hand, C and R are homogeneous Hilbertian operator spaces. We refer to Chapiter 10 of [P3] for the proofs of the following two results.

Proposition 3.9. *Let E and F be two n-dimensional Hilbertian homogeneous operator spaces. Let $(e_1, ..., e_n)$ and $(f_1, ..., f_n)$ be orthonormal bases of E and F, respectively. Let $u : E \to F$ be the map defined by $u(e_i) = f_i$. Then*

$$d_{cb}(E,F) = \|u^{-1}\|_{cb}\|u\|_{cb}\,.$$

Corollary 3.10. *$d_{cb}(C^n, R^n) = n$ and $d_{cb}(C^n, \min(\ell_2^n)) = \sqrt{n}$. Consequently, C, R and $\min(\ell_2)$ are not completely isomorphic each other.*

Exercises:

1) Let E be a Banach space and F an operator space. Prove that any bounded maps $u : F \to \min(E)$ and $v : \max(E) \to F$ are c.b. and $\|u\|_{cb} = \|u\|$, $\|v\|_{cb} = \|v\|$.
2) Prove that C and R are homogeneous.
3) Prove Corollary 3.10.
4) Let $u : C \to R$. Prove $\|u\|_{cb} = \|u\|_{HS}$, where $\|u\|_{HS}$ denotes the Hilbert-Schmidt norm of u regarded as an operator on ℓ_2, i.e.,

$$\|u\|_{HS} = \Big(\sum_{i=1}^{\infty} \|u(e_i)\|_2^2\Big)^{1/2}.$$

4 Ruan's Theorem: Abstract Operator Spaces

The definition of concrete operator spaces presented in the previous section has a major drawback: it does not allow to do basic operations on concrete operator spaces. For instance, it is not clear at all how to introduce a nice matricial structure on the Banach dual E^* of E which reflects the one of E. This drawback is resorbed in Ruan's definition of abstract operator spaces.

We have already seen that a concrete operator space $E \subset B(H)$ possesses a natural matricial structure inherited from that of $B(H)$: for each n, $\mathbb{M}_n(E) \subset B(\ell_2^n(H))$ is again an operator space, equipped with the norm $\|\cdot\|_n$ induced by that of $B(\ell_2^n(H))$. This sequence $(\|\cdot\|_n)$ of matricial norms clearly satisfy the following properties

- (R_1): $\|\alpha x\beta\|_n \le \|\alpha\|\,\|x\|_n\|\beta\|,\ \forall\,\alpha,\beta \in \mathbb{M}_n, x \in \mathbb{M}_n(E), n \ge 1.$
- (R_2): $\|x\oplus y\|_{n+m} \le \max\big(\|x\|_n,\ \|y\|_m\big), \forall\, x \in \mathbb{M}_n(E), y \in \mathbb{M}_m(E), n,m \ge 1.$

Here the product is the usual matrix product. $x \oplus y$ denotes the $(n+m) \times (n+m)$-matrix

$$\begin{pmatrix} x & 0 \\ 0 & y \end{pmatrix}.$$

(R_1) and (R_2) above are usually called Ruan's axioms .

Theorem 4.1. (**Ruan's characterization**)
Let E be a vector space. Assume that each $\mathbb{M}_n(E)$ is equipped with a norm $\|\cdot\|_n$. If these norms $\|\cdot\|_n$ satisfy Ruan's axioms (R_1) and (R_2), then there are a Hilbert space H and a linear map $J : E \to B(H)$ such that

$$J_n = \mathrm{id}_{\mathbb{M}_n} \otimes J : \mathbb{M}_n(E) \to \mathbb{M}_n(B(H)) \quad \textit{is isometric for every}\, n.$$

In other words, the sequence $(\|\cdot\|_n)$ comes from the operator space structure of E given by the embedding $J : E \to B(H)$.

This theorem is proved in [R] (see also [ER] for an alternate proof).

Definition 4.2. An (*abstract*) *operator space* is a Banach space E together with a sequence $(\|\cdot\|_n)$ of norms satisfying (R_1) and (R_2) (with $\|\cdot\|_1$ equal to the original norm of E).

Henceforth, we will drop the adjective "concrete" or "abstract" by saying only operator spaces. Thus to have an operator space structure on a Banach space E is to have a sequence of matricial norms verifying Ruan's axioms. In the remainder of this section we present some basic operations on operator spaces. The complex interpolation is postponed, however, to the next one, where Pisier's operator Hilbert space will be also introduced.

Spaces of c.b. maps. If E and F are two operator spaces, $CB(E,F)$ denotes again the space of all c.b. maps from E to F. This is a Banach space equipped with the norm $\|\cdot\|_{cb}$. Now we wish to turn $CB(E,F)$ an operator space. Let $u=(u_{ij})\in\mathbb{M}_n(CB(E,F))$. We view u as a map from E into $\mathbb{M}_n(F)$ by defining $u(x)=\big(u_{ij}(x)\big)$ for $x\in E$. Then the matricial norm on $\mathbb{M}_n(CB(E,F))$ is defined by

$$\|u\|_n=\big\|u:E\to\mathbb{M}_n(F)\big\|_{cb}\,.$$

Namely, we have the identification

$$\mathbb{M}_n(CB(E,F))=CB(E,\mathbb{M}_n(F)).$$

It is easy to show that Ruan's axioms are verified. Thus $CB(E,F)$ becomes an operator space.

Duality. Specializing the previous discussion to $F=\mathbb{C}$, we see that $CB(E,\mathbb{C})$ is an operator space. However, Proposition 3.3 implies that $CB(E,\mathbb{C})=E^*$ isometrically. Therefore, E^* becomes an operator space. The norm of $\mathbb{M}_n(E^*)$ is that of $CB(E,\mathbb{M}_n)$. This is usually called the *standard dual* of E. We will simply say the dual of E since only standard duals are used in the sequel. The bidual $E^{**}=(E^*)^*$ is an operator space too. Then it is easy to check that the natural inclusion $E\hookrightarrow E^{**}$ is completely isometric. This allows to view E as a subspace of E^{**}.

Thus the duals of C*-algebras and the preduals of von Neumann algebras are operator spaces.

Let $u:E\to F$ be a map between two operator spaces. Then u is c.b. iff its adjoint $u^*:F^*\to E^*$ is c.b.. If this is the case, $\|u\|_{cb}=\|u^*\|_{cb}$.

Quotient. Let E be an operator space and $F\subset E$ a closed subspace. We equip $\mathbb{M}_n(E/F)$ with the quotient norm of $\mathbb{M}_n(E)/\mathbb{M}_n(F)$. Then it is easy to check that these norms satisfy (R_1) and (R_2), so E/F becomes an operator space. The usual duality between subspaces and quotients in Banach space theory remains available now:

$$F^*=\frac{E^*}{F^\perp}\quad\text{and}\quad\Big(\frac{E}{F}\Big)^*=F^\perp\quad\text{completely isometrically.}$$

Direct sum. Let (E_k) be a sequence of operator spaces, $E_k\subset B(H_k)$ (the sequence may be finite). Let $\ell_\infty((E_k))$ denote the space of all sequences (x_k) with $x_k\in E_k$ such that $\sup_k\|x_k\|<\infty$. This is a Banach space when equipped with the norm

$$\|(x_k)\|=\sup_k\|x_k\|.$$

$\ell_\infty((E_k))$ naturally inherits a matricial structure from $\ell_\infty((B(H_k)))$, the latter being a C*-algebra. Thus we have

$$\mathbb{M}_n\big(\ell_\infty((E_k))\big)=\ell_\infty\big((\mathbb{M}_n(E_k))\big).$$

$c_0((E_k))$ denotes the subspace of $\ell_\infty((E_k))$ consisting of all (x_k) such that $\|x_k\| \to 0$.

On the other hand, we define $\ell_1((E_k))$ to be the space of all sequences (x_k) with $x_k \in E_k$ such that $\sum_k \|x_k\| < \infty$. This is again a Banach space with the natural norm. Recall that

$$\big(\ell_1((E_k))\big)^* = \ell_\infty((E_k^*)) \quad \text{isometrically.}$$

Thus $\ell_1((E_k))$ is a predual of $\ell_\infty((E_k))$, which allows us to view $\ell_1((E_k))$ as an operator space too. We often use the notations

$$\bigoplus_k {}_\infty\, E_k \quad \text{and} \quad \bigoplus_k {}_1\, E_k$$

instead of $\ell_\infty((E_k)_k)$ and $\ell_1((E_k)_k)$, respectively. If all E_k are equal, these spaces are denoted by $\ell_\infty(E)$ and $\ell_1(E)$, respectively. In particular, if $E = \mathbb{C}$, we recover ℓ_∞ and ℓ_1.

Let us introduce the continuous version of $c_0(E)$. Let Ω be a locally compact topological space and $E \subset B(H)$ an operator space. Let $C_0(\Omega; E)$ denote the space of continuous functions from Ω to E which vanish at infinity. $C_0(\Omega; E)$ is equipped with the uniform norm

$$\|f\| = \sup_{\omega \in \Omega} \|f(\omega)\|.$$

Then $C_0(\Omega; E) \subset C_0(\Omega; B(H))$. The latter space is a C*-algebra. In this way, we turn $C_0(\Omega; E)$ an operator space.

Sum and Intersection. Let (E_0, E_1) be a couple of operator spaces. Assume (E_0, E_1) is *compatible* in the sense that both E_0 and E_1 continuously embed into a common topological vector space V. This allows us to define

$$E_0 \cap E_1 = \big\{x \in V \ :\ x \in E_0,\ x \in E_1\big\}$$

and

$$E_0 + E_1 = \big\{x \in V \ :\ \exists\, x_0 \in E_0,\ x_1 \in E_1 \text{ s.t. } x = x_0 + x_1\big\},$$

equipped respectively with the intersection and sum norms

$$\|x\|_{E_0 \cap E_1} = \max\big(\|x\|_{E_0}\,,\ \|x\|_{E_1}\big),$$

$$\|x\|_{E_0 + E_1} = \inf\big\{\|x_0\|_{E_0} + \|x_1\|_{E_1} \ :\ x = x_0 + x_1, x_0 \in E_0,\ x_1 \in E_1\big\}.$$

Note that $E_0 \cap E_1$ can be regarded as the diagonal subspace of $E_0 \oplus_\infty E_1$. On the other hand, $E_0 + E_1$ is identifiable with the quotient space of $E_0 \oplus_1 E_1$ by Δ, where $\Delta = \{(x_0, x_1) \ :\ x_0 + x_1 = 0\}$. Equipped with the operator space structures induced by those of $E_0 \oplus_\infty E_1$ and $E_0 \oplus_1 E_1$, respectively, $E \cap E_1$ and $E_0 + E_1$ become operator spaces too.

Let us consider an important example. Take the column and row spaces C and R and view them as compatible by identifying both of them with ℓ_2 at the Banach space level. Thus if $x \in C$, we write

$$x = \sum_i x_i e_{i1} \quad \text{with} \quad x_i \in \mathbb{C}.$$

Recall that

$$\|x\|_C = (\sum_i |x_i|^2)^{1/2} = \|(x_i)\|_{\ell_2} = \|\sum_i x_i e_{1i}\|_R\,.$$

Then the compatibility above means that x is identified with the sequence (x_i). Accordingly, we often identify the canonical bases (e_{i1}) of C and (e_{1i}) of R with (e_i) of ℓ_2. Thus as Banach spaces, $C \cap R = C = R\,(= \ell_2)$. But this is no longer true in the category of operator spaces.

Let $x \in \mathbb{M}_n(C \cap R) = \mathbb{M}_n(C) \cap \mathbb{M}_n(R)$. Write

$$x = \sum_i x_i \otimes e_i \quad \text{with} \quad x_i \in \mathbb{M}_n.$$

Then

$$\begin{aligned}\|x\|_{\mathbb{M}_n(C\cap R)} &= \max\big(\|x\|_{\mathbb{M}_n(C)}\,,\ \|x\|_{\mathbb{M}_n(R)}\big)\\ &= \max\big(\|\sum_i x_i^* x_i\|^{1/2}\,,\ \|\sum_i x_i x_i^*\|^{1/2}\big).\end{aligned}$$

Using this, we easily check that $C \cap R$ is not completely isomorphic to C. Indeed, using Proposition 3.3, one easily shows that their n-dimensional versions satisfy the following

$$d_{cb}(C^n,\ C^n \cap R^n) = \sqrt{n}.$$

The operator space structure of $C + R$ is a little bit more complicated. Using the complete isomorphism between $E_1 \oplus_\infty E_2$ and $E_1 \oplus_1 E_2$ (see Exercise 6 below), we deduce that for $x = \sum_i x_i \otimes e_i \in \mathbb{M}_n(C + R)$

$$\frac{1}{2}\,\|x\|_{\mathbb{M}_n(C+R)} \le \inf\big\{\big\|\sum_i y_i^* y_i\big\|^{1/2} + \big\|\sum_i z_i z_i^*\big\|^{1/2}\big\} \le 2\|x\|_{\mathbb{M}_n(C+R)}\,,$$

where the infimum runs over all decompositions $x_i = y_i + z_i$ with $y_i,\, z_i \in \mathbb{M}_n$. We will give later a complete isometric description of $C + R$ in terms of the trace class S_1.

Exercises:

1) Prove that $C^* \simeq R$ and $R^* \simeq C$ completely isometrically. More precisely, the map $\xi \in C^* \mapsto \sum_i \xi(e_{i1}) e_{1i}$ establishes a complete isometry between C^* and R.
2) Show that the natural inclusion $E \hookrightarrow E^{**}$ is completely isometric.

3) Let $F \subset E$ be operator spaces. Prove

$$F^* = \frac{E^*}{F^\perp} \quad \text{and} \quad \Big(\frac{E}{F}\Big)^* = F^\perp \quad \text{completely isometrically.}$$

4) Prove that a map $u : E \to F$ is c.b. iff its adjoint $u^* : F^* \to E^*$ is c.b.. Moreover, $\|u\|_{cb} = \|u^*\|_{cb}$.
5) Prove

$$\big(c_0((E_k))\big)^* = \ell_1((E_k^*)) \quad \text{and} \quad \big(\ell_1((E_k))\big)^* = \ell_\infty((E_k^*))$$

completely isometrically.
6) Prove that the natural inclusion from $\ell_1((E_k))$ into $\ell_\infty((E_k))$ is completely contractive. Conversely, prove that the c.b. norm of the formal identity from $E_1 \oplus_\infty \cdots \oplus_\infty E_n$ to $E_1 \oplus_1 \cdots \oplus_1 E_n$ is equal to n.
7) Let (E_0, E_1) be a compatible couple of operator spaces such that $E_0 \cap E_1$ is dense in both E_0 and E_1. Prove

$$\big(E_0 \cap E_1\big)^* = E_0^* + E_1^*, \quad \big(E_0 + E_1\big)^* = E_0^* \cap E_1^* \quad \text{completely isometrically.}$$

5 Complex Interpolation and Operator Hilbert Spaces

Hilbert spaces are in the center of the family of Banach spaces and play a crucial role there. It is thus natural to find their operator space analogues. One way to define operator Hilbert spaces is complex interpolation, which is of great importance for its own right in operator space theory. Our references for this section are [P1] and [P3].

Interpolation. We first recall the definition of complex interpolation for Banach spaces. Let (E_0, E_1) be a compatible couple of complex Banach spaces. Let $S = \{z \in \mathbb{C} \,:\, 0 \le \operatorname{Re} z \le 1\}$, a strip in $\mathbb{C}$. Let $\mathcal{F}(E_0, E_1)$ be the family of all functions $f : S \to E_0 + E_1$ satisfying the following conditions:

- f is continuous on S and analytic in the interior of S;
- $f(k + it) \in E_k$ for all $t \in \mathbb{R}$ and the function $t \mapsto f(k + it)$ is continuous from $\mathbb{R}$ to E_k for $k = 0$ and $k = 1$;
- $\lim_{|t|\to\infty} \|f(k + it)\|_{E_k} = 0$ for $k = 0$ and $k = 1$.

We equip $\mathcal{F}(E_0, E_1)$ with the norm:

$$\|f\|_{\mathcal{F}(E_0,E_1)} = \max\big\{\sup_{t\in\mathbb{R}} \|f(it)\|_{E_0}\,,\ \sup_{t\in\mathbb{R}} \|f(1 + it)\|_{E_1}\big\}.$$

Then it is a routine exercise to check that $\mathcal{F}(E_0, E_1)$ is a Banach space. For $0 < \theta < 1$ the complex interpolation space $E_\theta = (E_0,\ E_1)_\theta$ is defined as the space of all those $x \in E_0 + E_1$ for which there exists $f \in \mathcal{F}(E_0, E_1)$ such that $f(\theta) = x$. Equipped with

$$\|x\|_\theta = \inf\left\{\left\|f\right\|_{\mathcal{F}(E_0,E_1)} \ : \ f(\theta)=x,\ f\in\mathcal{F}(E_0,E_1)\right\},$$

E_θ becomes a Banach space. Note that by the maximum principle, the map $f\mapsto f(\theta)$ is a contraction from $\mathcal{F}(E_0,E_1)$ to E_0+E_1. Then $(E_0,\ E_1)_\theta$ can be isometrically identified with the quotient of $\mathcal{F}(E_0,E_1)$ by the kernel of this map.

Now assume E_0 and E_1 are operator spaces. Then $(\mathbb{M}_n(E_0),\mathbb{M}_n(E_1))$ is again compatible for any $n\geq 1$. This allows to define

$$\mathbb{M}_n(E_\theta)=\big(\mathbb{M}_n(E_0),\ \mathbb{M}_n(E_1)\big)_\theta .$$

It is easy to show that Ruan's axioms are satisfied, so E_θ is an operator space. Let us express E_θ as a quotient of a subspace of $C_0(\mathbb{R};E_0)\oplus_\infty C_0(\mathbb{R};E_1)$. Using Poisson integral, one sees that $C_0(\mathbb{R};E_0)\oplus_\infty C_0(\mathbb{R};E_1)$ is just the space of functions $f:S\to E_0+E_1$ satisfying the same conditions as above for $\mathcal{F}(E_0,E_1)$ but only with "analytic" replaced by "harmonic". Then $\mathcal{F}(E_0,E_1)$ is the subspace of $C_0(\mathbb{R};E_0)\oplus_\infty C_0(\mathbb{R};E_1)$ consisting of all analytic functions. Therefore, E_θ is the quotient space of $\mathcal{F}(E_0,E_1)$ by the subspace of all f such that $f(\theta)=0$.

Operator Hilbert Spaces. Let H be a complex Hilbert space. Fixing an orthonormal basis $(e_i)_{i\in I}$ in H, we can identify H with $\ell_2(I)$. The classical Riesz representation theorem asserts that H^* is isometric to the conjugate $\bar{H}$ of H. The latter space is H itself with the same norm but with conjugate multiplication: $\lambda\cdot x=\bar{\lambda}x$ for $\lambda\in\mathbb{C}$ and $x\in H$. Viewed as a vector in $\bar{H}$, a vector $x\in H$ is often denoted by $\bar{x}$. Thus if $x=(x_i)\in\ell_2(I)$, then $\bar{x}=(\bar{x}_i)_{i\in I}$. The map $x\mapsto\bar{x}$ establishes an anti-linear isometry between H and $\bar{H}$. Consequently, $\overline{H^*}$ is isometric to H. In fact, the conjugation can be defined for any Banach space X. It is a well-known elementary fact that the Hilbert spaces are only Banach spaces X such that $\overline{X^*}$ is isometric to X.

Now we wish to consider the operator space analogue of this property. The resulting spaces are the so-called operator Hilbert spaces, introduced by Pisier. Note that if E is an operator space, so is $\bar{E}$ by defining $\mathbb{M}_n(\bar{E})=\overline{\mathbb{M}_n(E)}$.

Theorem 5.1. *Let I be an index set. For any $x=\sum_i x_i\otimes e_i\in\mathbb{M}_n(\ell_2(I))$ define*

$$\|x\|_n=\Big\|\sum_i x_i\otimes\bar{x}_i\Big\|^{1/2}_{\mathbb{M}_n\otimes\overline{\mathbb{M}}_n}=\Big\|\sum_i x_i\otimes\bar{x}_i\Big\|^{1/2}_{\mathbb{M}_{n^2}} .$$

Then $(\|\cdot\|_n)$ satisfy Ruan's axioms. The resulting operator space is denoted by $OH(I)$. Moreover, $OH(I)$ is the unique, up to complete isometry, operator space structure on $\ell_2(I)$ such that $\overline{OH(I)^*}$ is completely isometric to $OH(I)$.

If $I=\mathbb{N}$ or $I=\{1,...,n\}$, we denote $OH(I)$ simply by OH or OH^n . The space OH can be also obtained by interpolating the column and row spaces.

Theorem 5.2. *$OH = (C,\ R)_{1/2}$ completely isometrically.*

Exercises:

1) Let (E_0, E_1) and (F_0, F_1) be two compatible couples of operator spaces. Let $T : E_0 + E_1 \to F_0 + F_1$ be a linear map such that $T\big|_{E_k} : E_k \to F_k$ is c.b. of cb-norm c_k for $k = 0, 1$. Then T is c.b. from E_θ to F_θ for any $0 < \theta < 1$ and of cb-norm $\le c_0^{1-\theta} c_1^{\theta}$.
2) Show that OH is homogeneous and $d_{cb}(C^n,\ OH^n) = \sqrt{n}$. Consequently, OH is not completely isomorphic to C.

6 Vector-valued Noncommutative L_p-spaces

Since operator spaces are quantized Banach spaces, noncommutative L_p-spaces are quantized L_p-spaces. Thus it is not surprising that noncommutative L_p-spaces play the role in operator space theory as the usual L_p-spaces do in the category of Banach spaces. In this section we introduce the natural operator space structures on noncommutative L_p and Pisier's vector-valued Schatten classes. We will need essentially the cases $p = \infty$ and $p = 1$ (so the case $1 < p < \infty$ can be skipped). For these special cases what is presented below becomes extremely simple for noncommutative L_∞ and L_1 are nothing but von Neumann algebras and their preduals.

6.1 Noncommutative L_p-spaces. Let M be a von Neumann algebra equipped with a normal faithful tracial state τ. For $1 \le p < \infty$ and $x \in M$ define

$$\|x\|_p = [\tau(|x|^p)]^{1/p}, \quad \text{where} \quad |x| = (x^*x)^{1/2}\,.$$

Then $(M, \|\cdot\|_p)$ is a normed space, whose completion is the noncommutative L_p-space associated with (M, τ), denoted by $L_p(M)$. By convention, $L_\infty(M) = M$ with the operator norm. Then for any $1 \le p < \infty$, the dual space of $L_p(M)$ is $L_{p'}(M)$ (p' being the conjugate index of p):

$$L_p(M)^* = L_{p'}(M) \quad \text{isometrically}$$

with respect to the duality bracket

$$\langle x,\ y\rangle = \tau(xy), \quad x \in L_p(M),\ y \in L_{p'}(M).$$

Consequently, $L_1(M)$ is the predual of M.

Let us consider two special cases. The first is where M is commutative, say, $M = L_\infty(\Omega, \mu)$ for some probability space (Ω, μ) (μ can be, of course, assumed to be a σ-finite measure). Then we recover the usual L_p-spaces $L_p(\Omega)$. The second case concerns $M = B(\ell_2^n)$, equipped with the usual trace Tr (which can be normalized to a state if we wish). Then we get the Schatten classes S_p^n. The infinite dimensional algebra $B(\ell_2)$ is not covered by this definition since the usual trace Tr on $B(\ell_2)$ is not finite. However, it still has a nice trace in the sense that it is *normal, semifinite and faithful.* The preceding construction can be done for normal semifinite faithful traces too. The resulting spaces for $(B(\ell_2), \mathrm{Tr})$ are the Schatten classes S_p. Recall that S_1 and S_2 are respectively the trace and Hilbert-Schmidt classes. Note that by definition S_∞ is the whole $B(\ell_2)$.

The previous definition does not apply to type III von Neumann algebras. There are several equivalent constructions of noncommutative L_p-spaces in the type III case. Here we adopt the one by Kosaki [Ko] via complex interpolation. Let M be a von Neumann algebra equipped with a normal faithful state φ. Define $L_\infty(M) = M$ as before and $L_1(M) = M_*$. Consider the left injection j of $L_\infty(M)$ into $L_1(M)$ by $j(x) = x\varphi$. The faithfulness of φ implies that j is injective and its range is dense in $L_1(M)$. This injection makes $(L_\infty(M),\ L_1(M))$ compatible. Thus we can consider the complex interpolation spaces between them. Now for $1 < p < \infty$ define

$$L_p(M) = \big(L_\infty(M),\ L_1(M)\big)_{\frac{1}{p}}\,.$$

We refer to the survey paper [PX] for more information and historical references on noncommutative L_p-spaces.

6.2 Operator Space Structures on Noncommutative L_p. Now we turn to describe the natural operator space structure on $L_p(M)$ (see [P3] for more information). For $p = \infty$, $L_\infty(M) = M$ has its natural operator space structure as a von Neumann algebra. This also yields an operator space structure on M^*, the standard dual of M. To deal with the case $p = 1$ we consider the opposite von Neumann algebra M^{op} of M. M^{op} is the same as M but with the new multiplication which is opposite to that of M: $x \cdot y$ in M^{op} is equal to $yx \in M$. Note that if M acts on H, then M^{op} acts on H^* and coincides with $\{x^t\ :\ x \in M\}$, where x^t denotes the transpose (= Banach space adjoint) of x. It is clear that the map $x \mapsto \overline{x^*}$ establishes an isomorphism between M and $\overline{M^{\mathrm{op}}}$. Thus $L_1(M)$ is isometric to $L_1(M^{\mathrm{op}})$ at the Banach space level. This allows us to equip $L_1(M)$ with the operator space structure inherited from $(M^{\mathrm{op}})^*$. The main reason for this choice is that it insures that the equality $L_1(\mathbb{M}_n \otimes M) = S_1^n \widehat{\otimes} L_1(M)$ (operator space projective tensor product) holds true. Finally, the operator space structure of $L_p(M)$ is obtained by complex interpolation. It is worth to mention that $L_2(M)$ is an operator Hilbert space by virtue of a theorem of Pisier.

Thus for every σ-finite measure space (Ω, μ), the commutative L_p-spaces $L_p(\Omega)$ are equipped with their natural operator space structures. In particular, the ℓ_p are operator spaces and $\ell_2 = OH$.

The same happens to the Schatten classes S_p too. If $1 \le p < \infty$, the dual space of S_p is $S_{p'}$ with respect to the so-called parallel duality bracket

$$\langle x,\ y\rangle = \mathrm{Tr}(xy^t) = \sum_{i,j} x_{ij} y_{ij}$$

for $x = (x_{ij}) \in S_p$ and $y = (y_{ij}) \in S_{p'}$. This is due to our definition that S_1 is defined as the predual of $B(\ell_2)^{\mathrm{op}}$.

6.3 Vector-valued Schatten Classes. We wish to define Schatten classes with values in operator spaces. To this end we first recall the *minimal tensor product* in the category of operator spaces. Let $E \subset B(H)$ and $F \subset B(K)$ be two operator spaces. Let $x \in B(H)$ and $y \in B(K)$. The tensor $x \otimes y$ is an operator on the Hilbert space tensor product $H \otimes K$ defined by $x \otimes y(\xi \otimes \eta) = x(\xi) \otimes y(\eta)$. It is easy to check that $x \otimes y$ is bounded and $\|x \otimes y\| = \|x\| \, \|y\|$. Consequently, the algebraic tensor product $E \otimes F$ is a vector subspace of $B(H \otimes K)$. Then the minimal tensor product $E \otimes_{\min} F$ is defined to be the closure of $E \otimes F$ in $B(H \otimes K)$.

Now let E be an operator space. Define $S_\infty[E]$ to be $S_\infty \otimes_{\min} E$. The elements in $S_\infty[E]$ are often represented as infinite matrices with entries in E.

To define $S_1[E]$ we use duality. The operator space structure to be put in $S_1[E]$ will be such that the dual space of $S_1[E]$ is $S_\infty[E^*]$. More precisely, let $u \in S_1 \otimes E$. Write

$$u = \sum_k a_k \otimes x_k \quad \text{with} \quad a_k \in S_1, \ x_k \in E.$$

Consider u as a linear functional on $S_\infty[E^*]$ as follows. For $v = \sum_j b_j \otimes \xi_j \in S_\infty \otimes E^*$ define

$$\langle u, v \rangle = \sum_{k,j} \langle a_k, b_j \rangle \langle x_k, \xi_j \rangle = \sum_{k,j} \mathrm{Tr}(a_k b_j^t) \, \xi_j(x_k).$$

Then the norm of u is defined to be the linear functional norm of u on $S_\infty[E^*]$, which coincides with the norm of u in $CB(S_\infty[E^*], \mathbb{C})$ (see Proposition 3.3). We define $S_1[E]$ to be the closure of $S_1 \otimes E$ with respect to this norm. Next, we have to introduce a norm $\| \cdot \|_n$ on $\mathbb{M}_n(S_1[E])$ for any n. This is now easy. As before, every $u \in \mathbb{M}_n(S_1 \otimes E)$ induces a linear map from $S_\infty[E^*]$ to $\mathbb{M}_n$. Then define

$$\|u\|_n = \|u\|_{CB(S_\infty[E^*], \mathbb{M}_n)}.$$

It is then routine to check that these norms satisfy Ruan's axioms. Therefore, $S_1[E]$ becomes an operator space.

Having defined $S_\infty[E]$ and $S_1[E]$, we define $S_p[E]$ by interpolation for any $1 < p < \infty$:

$$S_p[E] = \big(S_\infty[E], \ S_1[E]\big)_{1/p}.$$

The elements of $S_p[E]$ are often represented as infinite matrices with entries in E. It is not hard to show that finite matrices (i.e., those with only a finite number of nonzero entries) are dense in $S_p[E]$ for $p < \infty$.

The following theorem of Pisier is very useful. The reader is referred to [P2] for its proof.

Theorem 6.1. *Let* $1 \le p < \infty$.

i) *Any* $x = (x_{ij}) \in S_p[E]$ *admits a factorization* $x = ayb$ *with* $a, b \in S_{2p}$ *and* $y \in S_\infty[E]$. *Here the product is the usual matrix product. Moreover, we have*

$$\|x\|_{S_p[E]} = \inf_{x=ayb} \big\{ \|a\|_{2p} \, \|y\|_{S_\infty[E]} \, \|b\|_{2p} \big\}.$$

ii) *Conversely, for any* $x = (x_{ij}) \in S_\infty[E]$

$$\|x\|_{S_\infty[E]} = \sup \big\{ \|axb\|_{S_p[E]} \ : \ a, b \in S_{2p}, \ \|a\|_{2p} \le 1, \|b\|_{2p} \le 1 \big\}.$$

Corollary 6.2. *Let* E *and* F *be two operator spaces. Let* $1 \le p < \infty$. *Then a linear map* $u : E \to F$ *is c.b. iff*

$$\sup_n \big\| I_{S_p^n} \otimes u : S_p^n[E] \to S_p^n[F] \big\| < \infty;$$

moreover in this case the supremum above is equal to $\|u\|_{cb}$. *Alternatively,* u *is c.b. iff* $I_{S_p} \otimes u$ *extends to a bounded map from* $S_p[E]$ *to* $S_p[F]$.

Proof. Assume that u is c.b., i.e.,

$$\|u\|_{cb} = \sup_n \big\| I_{S_\infty^n} \otimes u : S_\infty^n[E] \to S_\infty^n[F] \big\| < \infty.$$

Let $x = (x_{ij})$ be a matrix in $S_p^n[E]$ with norm less than 1. Then x admits a factorization $x = ayb$ with

$$\|a\|_{S_{2p}^n} \le 1, \quad \|y\|_{S_\infty^n[E]} \le 1, \quad \|b\|_{S_{2p}^n} \le 1.$$

We have

$$I \otimes u(x) = a(I \otimes u)(y)b.$$

Therefore,

$$\big\| I \otimes u(x) \big\|_{S_p^n[F]} \le \|a\|_{S_{2p}^n} \big\| I \otimes u(y) \big\|_{S_\infty^n[F]} \|b\|_{S_{2p}^n} \le \|u\|_{cb}\,;$$

whence

$$\sup_n \big\| I_{S_p^n} \otimes u : S_p^n[E] \to S_p^n[F] \big\| \le \|u\|_{cb}\,.$$

The converse is proved similarly. □

The previous corollary is very useful notably for subspaces of noncommutative L_p-spaces for the following reason. Given $E \subset L_p(M)$ it is usually difficult to determine the norm of $\mathbb{M}_n(E)$; but it is extremely simple to describe the norm of $S_p[E]$, as shows the next paragraph.

We will only need the case where E is a subspace of a noncommutative $L_p(M)$ in which the previous theory becomes much simpler. Note that there is a natural algebraic identification of $L_p(\mathbb{M}_n \otimes M)$ with $\mathbb{M}_n(L_p(M))$. Then $S_p^n[L_p(M)]$ is nothing but the linear space $\mathbb{M}_n(L_p(M))$ equipped with the norm of $L_p(\mathbb{M}_n \otimes M)$. More generally, if $E \subset L_p(M)$ is a closed subspace, the norm of $S_p^n[E]$ is induced by that of $S_p^n[L_p(M)]$. In the infinite dimensional case, $S_p[L_p(M)]$ is completely isometrically identified with $L_p(B(\ell_2)\bar{\otimes}M)$ for all $1 \le p < \infty$. If $E \subset L_p(M)$, then $S_p[E]$ is the closure of $S_p \otimes E$ in $L_p(B(\ell_2)\bar{\otimes}M)$.

6.4 Column and Row p-spaces. The column and row spaces, C and R, are pillars of the whole theory of operator spaces. Recall that C and R are respectively the (first) column and row subspaces of S_∞. By analogy, let C_p (resp. R_p) denote the first column (resp. row) subspace of S_p. Since S_2 is an OH space, $C_2 \simeq R_2 \simeq OH$. The n-dimensional versions of these spaces are denoted by C_p^n and R_p^n.

Now let E be an operator space. We denote by $C_p[E]$ (resp. $R_p[E]$) the closure of $C_p \otimes E$ (resp. $R_p \otimes E$) in $S_p[E]$. If E is a subspace of a noncommutative $L_p(M)$, the norm of $C_p[E]$ is easy to determine. We consider only the case where M is semifinite. For any finite sequence $(x_k) \subset E$

$$\Big\|\sum_k x_k \otimes e_k\Big\|_{C_p[E]} = \Big\|\Big(\sum_k x_k^* x_k\Big)^{1/2}\Big\|_{L_p(M)},$$

where (e_k) denotes the canonical basis of C_p. More generally, if $a_k \in C_p$, then

$$\Big\|\sum_k x_k \otimes a_k\Big\|_{C_p[E]} = \Big\|\Big(\sum_{j,k}\langle a_j, a_k\rangle x_k^* x_j\Big)^{1/2}\Big\|_{L_p(M)},$$

where $\langle\ ,\ \rangle$ denotes the scalar product in C_p. (In terms of matrix product, $\langle a_j, a_k\rangle = a_k^* a_j$.) We also have a similar description for $R_p[E]$.

We end this section by describing the operator space structure of $C + R$ with help of Corollary 6.2. To this end we use the identification that $C \simeq R_1$ and $R \simeq C_1$ (see Exercise 2 below). Thus $C + R \simeq R_1 + C_1$, which is the quotient of $R_1 \oplus_1 C_1$ by the subspace $\{(x, y)\,;\ x + y = 0\}$. Therefore, for any finite sequence $(x_k) \subset S_1$

$$\begin{aligned}\big\|(x_k)\big\|_{S_1[C+R]} &= \inf\big\{\big\|(y_k)\big\|_{S_1[R_1]} + \big\|(z_k)\big\|_{S_1[C_1]}\big\}\\ &= \inf\Big\{\Big\|\Big(\sum_k \big(y_k y_k^*\big)^{1/2}\Big)\Big\|_{S_1} + \Big\|\Big(\sum_k \big(z_k^* z_k\big)^{1/2}\Big)\Big\|_{S_1}\Big\},\end{aligned}$$

where the infimum runs over all decompositions of $x_k = y_k + z_k$ in S_1. It follows that $S_1[C + R] = C_1[S_1] + R_1[S_1]$ with equal norms (even completely isometrically).

Exercises:

1) Let ℓ_1 have its natural operator space structure. Let $x \in \mathbb{M}_n(\ell_1)$ with $x = \sum_i x_i \otimes e_i$ (with (e_i) the canonical basis of ℓ_1). Prove

$$\|x\|_{\mathbb{M}_n(\ell_1)} = \sup\Big\{\big\|\sum_i x_i \otimes y_i\big\|_{\mathbb{M}_{mn}} \ : \ y_i \in \mathbb{M}_m, \|y_i\| \le 1, m \in \mathbb{N}\Big\}.$$

On the other hand, show $S_1[\ell_1] = \ell_1(S_1)$ completely isometrically.

2) Let $1 \le p \le \infty$ and p' be the conjugate index of p. Prove the following completely isometric identities:

$$(C_p)^* \cong C_{p'} \cong R_p \quad \text{and} \quad (R_p)^* \cong R_{p'} \cong C_p$$

by identifying the canonical bases in question.

3) Prove that C_p and R_p are homogeneous Hilbertian spaces.

4) Compute (or estimate) $d_{cb}(C_p^n,\ C_q^n)$ for $1 \le p, q \le \infty$. Then prove that C_p and C_q are not completely isomorphic for $p \ne q$.

7 Noncommutative Khintchine Type Inequalities

This section is devoted to Khintchine type inequalities in the noncommutative L_p-spaces. These inequalities are of paramount importance in operator space theory and noncommutative analysis.

7.1 The Classical Khintchine Inequalities. Let (ε_k) be a Rademacher sequence on a probability space (Ω, P), i.e., an independent sequence of random variables such that $P(\varepsilon_k = 1) = P(\varepsilon_k = -1) = 1/2$. The classical Khintchine inequality states that for any $1 \le p < \infty$ and any finite sequence $(x_n) \subset \mathbb{C}$

$$\big\|\sum_k x_k \varepsilon_k\big\|_p \sim_{c_p} \big\|\sum_k x_k \varepsilon_k\big\|_2 = \big(\sum_k |x_k|^2\big)^{1/2}. \tag{7.1}$$

Here as well as in the sequel we use $A \sim_c B$ to abbreviate $c^{-1}B \le A \le cB$. c_p denotes a positive constant depending only on p. Using the Fubini theorem, we deduce a similar inequality for coefficients x_n in a commutative L_p-space, say, in $L_p(0,1)$. Namely,

$$\big\|\sum_k x_k\, \varepsilon_k\big\|_{L_p(\Omega; L_p(0,1))} \sim_{c_p} \big\|\big(\sum_k |x_k|^2\big)^{1/2}\big\|_{L_p(0,1)}. \tag{7.2}$$

Note that the norm of $L_p(\Omega; L_p(0,1))$ in the above equivalence can be replaced by that of $L_q(\Omega; L_p(0,1))$ for any $1 \le q < \infty$. (The relevant constant then depends on q too.) This is because of the so-called Khintchine-Kahane inequalities (cf. [Ka]). Let E be a Banach space and $1 \le p, q < \infty$. Then for any finite sequence $(x_k) \subset E$ we have

$$\big\|\sum_k x_k\, \varepsilon_k\big\|_{L_p(\Omega; E)} \sim_{c_{p,q}} \big\|\sum_k x_k\, \varepsilon_k\big\|_{L_q(\Omega; E)}.$$

Now we wish to extend (7.2) to the noncommutative setting, i.e., replacing $L_p(0,1)$ by a noncommutative L_p. We will consider only the case where the coefficients x_k are in the Schatten classes S_p. All inequalities stated below are valid for general noncommutative L_p. On the other hand, we will concentrate mainly on the case $p=1$ (and the case $p=\infty$ in the free case). Thus our goal is to find a deterministic expression for

$$\big\|\sum x_k\varepsilon_k\big\|_{L_p(\Omega;S_p)}\,.$$

In view of the square function $\big(\sum|x_k|^2\big)^{1/2}$ in (7.2), we are naturally led to conjecture that the deterministic expression to be found should involve the term

$$\big\|\big(\sum|x_k|^2\big)^{1/2}\big\|_p=\big\|\big(\sum x_k^*x_k\big)^{1/2}\big\|_p\,.$$

This norm is also equal to $\|(x_k)\|_{C_p[S_p]}$. Here and in the sequel, we often identify a sequence (x_k) in E with the element $\sum_k x_k\otimes e_k$ in $C_p[E]$ or $R_p[E]$. But now because of the noncommutativity, we should also take into account the right modulus, i.e., the term

$$\big\|\big(\sum|x_k^*|^2\big)^{1/2}\big\|_p=\big\|\big(\sum x_kx_k^*\big)^{1/2}\big\|_p=\|(x_k)\|_{R_p[S_p]}\,.$$

Although $\|a\|_p=\|a^*\|_p$ for a *single* operator $a\in S_p$, the two terms above are not comparable at all if $p\neq 2$. For example, if $x_k=e_{k1}$, then clearly

$$\big\|\big(\sum_{k=1}^n x_k^*x_k\big)^{1/2}\big\|_p=n^{1/2}\quad\text{and}\quad\big\|\big(\sum_{k=1}^n x_kx_k^*\big)^{1/2}\big\|_p=n^{1/p}\,.$$

7.2 Column and Row Subspaces. In this subsection we collect some basic properties of the column and row subspaces $C_p[S_p]$ and $R_p[S_p]$.

Proposition 7.1. i) *The Hölder inequality: Let $1\le p,q,r\le\infty$ such that $1/r=1/p+1/q$. Then for any sequences $(x_k)\in C_p[S_p]$ and $(y_k)\in C_q[S_q]$ the series $\sum_k y_k^*x_k$ converges in S_r (with respect to the w^*-topology if $r=\infty$) and*

$$\big\|\sum_k y_k^*x_k\big\|_r\le\big\|(x_k)\big\|_{C_p[S_p]}\,\big\|(y_k)\big\|_{C_q[S_q]}\,.$$

ii) *Complementation: $C_p[S_p]$ and $R_p[S_p]$ are 1-complemented subspaces of $S_p(\ell_2\otimes\ell_2)$ for any $1\le p\le\infty$. More precisely, let $P:\ S_p(\ell_2\otimes\ell_2)\to S_p(\ell_2\otimes\ell_2)$ be defined by $P(x)=xe$, where $e=1\otimes e_{11}$. Then P is a contractive projection from $S_p(\ell_2\otimes\ell_2)$ onto $C_p[S_p]$.*

iii) *Duality: Let $1\le p<\infty$, and let p' be the conjugate index of p. Then*

$$C_p[S_p]^*=C_{p'}[S_{p'}]\quad\textit{and}\quad R_p[S_p]^*=R_{p'}[S_{p'}]$$

isometrically with respect to the anti-linear duality bracket:

$$\langle (x_k), (y_k)\rangle \mapsto \sum_{k\geq 1} \operatorname{Tr}(y_k^* x_k).$$

Proof. i) Given $(x_k) \subset S_p$ define

$$T((x_k)) = \begin{pmatrix} x_1 & 0 & \cdots \\ x_2 & 0 & \cdots \\ \vdots & \vdots & \end{pmatrix}.$$

We view $T((x_k))$ as an element in $S_p[S_p] = S_p(\ell_2 \otimes \ell_2)$. Now let $(y_k) \subset S_q$ be another finite sequence. Then

$$\sum_k y_k^* x_k = T((y_k))^* \, T((x_k)).$$

So the desired inequality follows from the Hölder inequality in $S_p(\ell_2 \otimes \ell_2)$.

ii) This is obvious. Note that $P(x)$ is the matrix whose first column is that of x and all others are zero.

iii) Using i) one sees that the duality is well-defined. The two duality equalities are immediate consequences of ii) and the duality between $S_p(\ell_2 \otimes \ell_2)$ and $S_{p'}(\ell_2 \otimes \ell_2)$. □

Proposition 7.2. *Let* $1 \leq p \leq \infty$ *and* $(x_k) \subset S_p$ *be a finite sequence.*

i) *If* $2 \leq p \leq \infty$*, then*

$$\max\left\{\big\|(x_k)\big\|_{C_p[S_p]},\ \big\|(x_k)\big\|_{R_p[S_p]}\right\} \leq \Big(\sum_k \|x_k\|_p^2\Big)^{1/2}.$$

ii) *If* $1 \leq p \leq 2$*, then*

$$\min\left\{\big\|(x_k)\big\|_{C_p[S_p]},\ \big\|(x_k)\big\|_{R_p[S_p]}\right\} \geq \Big(\sum_k \|x_k\|_p^2\Big)^{1/2}.$$

Proof. i) Let $p \geq 2$. By the triangle inequality in $S_{p/2}$ we have

$$\big\|(x_k)\big\|_{C_p[S_p]}^2 = \Big\|\sum_k |x_k|^2\Big\|_{p/2} \leq \sum_k \|x_k\|_p^2.$$

Passing to adjoints we get the inequality on the row norm.

ii) This follows from i) by duality. □

Corollary 7.3. i) *Let* (Σ, μ) *be a measure space, and let* f *belong to the algebraic tensor product* $L_2(\Sigma) \otimes S_p$*. Then if* $2 \leq p \leq \infty$*,*

$$\max\left\{\Big\|\Big[\int_\Sigma f(t)^* f(t) d\mu(t)\Big]^{1/2}\Big\|_p,\ \Big\|\Big[\int_\Sigma f(t) f(t)^* d\mu(t)\Big]^{1/2}\Big\|_p\right\} \leq \|f\|_{L_2(\Sigma; S_p)}.$$

and if $1 \le p \le 2$,

$$\|f\|_{L_2(\Sigma;S_p)} \le \min\big\{\big\|\big[\int_\Sigma f(t)^* f(t) d\mu(t)\big]^{1/2}\big\|_p,\ \big\|\big[\int_\Sigma f(t) f(t)^* d\mu(t)\big]^{1/2}\big\|_p\big\}.$$

ii) *In particular, if* (φ_k) *is an orthonormal sequence in* $L_2(\Sigma)$ *and* (x_k) *a finite sequence in* S_p*, then for* $2 \le p \le \infty$

$$\max\big\{\big\|(x_k)\big\|_{C_p[S_p]},\ \big\|(x_k)\big\|_{R_p[S_p]}\big\} \le \big\|\sum_k x_k\varphi_k\big\|_{L_2(\Sigma;S_p)};$$

and for $1 \le p \le 2$

$$\big\|\sum_k x_k\varphi_k\big\|_{L_2(\Sigma;S_p)} \le \inf\big\{\big\|(y_k)\big\|_{C_p[S_p]} + \big\|(z_k)\big\|_{R_p[S_p]}\big\},$$

where the infimum runs over all decompositions $x_k = y_k + z_k$ *with* y_k *and* z_k *in* S_p.

Proof. i) Note that since $f \in L_2(\Sigma) \otimes S_p$, the two integrals

$$\int_\Sigma f(t)^* f(t) d\mu(t) \quad \text{and} \quad \int_\Sigma f(t) f(t)^* d\mu(t)$$

are well-defined and belong to $S_{p/2}$. The desired inequalities follow from the corresponding ones in the previous proposition.

ii) The first inequality immediately follows from i) above. To prove the second take a decomposition $x_k = y_k + z_k$. Then again by the previous proposition

$$\begin{aligned}\big\|\sum_k x_k\varphi_k\big\|_{L_2(\Sigma;S_p)} &\le \big\|\sum_k y_k\varphi_k\big\|_{L_2(\Sigma;S_p)} + \big\|\sum_k z_k\varphi_k\big\|_{L_2(\Sigma;S_p)}\\ &\le \big\|(y_k)\big\|_{C_p[S_p]} + \big\|(z_k)\big\|_{R_p[S_p]};\end{aligned}$$

whence the desired inequality. □

Recall that (C, R) is considered as a compatible pair by identifying their canonical bases with that of ℓ_2. This identification is extended to all spaces C_p and R_p. Thus any pair (C_p, R_q) is also compatible. Then the maximum and infimum in Corollary 7.3, ii) are respectively $\|(x_k)\|_{C_p[S_p]\cap R_p[S_p]}$ and $\|(x_k)\|_{C_p[S_p]+R_p[S_p]}$. For notational simplicity, we introduce the following

Definition 7.4. For $1 \le p \le \infty$ define

$$CR_p[S_p] = C_p[S_p]\cap R_p[S_p] \text{ if } p \ge 2 \quad \text{and} \quad CR_p[S_p] = C_p[S_p]+R_p[S_p] \text{ if } p < 2.$$

Since $C_p[S_p] = S_p[C_p]$ and $R_p[S_p] = S_p[R_p]$,

$$C_p[S_p] \cap R_p[S_p] = S_p[C_p \cap R_p] \quad \text{and} \quad C_p[S_p] + R_p[S_p] = S_p[C_p + R_p]$$

with equivalent norms; moreover, the equivalence constants are controlled by a universal one. By Corollary 6.2, these identities are also completely isomorphic. Thus if we define $CR_p = C_p \cap R_p$ for $p \geq 2$ and $CR_p = C_p + R_p$ for $p < 2$, we obtain $CR_p[S_p] = S_p[CR_p]$ with complete equivalent norms.

We are now well prepared for our noncommutative Khintchine inequalities.

7.3 Rademacher Sequences. The following is the noncommutative Khintchine inequality for Rademacher variables (ε_k) due to Lust-Piquard and Pisier.

Theorem 7.5. *Let $1 \leq p < \infty$ and (x_k) be a finite sequence in S_p. Then*

$$\Big\| \sum_k x_k \varepsilon_k \Big\|_{L_p(\Omega; S_p)} \sim_{c_p} \big\| (x_k) \big\|_{CR_p[S_p]} .$$

More precisely,

i) *if $2 \leq p < \infty$, then*

$$\big\| (x_k) \big\|_{CR_p[S_p]} \leq \Big\| \sum_k x_k \varepsilon_n \Big\|_{L_p(\Omega; S_p)} \leq c\sqrt{p} \, \big\| (x_k) \big\|_{CR_p[S_p]} ;$$

ii) *if $1 \leq p < 2$, then*

$$c^{-1} \big\| (x_k) \big\|_{CR_p[S_p]} \leq \Big\| \sum_k x_k \varepsilon_k \Big\|_{L_p(\Omega; S_p)} \leq \big\| (x_k) \big\|_{CR_p[S_p]} ,$$

where c is a universal positive constant.

Proof. The lower estimate in i) and the upper estimate in ii) follow from Corollary 7.3. We will prove only the lower estimate in ii) for $p = 1$, following the recent approach of Haagerup and Musat [HM]. The reader is referred to [LPP] for the proof of all remaining cases and to [P2] for the optimal order of the best constant for the upper estimate in i).

By duality, the lower estimate of ii) for $p = 1$ is equivalent to the following statement:

$(*)$For any finite sequence $(x_k) \subset S_\infty$ there exists a function $f \in L_\infty(\Omega; S_\infty)$ such that

$$\widehat{f}(\varepsilon_k) = x_k \quad \text{and} \quad \|f\|_{L_\infty(\Omega; S_\infty)} \leq c \, \big\| (x_k) \big\|_{CR_\infty[S_\infty]} ,$$

where $\widehat{f}(\varepsilon_k) = \mathbb{E}(f \varepsilon_k)$ with $\mathbb{E}$ denoting the expectation on the probability space (Ω, P).

Let $x_k \in S_\infty$ be selfadjoint and such that $\big\| (x_k) \big\|_{CR_\infty[S_\infty]} \leq 1$. Let

$$g = \sum_k \varepsilon_k x_k .$$

Then

$$g^2 = \sum_k x_k^2 + \sum_{j<k} \varepsilon_j \varepsilon_k (x_j x_k + x_k x_j)$$

and

$$\begin{aligned}\mathbb{E}(g^4) &= \big(\sum_k x_k^2\big)^2 + \sum_{j<k} (x_j x_k + x_k x_j)^2 \\ &\le 1 + 2\sum_{j<k} (x_j x_k^2 x_j + x_k x_j^2 x_k) \\ &= 1 + 2\sum_j x_j \big(\sum_{k\neq j} x_k^2\big) x_j \le 3.\end{aligned}$$

Now let λ be a positive number to be determined later. Set

$$f_\lambda = g\mathbb{1}_{[-\lambda,\,\lambda]}(g) \quad \text{and} \quad g_\lambda = g - f_\lambda\,,$$

where $\mathbb{1}_{[-\lambda,\,\lambda]}(g)$ denotes the spectral projection of g corresponding to the interval $[-\lambda,\ \lambda]$. By definition, $\|f_\lambda\|_{L_\infty(\Omega;S_\infty)} \le \lambda$. On the other hand, letting $z_k = \mathbb{E}(g_\lambda \varepsilon_k)$, we have

$$\sum_k z_k^2 \le \mathbb{E}(g_\lambda^2).$$

However,

$$\lambda^2 g_\lambda^2 \le g^4\,.$$

Therefore, combining the preceding inequalities, we find

$$\big\|\big(\sum_k z_k^2\big)^{1/2}\big\|_\infty \le \big\|\big(\mathbb{E}(g_\lambda^2)\big)^{1/2}\big\|_{L_\infty(\Omega;S_\infty)} \le \lambda^{-1}\big\|\big(\mathbb{E}(g^4)\big)^{1/2}\big\|_{L_\infty(\Omega;S_\infty)} \le \frac{\sqrt{3}}{\lambda}.$$

For $\lambda = 2\sqrt{3}$ let

$$f^{(0)} = f_\lambda\,, \quad x_k^{(0)} = \mathbb{E}(f^{(0)}\varepsilon_k), \quad z_k^{(0)} = z_k.$$

Then

$$x_k = x_k^{(0)} + z_k^{(0)}\,, \quad \|f^{(0)}\|_{L_\infty(\Omega;S_\infty)} \le 2\sqrt{3}\,, \quad \big\|\big(z_k^{(0)}\big)\big\|_{CR_\infty[S_\infty]} \le \frac{1}{2}\,.$$

Repeating the same argument with $2z_k^{(0)}$ instead of x_k, we find a function $f^{(1)}$ and a finite sequence $\big(z_k^{(1)}\big)$ such that

$$2z_k^{(0)} = x_k^{(1)} + z_k^{(1)}\,, \quad \|f^{(1)}\|_{L_\infty(\Omega;S_\infty)} \le 2\sqrt{3}\,, \quad \big\|\big(z_k^{(1)}\big)\big\|_{CR_\infty[S_\infty]} \le \frac{1}{2}\,,$$

where

$$x_k^{(1)} = \mathbb{E}(f^{(1)}\varepsilon_k)\,.$$

Continuing this procedure we obtain a sequence $\left(f^{(n)}\right)$ of functions in $L_\infty(\Omega; S_\infty)$ and a sequence $\left(x_k^{(n)}\right)$ in S_∞ such that

$$x_k = \sum_{n\geq 0} 2^{-n} x_k^{(n)}, \quad \|f^{(n)}\|_{L_\infty(\Omega;S_\infty)} \leq 2\sqrt{3}, \quad x_k^{(n)} = \mathbb{E}(f^{(n)}\varepsilon_k).$$

Put

$$f = \sum_{n\geq 0} 2^{-n} f^{(n)}.$$

Then

$$\|f\|_{L_\infty(\Omega;S_\infty)} \leq 4\sqrt{3} \quad \text{and} \quad x_k = \mathbb{E}(f\varepsilon_k).$$

Thus the statement $(*)$ is proved for selfadjoint x_k. The general case is easily reduced to the selfadjoint one by decomposing each x_k into its real and imaginary parts. Note that the final constant c obtained in this way is $8\sqrt{3}$. We refer to [HM] for a more careful argument which yields $\sqrt{3}$ as constant. □

Remark 7.6. Let $\mathcal{R}_p$ be the closed subspace of $L_p(\Omega)$ generated by the ε_k. Using Corollary 6.2, we can rephrase Theorem 7.5 as the fact that $\mathcal{R}_p$ is completely isomorphic to CR_p. This remark also applies to Theorems 7.8 and 7.9 below.

Remark 7.7. The Rademacher sequence (ε_k) can be replaced by a standard Gaussian sequence. More generally, let (φ_k) be an independent sequence of random variables on (Ω, P). Assume that (φ_k) is symmetric in the sense that (φ_k) has the same distribution as $(\pm\varphi_k)$ for any sequence of signs. Assume further that

$$0 < \inf_k \|\varphi_k\|_p, \quad \sup_k \|\varphi_k\|_2 < \infty \quad \text{for } 1 \leq p < 2$$

and

$$0 < \inf_k \|\varphi_k\|_2, \quad \sup_k \|\varphi_k\|_p < \infty \quad \text{for } 2 \leq p < \infty.$$

Then Theorem 7.5 holds for (φ_k) instead of (ε_k) with relevant constants depending on (φ_k) too.

Since now we are in the noncommutative setting, it is natural to consider Khintchine type inequalities for noncommutative random variables instead of (ε_k). We first consider the tracial case by giving two important examples. Namely, free generators and semicircular systems. We start with free generators.

7.4 Free Generators. Consider a discrete group G. Let $(\delta_g)_{g\in G}$ be the canonical basis of $\ell_2(G)$, i.e., δ_g is the function on G that takes value 1 at g

and zero elsewhere. Let $\lambda :\ G \to B(\ell_2(G))$ be the left regular representation. Namely, for any $g \in G$, $\lambda(g)$ is the unitary operator on $\ell_2(G)$ defined by

$$\big(\lambda(g)\varphi\big)(h) = \varphi(g^{-1}h), \quad h, g \in G,\ \varphi \in \ell_2(G).$$

Note that $\lambda(g)\delta_h = \delta_{gh}$ for all $g, h \in G$. Then the group von Neumann algebra $VN(G)$ is the von Neumann subalgebra of $B(\ell_2(G))$ generated by $\{\lambda(g)\ :\ g \in G\}$. Namely, $VN(G)$ is the w*-closure of all finite sums $\sum \alpha_g \lambda(g)$ with $\alpha_g \in \mathbb{C}$. $VN(G)$ also coincides with the left convolution algebra of $\ell_2(G)$. Recall that if $\varphi, \psi \in \ell_2(G)$, their convolution is defined by

$$\varphi * \psi(g) = \sum_{h \in G} \varphi(h)\psi(h^{-1}g), \quad g \in G.$$

Then $x \in VN(G)$ iff there exists $\varphi \in \ell_2(G)$ such that $x\psi = \varphi * \psi$ for every $\psi \in \ell_2(G)$. Let τ_G be the vector state on $VN(G)$ determined by δ_e, i.e., $\tau_G(x) = \langle x\delta_e,\ \delta_e\rangle$ for any $x \in VN(G)$. Then it is easy to check that τ_G is faithful and tracial.

If we identify an operator $x \in VN(G)$ with its symbol $x\delta_e$ in $\ell_2(G)$, then $L_2(VN(G))$ is nothing but $\ell_2(G)$. $L_1(VN(G))$ is traditionally called the Fourier algebra of G and denoted by $A(G)$. Since an operator in $L_1(VN(G))$ is a product of two operators in $L_2(VN(G))$, a function φ on G belongs to $A(G)$ iff there exist two functions $\psi,\ \rho \in \ell_2(G)$ such that $\varphi = \psi\,\rho$. We refer to [KR] for more information.

If G is abelian, $VN(G)$ ie equal to $L_\infty(\widehat{G})$, so is commutative, where $\widehat{G}$ is the dual group of G.

An important example of non abelian groups is a free group $\mathbb{F}$ on n generators (g_k) with $n \in \mathbb{N} \cup \{\infty\}$. The sequence $(\lambda(g_k))_k$ of the unitary operators given by the generators is of particular interest. With a slight abuse of terminology, we will also call it a *sequence of free generators* . Note that $(\lambda(g_k))_k$ is orthonormal in $L_2(VN(\mathbb{F}))$. Let us determine its linear span in $VN(\mathbb{F})$. To this end let F_k be the closed subspace of $\ell_2(\mathbb{F})$ generated by all those basic vectors δ_g for which g is a reduced word starting with g_k^{-1}. The F_k, $k = 1, 2, ...$, are mutually orthogonal. Let $\mathcal{F}_k$ be the orthogonal projection from $\ell_2(\mathbb{F})$ onto F_k. Now, given a finite sequence $(\alpha_k) \subset \mathbb{C}$ write

$$\sum_k \alpha_k \lambda(g_k) = \sum_k \alpha_k \lambda(g_k)\mathcal{F}_k + \sum_k \alpha_k \lambda(g_k)\mathcal{F}_k^{\perp}\,.$$

By the mutual orthogonality of the $\mathcal{F}_k$, we have

$$\begin{aligned}\big\|\sum_k \alpha_k \lambda(g_k)\mathcal{F}_k\big\|_\infty^2 &= \big\|(\sum_k \alpha_k \lambda(g_k)\mathcal{F}_k)(\sum_k \alpha_k \lambda(g_k)\mathcal{F}_k)^*\big\|_\infty \\ &= \big\|\sum_k |\alpha_k|^2 \lambda(g_k)\mathcal{F}_k \lambda(g_k)^*\big\|_\infty \le \sum_k |\alpha_k|^2\,.\end{aligned}$$

To treat another term, observe that for $k \neq j$ the range of $\lambda(g_k)^* \lambda(g_j) \mathcal{F}_j^\perp$ is contained in F_k, so $\mathcal{F}_k^\perp \lambda(g_k)^* \lambda(g_j) \mathcal{F}_j^\perp = 0$. Then it follows that

$$\Big\| \sum_k \alpha_k \lambda(g_k) \mathcal{F}_k^\perp \Big\|_\infty^2 = \Big\| \big(\sum_k \alpha_k \lambda(g_k) \mathcal{F}_k^\perp\big)^* \big(\sum_k \alpha_k \lambda(g_k) \mathcal{F}_k^\perp\big) \Big\|_\infty$$
$$= \Big\| \sum_k |\alpha_k|^2 \mathcal{F}_k^\perp \Big\|_\infty \le \sum_k |\alpha_k|^2 .$$

Therefore,

$$\Big\| \sum_k \alpha_k \lambda(g_k) \Big\|_\infty \le 2 \big(\sum_k |\alpha_k|^2 \big)^{1/2} .$$

The converse inequality with constant 1 is obvious for

$$\Big\| \sum_k \alpha_k \lambda(g_k) \Big\|_\infty \ge \Big\| \sum_k \alpha_k \lambda(g_k) \Big\|_2 = \big(\sum_k |\alpha_k|^2 \big)^{1/2} .$$

Consequently, for any $1 \le p \le \infty$ the closed subspace generated by the $\lambda(g_k)$ in $L_p(VN(\mathbb{F}))$ is isomorphic to ℓ_2. More precisely, for any finite sequence $(\alpha_k) \subset \mathbb{C}$,

$$\Big\| \sum_k \alpha_k \lambda(g_k) \Big\|_p \sim_c \big(\sum_k |\alpha_k|^2 \big)^{1/2} ,$$

where c is a universal constant. This inequality remains true if the scalar coefficients (α_k) are replaced by operator coefficients. The resulting inequalities are the Khintchine inequality for free generators . In the following statement $L_p(B(\ell_2) \bar{\otimes} VN(\mathbb{F}))$ is the noncommutative L_p-space associated with the von Neumann tensor product $B(\ell_2) \bar{\otimes} VN(\mathbb{F})$, equipped with the tensor trace $\mathrm{Tr} \otimes \tau_{\mathbb{F}}$, which is a normal semifinite faithful trace. Note that

$$L_p(B(\ell_2) \bar{\otimes} VN(\mathbb{F})) = S_p[L_p(VN(\mathbb{F}))].$$

The following theorem is due to Haagerup/Pisier [HP] for $p = \infty, 1$ and to Pisier [P2] for $1 < p < \infty$.

Theorem 7.8. *Let $1 \le p \le \infty$ and (x_k) be a finite sequence in S_p. Then*

$$\Big\| \sum_k x_k \otimes \lambda(g_k) \Big\|_{L_p(B(\ell_2) \bar{\otimes} VN(\mathbb{F}))} \sim_c \big\| (x_k) \big\|_{CR_p[S_p]} \tag{7.3}$$

with a universal constant c. Moreover, the closed subspace of $L_p(VN(\mathbb{F}))$ generated by the $\lambda(g_k)$ is completely complemented in $L_p(VN(\mathbb{F}))$ with relevant constant ≤ 2.

Proof. Here we prove (7.3) only in the cases $p = \infty, 1$ and the complementation assertion. The remaining cases are postponed to subsection 7.6. For $p = \infty$ we have the following inequalities

$$\big\|(x_k)\big\|_{CR_\infty[S_\infty]} \le \big\|\sum_k x_k \otimes \lambda(g_k)\big\|_{B(\ell_2)\bar{\otimes}VN(\mathbb{F})} \le 2\big\|(x_k)\big\|_{CR_\infty[S_\infty]} \tag{7.4}$$

for any finite sequence $(x_k) \subset S_\infty$. The proof of the second inequality above is the same as in the scalar case. Let us show the first one. Take a unit vector $\xi \in \ell_2$. Then

$$\begin{aligned}\big\|\sum_k x_k \otimes \lambda(g_k)\big\|_\infty^2 &\ge \langle \sum_k x_k \otimes \lambda(g_k)(\xi \otimes \delta_e),\ \sum_k x_k \otimes \lambda(g_k)(\xi \otimes \delta_e)\rangle \\ &= \langle \sum_k x_k(\xi) \otimes \delta_{g_k},\ \sum_k x_k(\xi) \otimes \delta_{g_k}\rangle \\ &= \sum_k \langle x_k(\xi),\ x_k(\xi)\rangle = \langle \sum_k x_k^* x_k(\xi),\ \xi\rangle;\end{aligned}$$

whence

$$\big\|\big(\sum_k x_k^* x_k\big)^{1/2}\big\|_\infty \le \big\|\sum_k x_k \otimes \lambda(g_k)\big\|_\infty .$$

Taking adjoints, we find

$$\big\|\big(\sum_k x_k x_k^*\big)^{1/2}\big\|_\infty \le \big\|\sum_k x_k \otimes \lambda(g_k)\big\|_\infty .$$

Therefore, the lower estimate of (7.4) is proved.

Dualizing (7.4), we get the case $p = 1$:

$$\frac{1}{2}\big\|(x_k)\big\|_{CR_1[S_1]} \le \big\|\sum_k x_k \otimes \lambda(g_k)\big\|_{L_1(B(\ell_2)\bar{\otimes}VN(\mathbb{F}))} \le \big\|(x_k)\big\|_{CR_1[S_1]} \tag{7.5}$$

for any finite sequence $(x_k) \subset S_1$. Indeed, let $(y_k) \subset S_\infty$ be such that

$$\big\|(x_k)\big\|_{CR_1[S_1]} = \sum_k \mathrm{Tr}(y_k^* x_k) \quad \text{and} \quad \big\|(y_k)\big\|_{CR_\infty[S_\infty]} \le 1$$

(see Proposition 7.1 iii)). Set

$$x = \sum_k x_k \otimes \lambda(g_k) \in L_1(B(\ell_2)\bar{\otimes}VN(\mathbb{F})), \quad y = \sum_k y_k \otimes \lambda(g_k) \in B(\ell_2)\bar{\otimes}VN(\mathbb{F}).$$

Then by (7.4)

$$\sum_k \mathrm{Tr}(y_k^* x_k) = \mathrm{Tr} \otimes \tau_{\mathbb{F}}(y^* x) \le \|y\|_\infty \|x\|_1 \le 2\|(y_k)\|_{CR_\infty[S_\infty]} \|x\|_1 \le 2\|x\|_1 .$$

This is the lower estimate of (7.5). To show the upper estimate we consider the projection P from the algebra of all finite sums $\sum \alpha_g \lambda(g)$ with $\alpha_g \in \mathbb{C}$ onto the linear span of the $\lambda(g_k)$. Let $Q = I - P$. It is easy to see that $P(x)$ and $Q(x)$ are orthogonal relative to the scalar product of $L_2(VN(\mathbb{F}))$. Thus the extension of P on $L_2(VN(\mathbb{F}))$ is the orthogonal projection from $L_2(VN(\mathbb{F}))$ onto the closed subspace generated by the $\lambda(g_k)$. Now let $x = \sum_{g\in\mathbb{F}} x_g \otimes \lambda(g)$ be a finite sum with $x_g \in S_\infty$. Write

$$x = \mathrm{id}_{S_\infty} \otimes P(x) + \mathrm{id}_{S_\infty} \otimes Q(x) = \sum_k x_k \otimes \lambda(g_k) + \mathrm{id}_{S_\infty} \otimes Q(x).$$

Then using the argument yielding the first inequality of (7.4), we get

$$\big\|(x_k)\big\|_{CR_\infty[S_\infty]} \le \|x\|_\infty \,. \tag{7.6}$$

Together with a duality argument as above, this inequality implies the upper estimate of (7.5).

Combining (7.4) and (7.6), we get

$$\|P(x)\|_\infty \le 2\|x\|_\infty \,.$$

On the other hand, note that

$$\mathrm{Tr} \otimes \tau_{\mathbb{F}}(y^* P(x)) = \mathrm{Tr} \otimes \tau_{\mathbb{F}}(P(y)^* x)$$

for all finite sums $x = \sum_{g\in\mathbb{F}} x_g \otimes \lambda(g)$ and $y = \sum_{g\in\mathbb{F}} y_g \otimes \lambda(g)$ with $x_g \in S_\infty$ and $y_g \in S_1$. We then deduce that P extends to a completely bounded map P_1 on $L_1(VN(\mathbb{F}))$ (with $\|P_1\|_{cb} \le 2$), which is a pre-adjoint of P. This implies that P extends to a completely bounded normal projection on $VN(\mathbb{F})$. Note that P_1 coincides with P on the family of finite sums as above, which allows us to denote P_1 still by P. Finally, by interpolation P extends to a complete bounded projection on $L_p(VN(\mathbb{F}))$ for every $1 < p < \infty$. □

7.5 Semicircular Systems. Let H be a complex Hilbert space. The associated free (or full) Fock space is defined by

$$\mathcal{F}(H) = \bigoplus_{n\ge 0} H^{\otimes n},$$

where $H^{\otimes 0} = \mathbb{C}\mathbb{1}$ ($\mathbb{1}$ being a unit vector, called vacuum), and $H^{\otimes n}$ is the n-th Hilbertian tensor power of H for $n \ge 1$. The (left) creator associated with a vector $\xi \in H$ is the operator on $\mathcal{F}(H)$ uniquely determined by

$$c(\xi)\, \eta_1 \otimes \cdots \otimes \eta_n = \xi \otimes \eta_1 \otimes \cdots \otimes \eta_n$$

for any $\eta_1, ..., \eta_n \in H$. Here $\eta_1 \otimes \cdots \otimes \eta_n$ is understood as the vacuum $\mathbb{1}$ if $n = 0$. It is clear that $c(\xi)$ is bounded and $\|c(\xi)\| = \|\xi\|$. The adjoint of $c(\xi)$ is given by

$$c(\xi)^*\, \eta_1 \otimes \cdots \otimes \eta_n = \langle \eta_1,\ \xi\rangle\, \eta_2 \otimes \cdots \otimes \eta_n$$

for any $\eta_1, ..., \eta_n \in H$ with $n \ge 1$ and $c(\xi)^*\mathbb{1} = 0$. This is the annihilator associated with ξ and is denoted by $a(\xi)$. Note that the map $\xi \mapsto c(\xi)$ is linear, while $\xi \mapsto a(\xi)$ is anti-linear. We have the following free commutation relation:

$$a(\eta)c(\xi) = \langle \xi,\ \eta \rangle 1, \quad \forall\, \xi,\ \eta \in H. \tag{7.7}$$

Now assume that H is the complexification of a real Hilbert space $H_{\mathbb{R}}$. The vectors in $H_{\mathbb{R}}$ are called *real.* Let $\xi \in H$ be real and define

$$s(\xi) = c(\xi) + a(\xi).$$

$s(\xi)$ is a *semicircular element* in Voiculescu's sense. We will also call it a *free Gaussian variable* . Note that the map $\xi \mapsto s(\xi)$ is real linear from $H_{\mathbb{R}}$ into $B(\mathcal{F}(H))$. Then the *free von Neumann algebra* $\Gamma(H)$ associated with H is the von Neumann subalgebra of $B(\mathcal{F}(H))$ generated by all $s(\xi)$ with real $\xi \in H$:

$$\Gamma_0(H) = \big\{ s(\xi) : \xi \in H_{\mathbb{R}} \big\}'' \subset B(\mathcal{F}(H))\,.$$

The vector state τ_0 defined by the vacuum, $x \mapsto \langle x\mathbb{1},\ \mathbb{1} \rangle$ is faithful and tracial on $\Gamma_0(H)$. We refer to [VDN] for more information.

Let us mention some basic properties of free Gaussian variables. Let $\xi \in H$ be a unit real vector. By definition, $s(\xi)$ is selfadjoint; its spectrum is $[-2, 2]$ and the corresponding measure induced by τ_0 is the so-called Wigner measure

$$d\mu(t) = \frac{1}{2\pi}\sqrt{4-t^2}\,dt.$$

Thus for any $1 \le p < \infty$

$$\big\| s(\xi) \big\|_p = \Big[\int_{-2}^{2} |t|^p \sqrt{4-t^2}\,\frac{dt}{2\pi} \Big]^{1/p}.$$

Therefore,

$$\big\| s(\xi) \big\|_\infty = 2, \quad \big\| s(\xi) \big\|_2 = 1, \quad \big\| s(\xi) \big\|_1 = \frac{8}{3\pi}\,.$$

Now let (ξ_k) be an orthonormal sequence of real vectors of H. $(s(\xi_k))$ is then called a *standard semicircular system.* Like the classical standard Gaussian variables, $(s(\xi_k))$ has the following invariance property. Let $(\alpha_k) \subset \mathbb{R}$ be such that $\sum_k |\alpha_k|^2 = 1$. Then $\sum_n \alpha_k s(\xi_k)$ (convergence in the strong operator topology) is again a free Gaussian variable, i.e., $s(\xi)$ with $\xi = \sum_k \alpha_k\,\xi_k$. More generally, if $s(\xi_1), ..., s(\xi_n)$ is a standard semicircular system and $u = (u_{jk})$ an orthogonal $n \times n$ matrix, then

$$\big(\sum_{k=1}^{n} u_{jk} s(\xi_k) \big)_{1 \le j \le n}$$

is still a standard semicircular system. Indeed,

$$\sum_{k=1}^{n} u_{jk} s(\xi_k) = s(\sum_{k=1}^{n} u_{jk}\,\xi_k) = s(\eta_j),$$

where $\eta_j = \sum_k u_{jk}\, \xi_k$. The η_j form an orthonormal family. This orthogonal invariance implies that if $(s(\xi_k))$ is a standard semicircular system, then for $(\alpha_k) \subset \mathbb{R}$ such that $\sum_k |\alpha_k|^2 < \infty$ and any $1 \le p \le \infty$

$$\big\| \sum_{k\ge 1} \alpha_k\, s(\xi_k) \big\|_p = \big(\sum_{k\ge 1} |\alpha_k|^2 \big)^{1/2} \big\| s(\xi) \big\|_p \, .$$

In particular, $(s(\xi_k))$ is an orthonormal sequence in $L_2(\Gamma(H))$.

For simplicity we now assume that H is infinite dimensional and separable and put $\Gamma_0 = \Gamma_0(H)$. Let (e_k) be an orthonormal basis of H and set $s_k = s(e_k)$. Thus (s_k) is a semicircular sequence and Γ_0 is generated by the s_k. The following inequality for semicircular systems comes from [P2] .

Theorem 7.9. *Let $1 \le p \le \infty$ and (x_k) be a finite sequence in S_p. Then*

$$\big\| \sum_k x_k \otimes s_k \big\|_{L_p(B(\ell_2)\bar{\otimes}\Gamma_0)} \sim_c \big\| (x_k) \big\|_{CR_p[S_p]} \, . \tag{7.8}$$

Moreover, the closed subspace of $L_p(\Gamma_0)$ generated by the s_k is completely complemented in $L_p(\Gamma_0)$ with constant 2.

Proof. This proof is similar to that of Theorem 7.8. Again, the case $1 < p < \infty$ will be proved later. By the free commutation relation (7.7), we have

$$\big\| \sum_k x_k \otimes c(e_k) \big\|_\infty^2 = \big\| \big(\sum_k x_k \otimes c(e_k) \big)^* \big(\sum_k x_k \otimes c(e_k) \big) \big\|_\infty = \big\| \sum_k x_k^* x_k \big\|_\infty .$$

Similarly,

$$\big\| \sum_k x_k \otimes a(e_k) \big\|_\infty^2 = \big\| \sum_k x_k x_k^* \big\|_\infty \, .$$

It follows that

$$\big\| \sum_k x_k \otimes s_k \big\|_\infty \le \big\| \big(\sum_k x_k^* x_k \big)^{1/2} \big\|_\infty + \big\| \big(\sum_k x_k x_k^* \big)^{1/2} \big\|_\infty \, .$$

For the lower estimate, take a unit vector $\xi \in \ell_2$. Then

$$\begin{aligned} \big\| \sum_k x_k \otimes s_k \big\|_\infty^2 &\ge \langle \sum_k x_k \otimes s_k (\xi \otimes \mathbb{1}),\ \sum_k x_k \otimes s_k (\xi \otimes \mathbb{1}) \rangle \\ &= \langle \sum_k x_k(\xi) \otimes e_k,\ \sum_k x_k(\xi) \otimes e_k \rangle \\ &= \langle \sum_k x_k^* x_k(\xi),\ \xi \rangle ; \end{aligned}$$

whence

$$\big\|\big(\sum_k x_k^* x_k\big)^{1/2}\big\|_\infty \le \big\|\sum_k x_k \otimes s_k\big\|_\infty .$$

Similarly,

$$\big\|\big(\sum_k x_k x_k^*\big)^{1/2}\big\|_\infty \le \big\|\sum_k x_k \otimes s_k\big\|_\infty .$$

Thus the lower estimate of (7.8) for $p = \infty$ follows.

(7.8) for $p = 1$ and the complementation assertion are proved in the same way as the corresponding assertions of Theorem 7.8. The only difference is the fact that the linear span of the s_k is no longer w*-dense in Γ_0. Instead, we have to use the family of polynomials in the s_k which is w*-dense in Γ_0. This family is the linear span of all Wick products associated with the elementary tensors formed from the basis vectors e_k. It then remains to note that these Wick products form an orthonormal basis of $L_2(\Gamma_0)$. We omit the details. □

Remark 7.10. The free Gaussian variables in the theorem above can be replaced by Bożejko-Speicher's q-Gaussians for $-1 < q < 1$ (see [BKS] and [BS]). This inequality remains also true for the case $q = -1$, for which the corresponding Gaussians become the so-called Fermions. Note that the case $q = 1$ corresponds to the classical Gaussian case. In strong contrast with the case $-1 < q < 1$, the analogue for $q = \pm 1$ of Theorem 7.9 fails for $p = \infty$.

7.6 Complete Unconditionality. Noncommutative Khintchine inequalities are closely related to complete unconditionality. Let M be a von Neumann algebra equipped with a normal faithful tracial state τ. Let (a_k) be a sequence in $L_p(M)$, $1 \le p \le \infty$. Assume that the noncommutative Khintchine inequality holds for (a_k): for any finite sequence (x_k) in S_p

$$\big\|\sum_k x_k \otimes a_k\big\|_{L_p(B(\ell_2)\bar{\otimes} M)} \sim \big\|(x_k)\big\|_{CR_p[S_p]} .$$

It then follows that the subspace E generated by the a_k in $L_p(M)$ is completely isomorphic to CR_p (see Remark 7.6). Since the canonical basis of CR_p is *completely unconditional* , so is the sequence (a_k). Namely, there exists a constant λ such that

$$\big\|\sum_k \varepsilon_k x_k \otimes a_k\big\|_p \le \lambda \big\|\sum_k x_k \otimes a_k\big\|_p \tag{7.9}$$

for any finite sequence $(x_k) \subset S_p$ and any $\varepsilon_k = \pm 1$. This property can be rephrased as follows. Given any sequence (ε_k) of signs the map $\sum_k \alpha_k a_k \mapsto \sum_k \varepsilon_k \alpha_k a_k$ on E is c.b. with cb-norm $\le \lambda$. Therefore, if the noncommutative Khintchine inequality holds for (a_k), then (a_k) is a completely unconditional basic sequence. The converse is also true with some additional mild conditions for $p < \infty$. We consider here only the case $1 \le p < 2$. The following result is proved independently by the author and Junge/Oikhberg [JO]. The latter paper contains more results of the same type.

Theorem 7.11. *Let M be a von Neumann algebra equipped with a normal faithful tracial state τ. Let $1 \le p < 2$ and $(a_k)_{k\ge 1} \subset L_p(M)$ be a completely unconditional basic sequence with constant λ. Assume that*

$$\delta = \inf_k \|a_k\|_p > 0 \quad \textit{and} \quad \Delta = \sup_k \|a_k\|_2 < \infty.$$

Then the noncommutative Khintchine inequality holds for (a_k) with relevant constants depending only on λ, δ and Δ. More precisely, for any finite sequence $(x_k) \subset S_p$

$$c\,\delta\lambda^{-1}\big\|(x_k)\big\|_{CR_p[S_p]} \le \Big\|\sum_k x_k \otimes a_k\Big\|_p \le \Delta\lambda\,\big\|(x_k)\big\|_{CR_p[S_p]}\,, \tag{7.10}$$

where c is an absolute positive constant.

Proof. Let $(x_k) \subset S_p$ be a finite sequence. We then have (7.9). Averaging the left hand side of (7.9) over the ε_n and using the noncommutative Khintchine inequality in Theorem 7.5, we get

$$\inf\Big\{\Big\|\Big(\sum_k Y_k^* Y_k\Big)^{1/2}\Big\|_p + \Big\|\Big(\sum_k Z_k Z_k^*\Big)^{1/2}\Big\|_p\Big\} \le c\,\lambda\,\Big\|\sum_k x_k \otimes a_k\Big\|_p\,,$$

where the infimum runs over all decompositions $x_k \otimes a_k = Y_k + Z_k$ with Y_k and Z_k in $L_p(B(\ell_2)\bar{\otimes}M)$. Fix such a decomposition $x_k \otimes a_k = Y_k + Z_k$. Now choose $b_k \in L_{p'}(M)$ such that

$$\tau(a_k b_k) = 1 \quad \text{and} \quad \|b_k\|_{p'} = \|a_k\|_p^{-1}\,.$$

Then

$$x_k = \mathrm{id}\otimes\tau\big((x_k\otimes a_k)(1\otimes b_k)\big) = \mathrm{id}\otimes\tau(Y_k(1\otimes b_k)) + \mathrm{id}\otimes\tau(Z_k(1\otimes b_k)) \overset{\text{def}}{=} y_k + z_k.$$

Note that $\mathrm{id}\otimes\tau$ is the natural conditional expectation from $B(\ell_2)\bar{\otimes}M$ onto $B(\ell_2)$ ($B(\ell_2)$ being viewed as a von Neumann subalgebra of $B(\ell_2)\bar{\otimes}M$ via $x \leftrightarrow x\otimes 1$). Also note that y_k and z_k belong to S_p. We need to majorize $\|(\sum y_k^* y_k)^{1/2}\|_p$ (resp. $\|(\sum z_k z_k^*)^{1/2}\|_p$) by $\|(\sum Y_k^* Y_k)^{1/2}\|_p$ (resp. $\|(\sum Z_k Z_k^*)^{1/2}\|_p$). To this end, let $(u_k) \subset S_{p'}$ be such that $\|(\sum_k u_k u_k^*)^{1/2}\|_{p'} \le 1$. By the Hölder inequality in Proposition 7.1

$$\begin{aligned}\Big|\sum_k \mathrm{Tr}(y_k u_k)\Big| &= \Big|\sum_k \mathrm{Tr}[\mathrm{id}\otimes\tau(Y_k(1\otimes b_k))u_k]\Big| = \Big|\sum_k \mathrm{Tr}\otimes\tau[Y_k(u_k\otimes b_k)]\Big|\\ &\le \Big\|\Big(\sum_k u_k u_k^*\otimes b_k b_k^*\Big)^{1/2}\Big\|_{p'}\,\Big\|\Big(\sum_k Y_k^* Y_k\Big)^{1/2}\Big\|_p\,.\end{aligned}$$

We claim that

$$\Big\|\Big(\sum_k u_k u_k^* \otimes b_k b_k^*\Big)^{1/2}\Big\|_{p'} \le \sup_k \|b_k\|_{p'} \,\Big\|\Big(\sum_k u_k u_k^*\Big)^{1/2}\Big\|_{p'}\,.$$

Indeed, this is obvious for $p' = 2$ and $p' = \infty$. Then complex interpolation yields the case $2 < p' < \infty$. Combining the preceding inequalities, we find

$$\begin{aligned}\Big|\sum_k \mathrm{Tr}(y_k u_k)\Big| &\le \sup_k \|b_k\|_{p'}\Big\|\Big(\sum_k u_k u_k^*\Big)^{1/2}\Big\|_{p'}\,\Big\|\Big(\sum_k Y_k^* Y_k\Big)^{1/2}\Big\|_p\\ &\le \delta^{-1}\Big\|\Big(\sum_k Y_k^* Y_k\Big)^{1/2}\Big\|_p\,.\end{aligned}$$

Thus taking the supremum over all (u_k), we get

$$\Big\|\Big(\sum_k y_k^* y_k\Big)^{1/2}\Big\|_p \le \delta^{-1}\Big\|\Big(\sum_k Y_k^* Y_k\Big)^{1/2}\Big\|_p\,.$$

Similarly,

$$\Big\|\Big(\sum_k z_k z_k^*\Big)^{1/2}\Big\|_p \le \delta^{-1}\Big\|\Big(\sum_k Z_k Z_k^*\Big)^{1/2}\Big\|_p\,.$$

Therefore, we deduce

$$\big\|(x_k)\big\|_{CR_p[S_p]} \le c\,\delta^{-1}\lambda\,\Big\|\sum_k x_k \otimes a_k\Big\|_p\,.$$

To prove the upper estimate we use again the complete unconditionality of (a_k) and the noncommutative Khintchine inequality. Then we have

$$\begin{aligned}\Big\|\sum_k x_k \otimes a_k\Big\|_p \le \lambda \inf_{x_k = y_k + z_k}\Big\{&\Big\|\Big(\sum_k y_k^* y_k \otimes a_k^* a_k\Big)^{\frac12}\Big\|_p\\ &+\Big\|\Big(\sum_k z_k z_k^* \otimes a_k a_k^*\Big)^{\frac12}\Big\|_p\Big\}.\end{aligned}$$

Now our task is to remove $a_k^* a_k$ and $a_k a_k^*$ from the terms on the right. To this end we use the natural conditional expectation $\mathbb{E}$ from $B(\ell_2)\bar\otimes M$ onto $B(\ell_2)$, already mentioned earlier. $\mathbb{E}$ is determined by $\mathbb{E}(x \otimes u) = \tau(u)x \otimes 1 \sim \tau(u)x$ for $x \in B(\ell_2)$ and $u \in M$, i.e., $\mathbb{E} = \mathrm{id} \otimes \tau$. $\mathbb{E}$ is normal and faithful. As usual, $\mathbb{E}$ extends to a contractive projection on $L_q(B(\ell_2)\bar\otimes M)$ for every $1 \le q < \infty$. For our purpose here we need to consider the case $q \le 1$. We claim that if X is a positive operator in $L_q(B(\ell_2)\bar\otimes M) \cap L_1(B(\ell_2)\bar\otimes M)$ with $q \le 1$, then

$$\|X\|_q \le \|\mathbb{E}(X)\|_q\,. \tag{7.11}$$

This is a consequence of the operator concavity of the map $X \mapsto X^q$ for $0 < q \le 1$. Indeed, using Stinespring's dilation theorem and Hansen's inequality [Ha], we deduce that $(\mathbb{E}(X))^q \geq \mathbb{E}(X^q)$ for any positive $X \in B(\ell_2)\bar{\otimes}M$. This clearly implies (7.11).

Return back to our task. Using (7.11) with $q = p/2$ (recalling that $1 \leq p < 2$), we deduce that

$$\begin{aligned}\big\|\big(\sum_k y_k^* y_k \otimes a_k^* a_k\big)^{1/2}\big\|_p^2 &= \big\|\sum_k y_k^* y_k \otimes a_k^* a_k\big\|_{p/2} \\ &\leq \big\|\mathbb{E}\big[\sum_k y_k^* y_k \otimes a_k^* a_k\big]\big\|_{p/2} \\ &= \big\|\sum_k y_k^* y_k \otimes \tau(a_k^* a_k)1\big\|_{p/2} \\ &\leq \sup_k \|a_k\|_2^2 \, \big\|\big(\sum_k y_k^* y_k\big)^{1/2}\big\|_p^2 .\end{aligned}$$

Therefore,

$$\big\|\big(\sum_k y_k^* y_k \otimes a_k^* a_k\big)^{1/2}\big\|_p \leq \Delta \big\|\big(\sum_k y_k^* y_k\big)^{1/2}\big\|_p .$$

A similar inequality holds for another term involving the z_k. It thus follows that

$$\big\|\sum_k x_k \otimes a_k\big\|_p \leq \Delta\,\lambda\, \big\|(x_k)\big\|_{CR_p[S_p]}.$$

This is the desired upper estimate, and so the proof of the theorem is complete. □

End of the proofs of Theorems 7.8 and 7.9. The $\lambda(g_k)$ are unitary, so $\|\lambda(g_k)\|_p = 1$ for any $1 \leq p \leq \infty$. On the other hand, for any sequence (ε_k) of signs, there exists a unique representation π of $VN(\mathbb{F})$ determined by $\pi(\lambda(g_k)) = \varepsilon_k \lambda(g_k)$. Moreover, π is trace preserving: $\tau_{\mathbb{F}} \circ \pi = \tau_{\mathbb{F}}$. It follows that π extends to a complete isometry on $L_p(VN(\mathbb{F}))$ for every $1 \leq p \leq \infty$. Therefore, for any finite sequence $(x_k) \subset S_p$ we have

$$\big\|\sum_k \varepsilon_k x_k \otimes \lambda(g_k)\big\|_p = \big\|\sum_k x_k \otimes \lambda(g_k)\big\|_p .$$

Thus the sequence $(\lambda(g_k))$ is completely unconditional with constant 1. Then Theorem 7.11 implies (7.3) for $1 \leq p < 2$. The case $p = 2$ is trivial. The case $2 < p < \infty$ is obtained by duality and using the complementation property in Theorem 7.11.

The proof of Theorem 7.9 is similar. This time to get the representation π of Γ_0 such that $\pi(s_k) = \varepsilon_k s_k$, we have to use second quantization (see [VDN]). □

Remark 7.12. There exist many examples satisfying the assumption of Theorem 7.11. This is the case of a sequence of q-Gaussians mentioned in Remark 7.10. In particular, for $q = -1$, we get the noncommutative Khintchine inequality for a sequence of Fermions.

7.7 Generalized Circular Systems. Remind that we wish to embed OH into a noncommutative L_1-space by using a certain noncommutative Khintchine type inequality. Namely, we have to prove that OH is completely isomorphic to the closed subspace generated by a sequence of random variables in an $L_1(M)$ for a von Neumann algebra M. Such a sequence cannot satisfy the assumption of Theorem 7.11 for OH is not completely isomorphic to CR_1. In fact, Pisier [P5] showed that OH cannot completely embed into an $L_1(M)$ with M semifinite (i.e., of type I or II). This explains why we are forced to seek for Khintchine type inequalities for random variables in a non tracial probability space, i.e., the underlying von Neumann algebra is of type III. We give below only one example of this kind.

Fix an infinite dimensional separable Hilbert space H as in subsection 7.5. Let $\{e_{\pm k}\}_{k\geq 1}$ be an orthonormal basis of H. We also fix a sequence $\{\lambda_k\}_{k\geq 1}$ of positive numbers. Let

$$g_k = c(e_k) + \sqrt{\lambda_k}\, a(e_{-k}).$$

$(g_k)_{k\geq 1}$ is a *generalized circular system* in Shlyakhtenko's sense [S]. Let Γ be the von Neumann algebra on the full Fock space $\mathcal{F}(H)$ generated by the g_k. Let ρ be the vector state on Γ determined by the vacuum $\mathbb{1}$. Then ρ is faithful on Γ. By the identification of $L_1(\Gamma)$ with the predual Γ_*, ρ is a positive unit element of $L_1(\Gamma)$, so for any $1 \leq p \leq \infty$, $\rho^{1/p}$ is a positive unit element of $L_p(\Gamma)$, and thus $g_k\, \rho^{1/p} \in L_p(\Gamma)$ for any k.

Shlyakhtenko proved that the algebra Γ is a type III$_\lambda$ factor $(0 < \lambda \leq 1)$ if not all λ_k are equal to 1. Γ is not hyperfinite. Recall that Γ is the free analogue of the classical Araki-Woods quasi-free CAR factors. The latter factors are hyperfinite type III$_\lambda$.

The following is the noncommutative Khintchine type inequalities for generalized circular systems , proved in [PS] for $p = \infty$ and in [X2] for $p < \infty$.

Theorem 7.13. *Let (x_n) be a finite sequence in S_p, $1 \leq p \leq \infty$.*

i) *If $p \geq 2$,*

$$\Big\|\sum_k x_k \otimes g_k \rho^{\frac{1}{p}}\Big\|_{L_p(B(\ell_2)\bar{\otimes}\Gamma)} \sim_c \max\Big\{\Big\|\Big(\sum_k x_k^* x_k\Big)^{\frac{1}{2}}\Big\|_p,\ \Big\|\Big(\sum_k \lambda_k^{1-\frac{2}{p}}\, x_k x_k^*\Big)^{\frac{1}{2}}\Big\|_p\Big\}.$$

ii) *If $p < 2$,*

$$\Big\|\sum_k x_k \otimes g_k \rho^{\frac{1}{p}}\Big\|_{L_p(B(\ell_2)\bar{\otimes}\Gamma)} \sim_c \inf\Big\{\Big\|\Big(\sum_k y_k^* y_k\Big)^{\frac{1}{2}}\Big\|_p + \Big\|\Big(\sum_k \lambda_k^{1-\frac{2}{p}}\, z_k z_k^*\Big)^{\frac{1}{2}}\Big\|_p\Big\},$$

where the infimum runs over all decompositions $x_k = y_k + z_k$ in S_p.

iii) *Let* $\mathcal{G}_p$ *be the closed subspace of* $L_p(\Gamma)$ *generated by* $\{g_k\rho^{1/p}\}_{k\geq 1}$*. Then* $\mathcal{G}_p$ *is completely complemented in* $L_p(\Gamma)$ *with constant* 2*.*

Proof. We prove only the cases $p=\infty, 1$ and the complementation assertion. The proof of i) for $p=\infty$ is the same as that of (7.4). Let us prove iii), which will imply ii) for $p=1$ by duality. As in the semicircular case, consider the projection P from the algebra of polynomials on the g_k onto the linear span of the g_k. Let $Q=I-P$. It is easy to see that $P(x)$ and $Q(x)$ are orthogonal relative to both scalar products $(a,b)\mapsto\rho(b^*a)$ and $(a,b)\mapsto\rho(ab^*)$. Now let x be a polynomial on the g_k with coefficients in S_∞. Write x as

$$x=\mathrm{id}_{S_\infty}\otimes P(x)+\mathrm{id}_{S_\infty}\otimes Q(x)=\sum_k a_k\otimes g_k+\mathrm{id}_{S_\infty}\otimes Q(x).$$

Then using the argument yielding the first inequality of (7.4), we get

$$\max\Big\{\big\|\big(\sum_k a_k^*a_k\big)^{1/2}\big\|_\infty\,,\ \big\|\big(\sum_k \lambda_k\,a_ka_k^*\big)^{1/2}\big\|_\infty\Big\}\leq\|x\|_\infty\,.$$

Therefore, using i) in the case $p=\infty$, we deduce that P is completely bounded. This implies, in turn, ii) for $p=1$ by duality. Let us also note that P extends to a completely bounded normal projection on Γ. Indeed, by the density of $\{x\rho\ :\ x \text{ polynomial on the } g_k\}$ in $L_1(\Gamma)$, we find that ii) in the case $p=1$ shows that P admits a pre-adjoint on $L_1(\Gamma)$ which is completely bounded. Finally, by interpolation we obtain iii) for $1<p<\infty$. □

Remark 7.14. In the spirit of Remark 7.6, Theorem 7.13 can be reformulated as a complete isomorphism between the subspace $\mathcal{G}_p$ and a weighted version of CR_p. Given a sequence (μ_k) of positive numbers we denote by $C((\mu_k))$ the weighted ℓ_2-space $\ell_2((\mu_k))$ equipped with the column Hilbert space structure. More generally, for any $p\geq 1$ we define $C_p((\mu_k))$ to be the weighted version of C_p. Note that $C_p((\mu_k))$ is completely isometric to C_p and its operator space structure is determined as follows: for any finite sequence $(x_k)\subset S_p$

$$\big\|\sum_k x_k\otimes e_k\big\|_{S_p[C_p((\mu_k))]}=\big\|\big(\sum_k \mu_k\,x_k^*x_k\big)^{1/2}\big\|_{S_p}\,.$$

Similarly, we define the weighted p-row space $R_p((\mu_k))$. Then Theorem 7.13 implies that $\mathcal{G}_p$ is completely isomorphic to $C_p\cap R_p((\mu_k))$ for $p\geq 2$ and to $C_p+R_p((\mu_k))$ for $p<2$, where $\mu_k=\lambda_k^{1-2/p}$.

Remark 7.15. It is worth to note that the proof of the previous Khintchine inequalities in the free case (i.e., for free generators, semicircular systems and generalized circular systems) is relatively easy. The main obstruction in proving these inequalities in the case $1<p<\infty$ is the fact that one cannot proceed by interpolation. Indeed, it is a priori not clear why the spaces $CR_p[S_p]$ form a (complex) interpolation scale. A posteriori this is a consequence of the Khintchine inequalities and the complete complementation in

Theorem 7.8 or Theorem 7.9. This is how Pisier shows that the $CR_p[S_p]$ form a complex interpolation scale (see [P2, Theorem 8.4.8]). In the same way, using Theorem 7.13 one deduces that the weighted versions of $CR_p[S_p]$ defined in the previous remark are also an interpolation scale (see [JPX] for more details).

Remark 7.16. Theorem 7.13 admits a Fermionic analogue. In this case the corresponding algebra is an Araki-Woods hyperfinite type III factor. The resulting inequality holds only for $p < \infty$ and the relevant constants depend only on p and blow up as $p \to \infty$. We refer to [J3] and [X1] for more information (see also [HM] for an alternate approach for the case $p = 1$).

Exercises:

1) Prove the classical Khintchine inequality (7.1). (Consider first the case of an even integer p.)
2) Prove by counterexample that there exists no constant c_p depending on p such that

$$\big\|\sum_k x_k \varepsilon_n\big\|_{L_p(\Omega;S_p)} \le c_p \,\big\|(x_k)\big\|_{C_p[S_p]} \quad \text{if } p > 2$$

or

$$\big\|(x_k)\big\|_{C_p[S_p]} \le c_p \,\big\|\sum_k x_k \varepsilon_n\big\|_{L_p(\Omega;S_p)} \quad \text{if } p < 2$$

holds for all finite sequences $(x_k) \subset S_p$.
3) Prove Remark 7.7.
4) Let G be a discrete group. Prove that the vector state τ_G determined by δ_e is faithful and tracial on $VN(G)$.
5) Prove that the vector state τ_0 determined by the vacuum $\mathbb{1}$ is faithful and tracial on the free von Neumann algebra $\Gamma_0(H)$.

8 Embedding of OH into Noncommutative L_1

Now we use the Khintchine inequality for generalized circular systems to embed OH completely isomorphically into a noncommutative L_1-space, i.e., to show that OH is completely isomorphic to a subspace of a noncommutative L_1. This is a remarkable theorem of Junge [J2]. The following representation of OH as a quotient of a subspace of $C \oplus R$ will be crucial.

Theorem 8.1. *OH is completely isometric to a quotient of a subspace of $C \oplus_\infty R$.*

The direct sum in the ℓ_∞-sense can be replaced by a direct sum in the ℓ_1-sense at the price of a constant 2. Since the complete embeddings in the sequel are only completely isomorphic, we will forget the index ∞ or 1 in all direct sums. The preceding theorem is Exercise 7.8 of [P3]. The proof there gives the following more precise statement.

Theorem 8.2. *There exists an injective positive selfadjoint (unbounded) operator $\Delta : C \to R$ such that OH is completely isometric to a quotient of $G(\Delta)$, where $G(\Delta)$ is the graph of Δ*

$$G(\Delta) = \big\{(h, \Delta h) \ : \ h \in D(\Delta)\big\} \subset C \oplus R,$$

considered as a subspace of $C \oplus R$.

Recall that both C and R are isometric to ℓ_2 as Banach spaces. Thus Δ is an operator on ℓ_2 with domain $D(\Delta)$. Since Δ is positive and injective, its range is also dense. Passing to duality, we see that OH^* is completely isometric to a subspace of $G(\Delta)^*$. Since $\overline{OH^*} = OH$ completely isometrically, embedding OH into an L_1 is reduced to embedding $G(\Delta)^*$ into an L_1.

To see why Khintchine type inequalities can help us for such a matter, let us describe the operator space structure of $G(\Delta)$:

$$G(\Delta) = \{(h,\ \Delta(h)) \ : \ h \in D(\Delta)\} \subset C \oplus_\infty R\,.$$

Let $x_k \in S_\infty$ and $h_k \in D(\Delta)$. Let $x = \sum_k x_k \otimes (h_k,\ \Delta(h_k)) \in S_\infty \otimes_{\min} G(\Delta)$. Then

$$\begin{aligned}&\|x\|_{S_\infty \otimes_{\min} G(\Delta)}\\ &\quad = \max\Big\{\Big\|\sum_{k,j}\langle h_k,\ h_j\rangle x_j^* x_k\Big\|_{S_\infty}^{1/2},\ \Big\|\sum_{k,j}\langle \Delta(h_k),\ \Delta(h_j)\rangle x_k x_j^*\Big\|_{S_\infty}^{1/2}\Big\}.\end{aligned}$$

This is a continuous version of the space (for $p = \infty$) introduced in Remark 7.14. To simplify our discussion and without loss of generality by a simple argument of approximation, we may assume that Δ has pure point spectrum, i.e., ℓ_2 has an orthonormal basis (e_k) of eigenvectors of Δ. Let (μ_k) be the associated eigenvalues: $\Delta e_k = \mu_k e_k$. It then follows that $G(\Delta)$ coincides (completely isometrically) with the diagonal subspace $C \cap R((\lambda_k))$ of $C \oplus_\infty R((\lambda_k))$, where $\lambda_k = \mu_k^2$.

By duality, we deduce that $G(\Delta)^* = C_1 + R_1((\lambda_k^{-1}))$. More precisely, the operator space structure of $G(\Delta)^*$ is determined as follows: for any finite sequence $(x_k) \subset S_1$:

$$\|x\|_{S_1[G(\Delta)^*]} = \inf\Big\{\Big\|\Big(\sum_k y_k^* y_k\Big)^{1/2}\Big\|_{S_1} + \Big\|\Big(\sum_k \lambda_k^{-1} z_k z_k^*\Big)^{1/2}\Big\|_{S_1}\Big\},$$

where the infimum runs over all decompositions $x_k = y_k + z_k$ in S_1. Therefore, by the Khintchine inequality in Theorem 7.13 with $p = 1$, $G(\Delta)^*$ is completely isomorphic to $\mathcal{G}_1$ there. Thus we have proved the following

Theorem 8.3. *OH is completely isomorphic to a subspace of a noncommutative L_1-space.*

Remark 8.4. i) The proof of Theorem 8.3 gives much more. In fact, it shows that the dual space of any graph in $C \oplus R$ completely embeds into an L_1. From this one can deduce that a quotient of a subspace of $C \oplus R$ completely embeds into an L_1. We refer to [J2], [P4] and [X1] for more information.

ii) The von Neumann algebra Γ is not hyperfinite. OH also completely embeds into the predual of a hyperfinite algebra (see [J3], [HM]).

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Dirichlet Forms on Noncommutative Spaces

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Abstract We show how Dirichlet forms provide an approach to potential theory of noncommutative spaces based on the notion of energy. The correspondence with KMS-symmetric Markovian semigroups is explained in details and applied to the dynamical approach to equilibria of quantum spin systems. Second part focuses on the differential calculus underlying a Dirichlet form. Applications are given in Riemannian Geometry to a potential theoretic characterization of spaces with positive curvature and to the construction of Fredholm modules in Noncommutative Geometry.

1 Introduction

Our purpose in these notes is to introduce the reader to those aspects of Potential Theory underlying the notion of energy on noncommutative spaces such as

- fractal spaces whose topology is not underlying any manifold structure
- Riemannian manifolds in spin geometry
- space of orbits of dynamical systems
- space of leaves of Riemannian foliations
- space of irreducible unitary representations of a discrete group
- space of observables of spin systems in Quantum Statistical Mechanics
- space of random variables in Free Probability.

To handle the complexity of spaces of this type, the classical tools of analysis like measure theory, topology and differential calculus, are unfitted or

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insufficient as they force to treating these spaces as *singular*. However, as emphasized by A. Connes in Noncommutative Geometry, the properties of these spaces are naturally encoded in algebras which, generalizing the familiar abelian ones of measurable, continuous or smooth functions, are in general *noncommutative*.

The aim of this introduction is to recall briefly the role of energy in Newtonian and Beurling-Deny generalized potential theories, then to show the natural emergence of a potential theory in various noncommutative spaces and then to describe the content of the sections of these notes.

Classical potential theory analyzes properties of force field F in Euclidean spaces $\mathbb{R}^d$, like incompressibility, irrotationality or conservativity, in which case one is looking, at least locally, for potentials U such that $F = \nabla U$. In regions Ω where charges are absent, the potential U is harmonic, as it solves the Laplace equation $\Delta U = 0$. One of the most important achievements of eighteenth century analysis was the solution of the Dirichlet problem, i.e. the determination of the potential U harmonic in Ω once its boundary values are known, under suitable regularity assumptions on $\partial\Omega$. One of the methods invented to solve this problem focuses on the construction of the Green's and Poisson's kernels on Ω, by which a solution U admits an integral representation in terms of its boundary values on $\partial\Omega$.
To recall the multiple connections of classical potential theory with other fields of mathematics, it suffices to mention those with *conformal geometry*. In fact, by methods dating back to B. Riemann and D. Hilbert (see [Abk] for a nice account of that long story), the conformal equivalence given by the Uniformization Theorem, between a simply connected region Ω having smooth enough boundary and the unit disk of the complex plane $\mathbb{C}$, gives rise to the Green function of Ω.
A second method to solve the Dirichlet problem is variational in nature and it consists of seeking the solution U as the unique minimizer of the *Dirichlet energy integral*

$$\mathcal{E}[u] = \int_\Omega |\nabla u(x)|^2\, dx \tag{1.1}$$

among the continuous functions having the prescribed boundary values. The characteristic property of this energy functional is that it does not increase upon modifying the function from u to $u \wedge 1 := \inf(u, 1)$:

$$\mathcal{E}[u \wedge 1] \leq \mathcal{E}[u]. \tag{1.2}$$

It is easy to recognize here a basic feature of the energy functional of many physical systems, such as the case where u is meant to describe the values of the potential at the vertices of an electrical circuit.

In the fall of the '50's of the previous century, A. Beurling and J. Deny developed in two seminal papers [BD1] and [BD2] a *generalized potential theory on locally compact spaces*. As their approach relies upon the notion of

energy where potentials appear as derived objects, it is a kernel-free point of view.
In that theory a *Dirichlet space* is a locally compact topological Hausdorff space X equipped with a *Dirichlet form* $\mathcal{E} : C_0(X) \to (-\infty, +\infty]$: this is just a quadratic, lower semi-continuous functional, defined on the algebra $C_0(X)$ of continuous functions vanishing at infinity, which is finite on a dense subspace and satisfies the *characteristic contraction property* (1.2).
In studying these functionals, Hilbertian methods are quite natural: by a result of G. Mokobodzki [Mok], there always exists a positive Radon measure m on X such that $\mathcal{E}$ admits a lower semi-continuous extension to $L^2(X, m)$. In other words, the functional $\mathcal{E}$ may be considered, in a natural way, as the closed quadratic form of a self-adjoint operator H on $L^2(X, m)$, with respect to a large family of reference measures on X.

The *nuance* between the theory on the algebra $C_0(X)$, and the one on the Hilbert space $L^2(X, m)$, relies on the *geometrical* character of the former and the *dynamical* character of the latter.

In this respect, A. Beurling and J. Deny discovered the fundamental dynamical characterization of the contraction property of an energy functional $\mathcal{E}$ on $L^2(X, m)$, in terms of the semigroup $\{e^{-tH} : t \geq 0\}$ generated by H: the contraction property of $\mathcal{E}$ is equivalent to the so called *Markovianity property.* This consists of *positivity*, in the sense that the maps e^{-tH} preserve positivity of functions, and of *contractivity*, by which e^{-tH} is contractive both with respect to the Hilbertian norm of $L^2(X, m)$ and with respect to the uniform norm of the algebra $L^\infty(X, m)$. In turn, by interpolation and duality, this implies contractivity with respect to the whole scale of Lebesgue spaces $L^p(X, m)$. In other terms, the solution $u(t) = e^{-tH}u(0)$ of the generalized heat equation $\partial_t u = -Hu$ associated to H satisfies a *maximum principle.*

The dynamical point of view is also fundamental for the *probabilistic* counterpart of the theory. By the work of M. Fukushima (see [FOT]), a Dirichlet form $\mathcal{E}$ on $C_0(X)$ gives rise to *a family of Markov-Hunt stochastic processes* on X. These processes are indexed, essentially, by the Radon measures m having X as support with respect to which $\mathcal{E}$ is closable in $L^2(X, m)$. In a sense, the various processes are essentially the same in that they differ one from another by a *random time change* only, associated to their *speed* measures m. In this sense *the functional* $\mathcal{E}$ on the algebra $C_0(X)$ *is a geometric object* representing an equivalence class of stochastic processes on X having the same paths.
The transition functions of these processes coincide with the *heat kernels* of the Markovian semigroups and one obtains a probabilistic interpretation of the solution of the generalized heat equation, which extends the well known relationships among *Laplace operator, heat equation and Brownian motion* on $\mathbb{R}^n$ (see for example [Do]).

The essential tool needed to associate a Markov process to a Dirichlet form $\mathcal{E}$ and a speed measure m on X, in the Beurling-Deny generalized potential theory are those functions u, called *potentials*, such that

$$\mathcal{E}[u+v] \geq \mathcal{E}[u] + \mathcal{E}[v] \tag{1.3}$$

for all positive functions v. The class of potentials then define a notion of smallness, called *polarity*, for subsets of X, which is well suited to discuss both the fine analytic properties of energy and the fine probabilistic properties of the process.

The need to extend tools like Dirichlet forms and Markovian semigroups, beyond the above commutative setting, was recognized a long time ago in Quantum Field Theory, where, for example, quadratic form techniques were employed to generate and analyze Hamiltonian operators representing the energy of the system.
In the second quantization of Boson systems the symmetric Fock space is isomorphic to the Lebesgue space $L^2(X\,,\gamma)$ over an infinite dimensional Gaussian space $(X\,,\gamma)$ and the number operator N into the generator of a symmetric Markovian semigroup over the commutative von Neumann algebra $L^\infty(X,\gamma)$. This allowed the developement of non perturbative techniques, like *hypercontractivity* and *logarithmic Sobolev inequalities*, helping the construction of interacting quantum fields (see [RS Section X.9, Notes]).
An extension of these methods, requiring *a noncommutative setting*, was developed by L. Gross in [G1], to deal with problems of *existence and uniqueness of ground states* of Hamiltonians describing Fermions systems. There, the relevant algebra is the *Clifford algebra* $Cl(h)$ of an infinite dimensional Hilbert space h. This is a *noncommutative von Neumann algebra*, with trivial center and finite normal trace τ, hence a II_1 factor, which is another example of those algebras (discovered by F.J. Murray and J. von Neumann [MvN] in the early days of the theory of operators algebras) displaying a *continuous geometry*.
L. Gross discovered that the Hamiltonian operators H of these systems are the generators of Markovian semigroups on the Clifford algebra, and then of a family of contraction semigroups on the noncommutative $L^p(Cl(h)\,,\tau)$ spaces associated to the trace. The construction of these spaces, which generalize Lebesgue's one in the commutative case, was achieved by I. Segal [Se] and reformulated by E. Nelson [Ne]. The method concerning the uniqueness problem may be seen as a *generalization of Perron's theory* of matrices with positive entries, while the tools needed to approach the existence problem exploit hypercontractivity again.

The study of Dirichlet forms in the noncommutative setting of a C* or von Neumann algebra $\mathfrak{M}$ and a semifinite trace τ on it was *pioneered by S. Albeverio and R. Hoegh-Krohn* in [AHK1,2], where, in particular, they

obtained the generalization of the Beurling-Deny characterization of Markovian semigroups, in terms of Dirichlet forms.
This theory was subsequently developed by J.-L. Sauvageot [S2,3], E. B. Davies-J. M. Lindsay [DL1,2]. In particular, D. Guido - T. Isola - S. Scarlatti [GIS] generalized the Beurling-Deny correspondence to non symmetric Dirichlet forms and Markovian semigroups.
This theory met several fields of application. In [S4] and [S7] the author constructed the *transverse Laplacian* operator and the corresponding *transverse heat semigroup* on the C*-algebra *of a Riemannian foliation*, defined by A. Connes in the framework of Noncommutative Geometry [Co2]. This Markovian semigroup was subsequently dilated in [S6] to a *noncommutative Markovian stochastic process* in the sense of Quantum Probability [AFLe], [Par].
In the framework of Riemannian Geometry, E. B. Davies - O. Rothaus proved [DR1] that the Bochner Laplacian of the Levi-Civita connection of a Riemannian manifold M generates a Markovian semigroup on the Clifford algebra of M, and used the result to investigate spectral bounds [DR2]. Markov structures on the Clifford algebra of a Riemannian manifold were also studied in [SU]. In [D2] E. B. Davies combined the technique of Dirichlet forms on von Neumann semifinite algebras with some ideas of A. Connes in Noncommutative Geometry, to obtain *sharp heat kernel bounds on graphs*, hence approaching through "noncommutative tools" a purely commutative classical problem. More recently, D. Goswami and K.B. Sinha [GS], using the first order *differential calculus associated to a Dirichlet form* developed in [CS1] and illustrated in Chapter below, see also [CS4], succeeded in constructing a *noncommutative stochastic process associated to a Dirichlet form, solving a quantum stochastic differential equation with unbounded generator.*

Despite the fact that traces on operators algebras are quite rare and even sometimes absent, the need to extend the theory to non tracial states or weights on C* or von Neumann algebras was suggested by possible applications in at least two fields of Mathematical Physics.
In the theory of Quantum Open Systems [D1] and in Quantum Measurement Theory [B], Markovian semigroups, also called *dynamical semigroups*, appear naturally as solutions of the master equation: they model dissipative dynamics of quantum systems coupled to thermal reservoirs [AFLu] or continuous measurement processes of a "small" quantum system coupled to a larger one (which represents the instrument).
On the other hand, the progresses made by D. Stroock - B. Zegarlinski at the end of the eighties in the stochastic approach to the equilibrium in Classical Statistical Mechanics [Lig] suggested the developement of similar tools for KMS equilibrium states in Quantum Statistical Mechanics [MZ1], [MZ2], [MOZ]. *At finite temperature however, KMS-states are never tracial states but give rise to type III von Neumann algebras* [Del].

This led to a general formulation of Dirichlet forms and symmetric Markovian semigroups on von Neumann algebras and to an extension of the Beurling-Deny correspondence with respect to faithful and normal states [Cip1], [GL1,2] and to faithful, normal and semifinite weights [GL3]. This approach provides in particular a *maximum principle for solutions of Dirichlet problems on C^*-algebras* [S5], [Cip2], [CS3].
There are two main differences with respect to the tracial setting. While in the commutative and tracial cases $(\mathfrak{M}\,,\tau)$ it is quite clear how to construct the Hilbert space $L^2(\mathfrak{M},\tau)$ on which the Markovian semigroups should act, in case of a generic state ω on $\mathfrak{M}$ the situation offers several possible choices. Beside the GNS space $\mathcal{H}_\omega$ of the Gelfand-Neimark-Segal representation $(\pi_\omega,\mathcal{H}_\omega,\xi_\omega)$ of $\mathfrak{M}$, concrete situations may provide more natural candidates, as for example when $\mathfrak{M}$ is the group von Neumann algebra $\lambda(G)''$ of a locally compact group G.

The second difference concerns the order structure on the Hilbert space $L^2(\mathfrak{M}\,,\omega)$, with respect to which we will consider positivity and Markovianity of semigroups. In the commutative case, the positive cone of $L^2(X,m)$ is generated by the positive cone of the von Neumann algebra $L^\infty(X,m)$. This is still true in the tracial case as there is a preferred embedding of the von Neumann algebra $\mathfrak{M}$ into the the various choices of $L^2(\mathfrak{M}\,\tau)$. In case of a non tracial state ω there are infinitely many possible choices.

In Chapter 2 we explain how to overcome these difficulties, adopting the point of view of the Tomita-Takesaki modular theory and, in particular, using standard forms of von Neumann algebras. This will allow the generalization of Beurling-Deny theory to Markovian semigroups on von Neumann algebras satisfying the ω-symmetry condition with respect to a fixed, faithful, normal state ω.
In the same section, however, we introduce a more fundamental symmetry condition for maps and semigroups, not necessarily positive or Markovian, on a C*-algebra A. It is a symmetry relation to be verified with respect to a fixed $(\alpha\,,\beta)$-KMS state of a dynamical system $\alpha=\{\alpha_t : t\in\mathbb{R}\}$ on A.
The adopted name of *KMS symmetry* is intended to suggest that this property is deeply related to, and in fact a deformation of, the *KMS condition* characterizing the *equilibrium states of quantum dynamical systems.*

By virtue of the KMS-symmetry, it is possible to study semigroups, not necessarily positive or Markovian, in the standard forms of the von Neumann algebra generated by the KMS state ω. In Chapter 3 we illustrate applications to the *convergence to equilibrium in Quantum Statistical Mechanics* initially developed by Y. M. Park [P1,2].
We emphasize the fact that the KMS symmetry condition, despite its similarity with the *detailed balance conditions* often considered in literature when dealing with Quantum Open Systems, *does not imply the semigroup commutes with the dynamics.* This fact is crucial for applications to the convergence to equilibrium in Quantum Statistical Mechanics.

In Chapter 4 we describe the construction of the canonical *first order differential calculus associated to regular Dirichlet forms* on a C*-algebra endowed with a faithful and semifinite trace, developed in [CS1]. When this calculus is applied to classical potential theory, on a Riemmannian space M say, this process allows the reconstruction of the Hilbert space of square integrable vector fields $L^2(TM)$ and the gradient operator ∇ from the energy integral

$$\mathcal{E}[a] = \int_M |\nabla a|^2 dm\,.$$

The differential calculus is understood in terms of *derivations with values in Hilbert bimodules over A, i.e. in terms of representations of the maximal tensor product $A \otimes_{\max} A^\circ$*. The content of this section is taken from [CS1]. Under the stronger hypothesis that the domain of the self-adjoint generator associated to the Dirichlet form contains a dense sub-algebra, it was previously proved in [S2,3]. Applying decomposition theory of representations of C*-algebras, we clarify the meaning of this differential calculus analyzing the Beurling-Deny-Le Jan decomposition of Dirichlet forms $\mathcal{E}$ on commutative C*-algebras. Other noncommutative examples of this differential calculus are illustrated on groups and Clifford C*-algebras. In Section 4.4 we describe certain derivations appearing in D. V. Voiculescu's Free Probability.

The last two chapters are devoted to illustrating two applications of the canonical differential calculus.

The first one, Chapter 5, concerns the relationships between noncommutative potential theory and Riemannian geometry. We first illustrate the work of E. B. Davies and O. S. Rothaus [DR1,2] showing that the Bochner Laplacian $\nabla^*\nabla$ is the generator of a Markovian semigroup on the Clifford algebra $Cl(M)$ of a Riemannian manifold M. *Then we characterize Riemannian manifolds with nonnegative curvature operator as those in which the Dirac Laplacian D^2, the square of the Dirac operator D on $Cl(M)$, generates a Markovian semigroup on the Clifford algebra.*

The aim of the final section, Chapter 6, is to convince the reader that Dirichlet forms, commutative or not, share a flavor of geometry, in the sense of A. Connes' Noncommutative Geometry ([Co2]). In particular we show how a regular Dirichlet form $\mathcal{E}$ on a compact space X gives rise to a Fredholm module, in the sense of M. Atiyah [At], on the function algebra $C(X)$, provided that the spectrum of the self-adjoint operator associated to $\mathcal{E}$ is discrete and its Green function G is finite [CS4]. This last condition implies the spectral dimension of $\mathcal{E}$ to be strictly less than two. Although very restrictive at first sight, it applies however to the regular harmonic structures, constructed by J. Kigami, on post critically finite self-similar fractal spaces [Ki]. These are interesting examples of spaces whose topology does not underlie any differentiable manifold structure in the classical sense. As a consequence of the boundedness of G, a finite energy function a on X has a *noncommutative differential*

$$da := i[F, a]$$

lying in the Hilbert-Schmidt class of compact operators, F being the *phase operator* of the Fredholm module. This reveals the direct role that the potential theory of Dirichlet forms may play in differential topology in the sense of Nnoncommutative Geometry.

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2 Dirichlet Forms on C*-algebras and KMS-symmetric Semigroups

In this chapter we show how the Beurling-Deny theory can be generalized, in a natural way, to situations in which the relevant algebra is no longer the commutative algebra of continuous functions $C_0(X)$ over a locally compact, metrizable Hausdorff space X or the commutative algebra of essentially bounded functions $L^\infty(X, m)$, but rather a noncommutative C*-algebra A or a noncommutative von Neumann algebra $\mathfrak{M}$.
The objects of interest will be maps, semigroups and quadratic forms which behave naturally, from the point of view of potential theory, with respect to the order structures of these types of spaces. The difficulties one encounters in dealing with these order structures, which are proportional to the degree of noncommutativity, are taken care of by the fundamental part of noncommutative measure theory concerned with the Tomita-Takesaki theory. This theory, essentially, develops the tools needed to generalize the Radon-Nikodym theorem at the level of von Neumann algebras. One of these tools, fundamental for our purposes, will be the existence and properties of the standard form of a von Neumann algebra.

Sesquilinear scalar product in Hilbert spaces will be assumed to be linear in the right-hand entry and conjugate linear in the left-hand one.

2.1 Tomita-Takesaki Modular Theory and Standard Forms of von Neumann Algebras

A detailed exposition of the Tomita-Takesaki modular theory would fall beyond the scope of these lectures. In this section we content ourselves with collecting some of the tools which will be in use throughout the paper. Nice references for this material are [BR1,2], [T1]. The background material about C*-algebras and von Neumann algebras may be found in [Arv], [Dix1,2], [Ped].

A C*-algebra is an involutive Banach algebra A, in which the norm, involution and product are related by

$$\|a^*a\| = \|a\|^2 \qquad a \in A\,.$$

The involution determines the positive cone $A_+ := \{a^*a \in A : a \in A\}$, so that A is, in particular, an ordered vector space. Assume for simplicity that A is unital and denote by 1_A its unit. A *state* $\omega \in A'_+$, i.e. a positive linear functional of norm one, gives rise to the *cyclic or Gelfand-Naimark-Segal representation* $(\pi_\omega, \mathcal{H}_\omega, \xi_\omega)$ of A, with cyclic and separating vector $\xi_\omega \in \mathcal{H}_\omega$. The double commutant $\mathfrak{M} := \pi_\omega(A)''$ is then a von Neumann algebra of operators in $\mathcal{H}_\omega$ whose positive cone $\mathfrak{M}_+$ coincides both with the set of elements of $\mathfrak{M}$ which are positive operators on $\mathcal{H}_\omega$ as well as with the weak closure of the image $\pi_\omega(A_+)$ of the positive cone of A.

To analyze at a Hilbert space level maps and semigroups on A and $\mathfrak{M}$, which leave globally invariant the positive cones, one is lead to consider in $\mathcal{H}_\omega$ the structure of an ordered vector space, and to relate it with those of A and $\mathfrak{M}$. There are, in general, several ways to do that, but only one is *standard*. This will be constructed and analyzed by the Tomita-Takesaki modular theory.

A natural choice for a positive cone in the GNS space $\mathcal{H}_\omega$ could be

$$\overline{\mathfrak{M}_+\, \xi_\omega} \tag{2.1}$$

as it is justified by the following

Example 2.1. (Self-polarity in classical measure theory) When A is commutative and unital, hence isomorphic to the algebra of continuous functions $C(X)$ over a compact Hausdorff space X, the state ω is represented by a positive Radon measure μ_ω on X, $\mathcal{H}_\omega$ is identified with $L^2(X, \mu_\omega)$, the representation π_ω is given by the obvious action of continuous functions on the square integrable ones and the von Neumann algebra $\mathfrak{M}$ coincides with $L^\infty(X, \mu_\omega)$. Since the cyclic vector ξ_ω corresponds to the constant function $1 \in L^2(X, \mu_\omega)$, in this setting positivity has the usual pointwise meaning and one realizes immediately that the positive cone $\mathcal{H}_\omega^+ = L^2_+(X, \mu_\omega)$ is *self-polar* in the sense that a function g in $L^2(X, \mu_\omega)$ is positive if and only if

$$\int_X f g \, d\mu_\omega \geq 0$$

for all functions f in the positive cone $L^2_+(X, \mu_\omega)$.

Re-writing the property above, using the scalar product of $L^2(X, \mu_\omega)$ as follows

$$L^2_+(X, \mu_\omega) = \{g \in L^2(X, \mu_\omega) : (f|g) \geq 0 \quad \forall f \in L^2_+(X, \mu_\omega)\},$$

one realizes that self-polarity can be considered in arbitrary Hilbert spaces.

Definition 2.2. (Self-polar cone) In a complex Hilbert space $\mathcal{H}$, a subset $\mathcal{H}^+ \subset \mathcal{H}$ is *self-polar* if it coincides with its polar

$$\mathcal{H}^+ = \{\xi \in \mathcal{H} : (\xi|\,\eta) \geq 0 \quad \forall\, \eta \in \mathcal{H}^+\}. \tag{2.2}$$

In particular a self-polar set is a closed convex cone.

Together with *facial homogeneity* and *orientability*, *self-polarity* is one of three fundamental properties characterizing von Neumann algebras in terms of ordered vector spaces [Co1]. Our interest in it relies upon the fact that self-polarity is the key property needed to treat Dirichlet forms and Markovian semigroups on general von Neumann algebras, avoiding being limited to type I or type II von Neumann algebras and to trace functionals on them.
A self-polar cone $\mathcal{H}^+$ endows a Hilbert space $\mathcal{H}$ with an order structure which behaves, in some respect, similarly to the one of Example 2.1. In particular we will make use of the following properties, referring to [Io] for the proof.

Proposition 2.3. *(Jordan decomposition in self-polar cones) Let $\mathcal{H}^+$ be a self-polar cone in a complex Hilbert space $\mathcal{H}$. Then*

i) $\mathcal{H}$ is the complexification $\mathcal{H} = \mathcal{H}^J \bigoplus i\mathcal{H}^J$ of its real subspace

$$\mathcal{H}^J := \{\xi \in \mathcal{H} : (\xi|\,\eta) \in \mathbb{R} \quad \forall \eta \in \mathcal{H}^+\};$$

ii) the cone $\mathcal{H}^+$ gives rise to the structure of an ordered real vector space on $\mathcal{H}^J$ and to an anti-unitary involution

$$J : \mathcal{H} \to \mathcal{H} \qquad J(\xi + i\eta) := \xi - i\eta\,, \qquad \xi\,, \eta \in \mathcal{H}^J\,;$$

iii) any J-real element $\xi \in \mathcal{H}^J$ can be written uniquely as a difference $\xi = \xi_+ - \xi_-$ of two orthogonal, positive elements $\xi_\pm \in \mathcal{H}^+$. This decomposition characterizes self-dual cones among the closed and convex ones. It is usually referred as the Jordan decomposition.

The positive part ξ_+ of a J-real element $\xi \in \mathcal{H}^J$ is, by definition, the Hilbertian projection of ξ onto the closed convex subset $\mathcal{H}^+ \subset \mathcal{H}^J$: ξ_+ is the unique element minimizing the distance between ξ and the positive cone $\mathcal{H}^+$. The negative part is defined by difference: $\xi_- := \xi_+ - \xi$.

Example 2.4. (Jordan decomposition in commutative von Neumann algebras) In the commutative case of Example 2.1, the Jordan decomposition of a square summable, complex function f into its real and imaginary parts and the splitting of these into their positive and negative pieces, has the usual familiar meaning. In this case, the positive part f_+ of a square summable, real function f can be understood as the composition of f with the real variable function $\phi(x) := x \vee 0$.

Example 2.5. (Jordan decomposition in type I and type II von Neumann algebras) Beyond the commutative case, the choice of the closed convex cone $\overline{\mathfrak{M}_+\xi_\omega}$ in the GNS Hilbert space $\mathcal{H}_\omega$ does not always match *self-duality* and it does if and only if the state ω is a *trace*:

$$\omega(ab) = \omega(b\,a) \qquad a, b \in A\,. \tag{2.3}$$

If this is the case, an element $x\xi_\omega$ is J-real if and only if $x = x^* \in \mathfrak{M}$ and its Jordan decomposition, given by $x\xi_\omega = x_+\xi_\omega - x_-\xi_\omega$, essentially reduces to the Jordan decomposition $x = x_+ - x_-$ in the von Neumann algebra $\mathfrak{M}$. Hence, even in noncommutative case, as long as the state ω is a trace, the order structure of the GNS space given by the cone $\overline{\mathfrak{M}_+\xi_\omega}$ is essentially the order structure of the von Neumann algebra $\mathfrak{M}$.

We will need the construction of a self-dual convex cone $\mathcal{H}_\omega^+$, in the case when the state ω is not necessarily a trace. This will be done with the help of the Tomita-Takesaki modular theory which we now briefly recall. The self-polar cone $\mathcal{H}_\omega^+$ will be, in a precise sense, intermediate among $\overline{\mathfrak{M}_+\,\xi_\omega}$ and $\overline{\mathfrak{M}'_+\,\xi_\omega}$, denoting by $\mathfrak{M}'$ the commutant von Neumann algebra of $\mathfrak{M}$ on $\mathcal{H}$:

$$\mathfrak{M}' = \{x \in B(\mathcal{H}) : xy = yx \quad y \in B(\mathcal{H})\}\,.$$

To work in complete generality, we consider a von Neumann algebra of operators $\mathfrak{M}$, acting on a Hilbert space $\mathcal{H}$, and a *cyclic* and *separating vector* ξ for it. The first property means that $\mathcal{H} = \overline{\mathfrak{M}\xi}$, while the second means that for $x \in \mathfrak{M}$, $x\xi = 0$ if and only if $x = 0$.
Equivalently, one may consider ξ to be the vector representing a faithful, normal state ω of $\mathfrak{M}$, in the GNS representation, having in mind, as a prototype, the case where $\mathfrak{M}$ is itself generated in a GNS representation of a given C*-algebra A and a state ω on it.

The isometric involution map $x \mapsto x^*$ on $\mathfrak{M}$ gives rise to the anti-linear map $x\xi \mapsto x^*\xi$ on $\mathcal{H}$, densely defined on $\mathfrak{M}\,\xi \subseteq \mathcal{H}$. This map is isometric if and only if the vector state $\omega(\cdot) = (\xi|\cdot\xi)$ is a trace on $\mathfrak{M}$. *The starting observation of the Tomita-Takesaki modular theory is that this map is always closable.* In the polar decomposition of its closure S_ξ

$$S_\xi = J_\xi \Delta_\xi^{1/2} \tag{2.4}$$

the anti-unitary part J_ξ is called the *modular conjugation* while $\Delta_\xi = S_\xi^* S_\xi$ is called the *modular operator* associated with the pair $(\mathfrak{M}, \xi)$. The modular operator Δ_ξ measures how the state ω differs from being a trace (in which case Δ_ξ reduces to the identity).

Theorem 2.6. (Tomita-Takesaki theorem) *Let $\mathfrak{M}$ be a von Neumann algebra, acting on the Hilbert space $\mathcal{H}$ and ξ be a cyclic and separating vector. Let Δ_ξ and J_ξ be the associated modular operator and modular conjugation, respectively. It follows that*

$$J_\xi \mathfrak{M} J_\xi = \mathfrak{M}' \tag{2.5}$$

and that

$$\Delta_\xi^{it} \mathfrak{M} \Delta_\xi^{-it} = \mathfrak{M} \qquad t \in \mathbb{R}. \tag{2.6}$$

Now let $\mathfrak{M}$ be a von Neumann algebra, ω a faithful normal state on it and $(\pi_\omega, \mathcal{H}_\omega, \xi_\omega)$ the associated cyclic representation. Denoting by Δ_ω the modular operator associated to the pair $(\pi_\omega(\mathfrak{M}), \xi_\omega)$, the Tomita-Takesaki theorem allows one to construct one of the main tools of the theory.

Definition 2.7. (Modular automorphisms group) The *modular automorphism group* $\sigma^\omega : \mathbb{R} \to \mathrm{Aut}(\mathfrak{M})$ of the pair $(\mathfrak{M}, \omega)$ is defined through

$$\sigma_t^\omega(x) := \pi_\omega^{-1}(\Delta_\omega^{it} \pi_\omega(x) \Delta_\omega^{-it}) \qquad x \in \mathfrak{M}\,, \quad t \in \mathbb{R}\,. \tag{2.7}$$

This construction shows that the pair $(\mathfrak{M}, \omega)$ is a dynamical object. The celebrated Connes' theorem of Radon-Nikodym type consists of a cocycle relation among the modular groups of different states on the same von Neumann algebra. A fundamental characterization of the modular group is the following.

Theorem 2.8. (Modular condition) *The modular group $\sigma^\omega : \mathbb{R} \to \mathrm{Aut}(\mathfrak{M})$ of the pair $(\mathfrak{M}, \omega)$ satisfies the following properties (referred to as the modular condition):*
i) $\{\sigma_t^\omega : t \in \mathbb{R}\}$ *leaves the state ω invariant,*

$$\omega = \omega \circ \sigma_t^\omega \qquad t \in \mathbb{R} \tag{2.8}$$

ii) *for all $x, y \in \mathfrak{M}$ there exists a bounded continuous function $F_{x,y}$ on the closed strip $\overline{D} = \{z \in \mathbb{C} : 0 \le \mathrm{Im} z \le 1\}$ which is holomorphic in the interior D of $\overline{D}$ and satisfies*

$$F(t) = \omega(\sigma_t^\omega(x) y)\,, \qquad F(t+i) = \omega(y \sigma_t^\omega(x)) \qquad t \in \mathbb{R}\,. \tag{2.9}$$

Moreover, given ω, the modular group is uniquely determined by the above modular condition.

The celebrated *KMS-condition* on one-parameter automorphism groups and states of C*-algebras, deeply related to the above relation (2.9), plays a fundamental role in Quantum Statistical Mechanics in association with the ideas of time evolution and equilibrium. See Section 2.3 and Chapter 3.

Example 2.9. (Modular automorphisms groups on type I factors) When $\mathfrak{M} = \mathcal{B}(H)$ is the algebra of all bounded operators on a separable Hilbert space H, a normal state ω can always be represented as

$$\omega(x) = \mathrm{Trace}(\rho\, x) \qquad x \in \mathcal{B}(H) \tag{2.10}$$

for some positive, trace-class operator $\rho \in \mathcal{B}(H)$, so that ω is faithful if and only if ρ is not singular. The modular automorphism group then reduces to $\sigma_t^\omega(x) = \rho^{it} x \rho^{-it}$ for all $x \in \mathcal{B}(H)$ and $t \in \mathbb{R}$. In particular, if $\mathfrak{M} = M_n(\mathbb{C})$, $\{e_{kl}; k, l = 1, \ldots, n\}$ is the system of matrix units and ρ is diagonal, one has

$$\sigma_t(e_{kl}) = \Big(\frac{\lambda_k}{\lambda_l}\Big)^{it} e_{kl} \qquad k, l = 1, \ldots, n\,,$$

where $\{\lambda_k : k = 1, \ldots, n\}$ denote the list of eigenvalues of ρ.

Example 2.10. (Modular automorphisms groups on Powers factors) Let $\mathfrak{M}_n$ be a copy of $M_2(\mathbb{C})$ for all $n \in \mathbb{N}^*$ and consider the sequence of states $\omega_n : \mathfrak{M}_n \to \mathbb{C}$, corresponding to a fixed $\lambda \in (0,1)$ and given by

$$\omega_n([x_{ij}]_{i,j=1}^2) = \lambda x_{11} + (1-\lambda) x_{22} \qquad [x_{ij}]_{i,j=1}^2 \in \mathfrak{M}_n\,.$$

Let A be the (unital) inductive limit of the C*-algebras

$$A_n := \mathfrak{M}_1 \otimes \mathfrak{M}_2 \otimes \ldots \mathfrak{M}_n\,,$$

obtained embedding A_n into A_{n+1} by $a \mapsto a \otimes 1$. On the C*-algebra A, a state ω is defined such that

$$\omega(x_1 \otimes \ldots x_n \otimes 1 \otimes \ldots) = \omega_1(x_1)\omega_2(x_2)\ldots\omega_n(x_n) \qquad n \in \mathbb{N}^*\,,$$

so that we may consider the von Neumann algebra $\mathfrak{M}$ generated by A in the GNS representation of ω. The modular automorphisms group of its normal extension is then given by

$$\sigma_t(x_1 \otimes \ldots x_n \otimes 1 \otimes \ldots) = \sigma_t^1(x_1)\sigma_t^2(x_2)\ldots\sigma_t^n(x_n) \qquad n \in \mathbb{N}^*\,,$$

where σ_t^n is the modular group of ω_n on $\mathfrak{M}_n = M_2(\mathbb{C})$, described in the previous example.

Let $\mathfrak{M}$ be a von Neumann algebra of operators acting on a Hilbert space $\mathcal{H}$ and let $\xi \in \mathcal{H}$ be a fixed cyclic and separating for $\mathfrak{M}$. To define the standard cone in $\mathcal{H}$, denote by $j_\xi : \mathfrak{M} \to \mathfrak{M}'$ the anti-linear, involutive isomorphism defined by the Tomita-Takesaki theorem:

$$j_\xi(x) := J_\xi x J_\xi \qquad x \in \mathfrak{M} \subseteq \mathcal{B}(\mathcal{H})\,. \tag{2.11}$$

Notice that if ξ is a *trace vector*, in the sense that the associated functional $\omega(\cdot) = (\xi| \cdot \xi)$ is a trace, this map coincides with the involution: $j_\xi(x) = x^*$ for all $x \in \mathfrak{M}$.

Definition 2.11. (Standard cone of a von Neumann algebra) The *standard cone* $\mathcal{H}_\xi^+$ associated with the pair $(\mathfrak{M}, \xi)$ is defined as the closure of the set

$$\{xj_\xi(x)\xi \in \mathcal{H} : x \in \mathfrak{M}\} .$$

Example 2.12. (Standard positive cone of finite von Neumann algebras) Since, by the Spectral Theorem, any positive element $y \in \mathfrak{M}_+$ can be written as $y = xx^*$ for some $x \in \mathfrak{M}$, in case ξ is the *trace vector* representing a finite trace on $\mathfrak{M}$, as in Example 2.5, the cone $\mathcal{H}_\xi^+$ coincides with $\overline{\mathfrak{M}_+ \xi_\omega}$. In particular, in the commutative case of Example 2.1, the definition above allows the recovery of the fact that positive, square integrable functions can be approximated by positive, essentially bounded ones.

The above example and the properties listed below suggest that the natural positive cone $\mathcal{H}_\xi^+$ should be considered as the analogue of the cone of positive L^2-functions of the commutative case. We omit the proof and refer to [BR1 2.5.4].

Proposition 2.13. *Let $\mathfrak{M}$ be a von Neumann algebra acting on the Hilbert space $\mathcal{H}$, with $\xi \in \mathcal{H}$ a cyclic and separating vector for $\mathfrak{M}$. The natural positive cone $\mathcal{H}_\xi^+$ has the following properties:*

i) $\mathcal{H}_\xi^+$ is a self-dual set and in particular is a closed, convex cone in $\mathcal{H}$;

ii) $\mathcal{H}_\xi^+ = \overline{\Delta_\xi^{1/4}\mathfrak{M}_+\xi} = \overline{\Delta_\xi^{-1/4}\mathfrak{M}'_+\xi}$

iii) $J_\xi\xi = \xi$ for all $\xi \in \mathcal{H}_\xi^+$;

iv) $xj_\xi(x)\mathcal{H}_\xi^+ \subseteq \mathcal{H}_\xi^+$ for all $x \in \mathfrak{M}$;

v) $\Delta_\xi^{it}\mathcal{H}_\xi^+ = \mathcal{H}_\xi^+$ for all $t \in \mathbb{R}$;

vi) $f(\log \Delta_\xi)\mathcal{H}_\xi^+ \subseteq \mathcal{H}_\xi^+$ for all positive-definite, continuous functions f on $\mathbb{R}$.

Property i), together with Proposition 2.3, implies that the Jordan decomposition can be achieved in the ordered vector space $(\mathcal{H}_\xi, \mathcal{H}_\xi^+)$, while property iii) reveals that J_ξ coincides with the anti-unitary involution associated to the positive cone $\mathcal{H}_\xi^+$, as in Proposition 2.3. Property iv) is a consequence of the very definition of $\mathcal{H}_\xi^+$ and the fact that for $x, y \in \mathfrak{M}$, $x \in \mathfrak{M}$ and $j_\xi(y) \in \mathfrak{M}'$ necessarily commute. The identities in item ii) show that the natural positive cone is an intermediate deformation of the cones $\overline{\mathfrak{M}_+ \xi_\omega}$ and $\overline{\mathfrak{M}'_+ \xi_\omega}$. Property v) provides a first natural example of a one-parameter family of *positive operators*, i.e. operators leaving globally invariant the natural positive cone. Maps and families of this type will be of interest below. Property vi) follows from v) since continuous, positive definite functions are, by a classical result S. Bochner on the Fourier transform of finite, positive measures. Examples of continuous, positive definite functions are $f^t(x) = e^{itx}$ for $t \in \mathbb{R}$, $f^t(x) = e^{-tx^2}$ for $t > 0$ and $f^t(x) = e^{-t|x|}$ for $t > 0$.

Remark 2.14. (Non self-polar cones) H. Araki studied in [Ara] properties analogous to those above, in particular generalizations of the Jordan decomposition, for the whole family of cones $V_\xi^\alpha = \overline{\Delta_\xi^\alpha \mathfrak{M}_+ \xi}$ for $\alpha \in [0, 1/2]$. Despite the lack of all the symmetries the cone $V_\xi^{1/4} = \mathcal{H}_\xi^+$ has, the positive cones corresponding to $\alpha \neq 1/4$, *although non self-polar*, are important constructing an interpolating family of spaces $L^p(\mathfrak{M})$, $1 \leq p \leq +\infty$, which generalizes at the von Neumann algebra level the familiar family of Lebesgue spaces (see [Ko], [Te]).

In the commutative case, equivalent measures μ, ν on a space X give rise to the same von Neumann algebra $L^\infty(X, \mu) = L^\infty(X, \nu)$. We can look at this as two different representations of the von Neumann algebra of essentially bounded functions defined by the σ-algebra of sets of vanishing measure. In a precise sense this holds true for general von Neumann algebras and to state it correctly we introduce the following definition.

Definition 2.15. (Standard form of a von Neumann algebra) A *standard form* $(\mathfrak{M}, \mathcal{H}, \mathcal{H}^+, J)$ of a von Neumann algebra $\mathfrak{M}$ acting on a Hilbert space $\mathcal{H}$ consists of a *self-dual cone* $\mathcal{H}^+$ and an anti-linear involution J, satisfying:

i) $J\mathfrak{M}J = \mathfrak{M}'$;

ii) $JxJ = x^* \qquad \forall x \in \mathfrak{M} \cap \mathfrak{M}' \qquad$ (the center of $\mathfrak{M}$);

iii) $J\eta = \eta \qquad \forall \eta \in \mathcal{H}^+$;

iv) $xJxJ(\mathcal{H}^+) \subseteq \mathcal{H}^+ \qquad \forall x \in \mathfrak{M}$.

In the commutative case, in which the von Neumann algebra is described as $L^\infty(X, \mu)$ for some finite measure μ on X, all standard forms appear as

$$(L^\infty(X, \mu), L^2(X, \nu), L^2_+(X, \nu), J)$$

for some measure ν equivalent to μ. Here the antilinear involution is just complex conjugation: $Ja(x) = \overline{a(x)}$, ν-a.e. on X.

Proposition 2.13 tells us that modular theory allows the constructionof standard forms of von Neumann algebras starting from faithful, normal state on them. As in the commutative case, we are going to see that all standard forms look essentially the same.

Proposition 2.16. *(Uniqueness of standard forms of von Neumann algebras) Let $(\mathfrak{M}_i, \mathcal{H}_i, \mathcal{H}_i^+, J_i)$, $i = 1, 2$, be standard forms of two von Neumann algebras $\mathfrak{M}_1, \mathfrak{M}_2$. If $\alpha : \mathfrak{M}_1 \to \mathfrak{M}_2$ is an isomorphism of $\mathfrak{M}_1$ onto $\mathfrak{M}_2$ then there exists a unique unitary $U : \mathcal{H}_1 \to \mathcal{H}_2$ such that:*

i) $\alpha(x) = UxU^* \qquad x \in \mathfrak{M}_1$*;*

ii) $J_2 = UJ_1U^*$*;*

iii) $\mathcal{H}_2^+ = U\mathcal{H}_1^+$*.*

iv) Moreover, when $\mathcal{H}_1 = \mathcal{H}_2$*, the map* $U \mapsto \alpha_U(\cdot) := U \cdot U^*$ *establishes a topological isomorphism between the subgroup*

$$\{U \in \mathcal{U}(\mathcal{H}) : U\mathfrak{M}U^* = \mathfrak{M}, \quad UJU^* = J, \quad U\mathcal{H}^+ = \mathcal{H}^+\}$$

of the group $\mathcal{U}(\mathcal{H})$ *of all unitary operators on* $\mathcal{H}$ *and the group* $\mathrm{Aut}(\mathfrak{M})$ *of all automorphisms of* $\mathfrak{M}$*.*

Hence, in the above sense, all standard forms of a von Neumann algebra are unitarily equivalent; a unified notation for them is $(\mathfrak{M}, L^2(\mathfrak{M}), L^2_+(\mathfrak{M}), J)$, as justified by the properties listed in Proposition 2.3, Proposition 2.13 and by the consideration of the commutative case discussed above.

We already met an example of property iv) in the above proposition, by which any automorphism, or group of them, can always be unitarily implemented in any standard form: namely the modular group of a faithful normal state (see Definition 2.7 and Proposition 2.13 v)).
A practical consequence of the uniqueness of a standard form is that in working with them we have the freedom to choose the most suitable for the problem at hand. Here are some illustrations of this.

Example 2.17. (Hilbert-Schmidt standard form of type I factors) Let $\mathfrak{M} = \mathcal{B}(H)$ be the type I factor of all bounded operator on a Hilbert space H. In the Hilbert space $\mathcal{L}^2(H)$ of all Hilbert-Schmidt operators on H, the cone $\mathcal{L}^2_+(H)$ of the positive ones is self-dual. The related involution J associates to the Hilbert-Schmidt operator ξ its adjoint ξ^*. Moreover

$$(\mathcal{B}(H)\,, \mathcal{L}^2(H)\,, \mathcal{L}^2_+(H)\,, J)$$

is a standard form of $\mathcal{B}(H)$. This standard form may be constructed by an extension of the Tomita-Takesaki theory which deal with faithful, semi-finite, normal weights on von Neumann algebras, as indeed is the trace $\mathrm{Tr} : \mathcal{B}(H)_+ \to [0, +\infty]$ on the algebra of all bounded operators. Notice that, under the identification $\mathcal{L}^2(H) = H \otimes \overline{H}$, the positive cone $\mathcal{L}^2_+(H)$ is generated by the elementary elements of the form $x \otimes \overline{x}$, $x \in H$ while the involution acts as $J(x \otimes \overline{y}) = y \otimes \overline{x}$, $x, y \in H$. Here $\overline{H}$ denotes the *opposite Hilbert space* and $\overline{x}\,, \overline{y}$ its elements. In terms of the Dirac's *bra-ket* notation: $x \otimes \overline{y} = |x\rangle\langle y|$.

Example 2.18. (Generalized Hilbert-Schmidt standard form) The construction above of standard forms of Type I factors, may be generalized to any von Neumann algebra using the *relative tensor product of Hilbert modules* (see [S1]).

Example 2.19. (Modular operators on type I factors) Consider on the above type I factor $\mathcal{B}(H)$, the normal state $\omega(x) := \mathrm{Tr}(\rho x)$ associated to a positive, trace-class operator $\rho \in \mathcal{B}(H)$. By Proposition 2.16 the standard form of the GNS representation of ω is isomorphic the Hilbert-Schmidt standard form considered in Example 2.17. We may then look for the realizations of the modular operators in this representation. Clearly the modular conjugation coincides with the operation of taking the adjoint, as it depends upon the positive cone only, by Proposition 2.3. The state ω can be represented as $\omega(x) = (\xi_\rho | x\xi_\rho)_{\mathcal{L}^2(H)}$ for a unique positive Hilbert-Schmidt operator $\xi_\rho \in \mathcal{L}^2_+(H)$ which then represents the cyclic and separating vector associated to ω. Since this means that $\mathrm{Tr}(\rho x) = \mathrm{Tr}(\xi_\rho x \xi_\rho)$ for all Hilbert-Schmidt operators x on H, one identifies $\xi_\rho = \rho^{1/2}$. To recover the action of the modular operator notice that, by definition,

$$J\Delta^{1/2}(x\xi_\rho) = x^*\xi_\rho\,, \qquad x \in \mathcal{B}(H)\,.$$

Then $\Delta^{1/2}(x\rho^{1/2}) = \rho^{1/2}x$ for all $x \in \mathcal{B}(H)$ so that

$$\Delta^{1/2}\xi = \rho^{1/2}\xi\rho^{-1/2}$$

for all $\xi \in D(\Delta^{1/2}) := \{\eta \in \mathcal{L}^2(H) : \rho^{1/2}\eta\rho^{-1/2} \in \mathcal{L}^2(H)\}$. One may check that the ideal of finite rank operators is an operator core for $\Delta^{1/2}$. This result then makes it easy to identify the action of the modular group:

$$\sigma_t^\omega(x) = \rho^{it}x\rho^{-it} \qquad x \in \mathcal{B}(H)\,, \qquad t \in \mathbb{R}\,.$$

An important example of standard form in harmonic analysis is the following one.

Example 2.20. (Standard forms of group von Neumann algebras and the Fourier transform) Consider a unimodular, locally compact group G and denote by $s, t \dots$ its elements and by $ds, dt \dots$ a fixed Haar measure on it. On the Hilbert space $L^2(G)$ the *left regular representation* λ of G is defined by

$$\lambda : G \to \mathcal{B}(L^2(G))\,, \qquad (\lambda(s)f)(t) = f(s^{-1}t) \quad s,t \in G\,, \quad f \in L^2(G)\,.$$

The associated von Neumann algebra is, by definition, the weak*-closure in $\mathcal{B}(L^2(G))$ of the group of unitaries $\lambda(G)$. By von Neumann's density theorem [Dix2] it coincides both with the double commutant $\lambda(G)''$ of $\lambda(G)$ and with the weak*-closure of the algebra $L^1(G)$ acting on $L^2(G)$ by left convolution

$$(f * g)(t) := \int_G f(s)g(s^{-1}t)ds \qquad t \in G\,, \qquad f \in L^1(G)\,, \qquad g \in L^2(G)\,.$$

A standard form of $\lambda(G)''$ is defined in the Hilbert space $L^2(G)$ by considering the involution

$$Jf(s) = \overline{f(s^{-1})}\,, \quad s \in G\,, \quad f \in L^2(G)$$

and the self-polar cone

$$\mathcal{H}_G^+ = \overline{\{f * Jf : f \in C_c(G)\}}\,,$$

where $C_c(G)$ denote the space of compactly supported continuous functions on G. $\mathcal{H}_G^+$ coincides with the cone of positive definite, square summable functions on G. These properties are proved in [Dix2]. Their generalization to a non unimodular group can be found in [Pen].

When G is commutative, the von Neumann algebra $\lambda(G)''$ is isomorphic to the abelian von Neumann algebra $L^\infty(\widehat{G})$ of essentially bounded functions on the Pontriagyn dual $\widehat{G}$, with respect to any of its Haar measures. The Fourier transform $F : L^2(G) \longrightarrow L^2(\widehat{G})$, is then a unitary operator with the properties i), ii) and iii) of Proposition 2.16, which implements that isomorphism.

2.2 Order Structures and Symmetric Embeddings

The positive cones $\mathfrak{M}_+$, $\mathcal{H}^+$ and $\mathfrak{M}_{*+}$ endow the von Neumann algebra $\mathfrak{M}$, the standard Hilbert space $\mathcal{H}$ and the pre-dual space $\mathfrak{M}_*$ with structures of ordered vector spaces. More precisely, what we get is a complex vector space E, complexification $E = E_\mathbb{R} \bigoplus E_\mathbb{R}$ of a real subspace $E_\mathbb{R}$, which in turn is linearly generated, over $\mathbb{R}$, by the cone E_+: $E_\mathbb{R} = E_+ - E_+$.
The order relation between real elements elements e_1, e_2 of an ordered vector space (E, E_+) will be indicated as customary: $e_1 \le e_2$ will mean that $e_2 - e_1 \in E_+$. The elements of E_+ are exactly those real vectors e in E such that $0 \le e$. The *order interval* $[e_1, e_2] \subset E$, defined by two real elements e_1, e_2 of E such that $e_1 \le e_2$, is defined by

$$[e_1, e_2] := \{e \in E : e_1 \le e \le e_2\}\,.$$

For example, the order interval $[0,1]$ in the abelian von Neumann algebra $L^\infty(X,m)$ (resp. in the standard Hilbert space $L^2(X,m)$) consists of those real valued functions a, m-a.e. defined on X (resp. belonging to $L^2(X,m)$) such that $0 \le a(x) \le 1$ for m-almost all $x \in X$.

Complex linear maps $L : E \longrightarrow F$ between complex ordered vector spaces (E, E_+) and (F, F_+), will be called *real* if $L(E_\mathbb{R}) \subseteq F_\mathbb{R}$ and *positive* if moreover $L(E_+) = F_+$.

The tools we need to compare maps and semigroups on von Neumann algebras, their standard Hilbert spaces and their pre-dual spaces, are the *symmetric embeddings*. These embeddings, for example, make it possible to *recognize* the elements of the von Neumann algebra $\mathfrak{M}$ within the standard Hilbert space $\mathcal{H}$, in such a way that an element is positive in $\mathfrak{M}$ if and only if is positive in $\mathcal{H}$. These embeddings generalize the commutative situation in which, for a finite measure m, one has

$$L^\infty(X,m) \subseteq L^2(X,m) \subseteq L^1(X,m)\,.$$

Let $(\mathfrak{M}, \mathcal{H}, \mathcal{H}^+, J)$ be a *standard form* of a von Neumann algebra $\mathfrak{M}$, with $J_0\,, \Delta_0$ the modular operators associated to a cyclic and separating vector $\xi_0 \in \mathcal{H}^+$ and $\omega_0(\cdot) = (\xi_0 | \cdot \xi_0)$ the corresponding normal state.

When $\mathfrak{M}$ is commutative, or at least when ξ_0 is a trace vector, the embedding $x \mapsto x\xi_0$ of the von Neumann algebra $\mathfrak{M}$ into the Hilbert space $\mathcal{H}$ *is injective, continuous with norm dense range and positivity preserving.* In case ξ_0 is not a trace vector, a "distortion" of the above embedding makes it possible to keep all these properties throughout.

Definition 2.21. (Symmetric embeddings) The symmetric embeddings associated to the standard form $(\mathfrak{M}, \mathcal{H}, \mathcal{H}^+, J)$ and a cyclic and separating vector $\xi_0 \in \mathcal{H}^+$ are defined as follows:

i) $i_0 : \mathfrak{M} \to \mathcal{H} \qquad i_0(x) := \Delta_0^{1/4} x\xi_0 \qquad x \in \mathfrak{M}$;

ii) $i_{0*} : \mathcal{H} \to \mathfrak{M}_* \qquad \langle i_{0*}(\xi), y\rangle = (i_0(y^*)|\,\xi) = (\Delta_0^{1/4} y^*\xi_0|\,\xi) \quad \xi \in \mathcal{H}\,, y \in \mathfrak{M}$;

iii) $j_0 : \mathfrak{M} \to \mathfrak{M}_* \qquad \langle j_0(x), y\rangle = (J_0 y\xi_0 | x\xi_0) \qquad x, y \in \mathfrak{M}$.

These maps are well defined because $\mathfrak{M}\xi_0 \subseteq D(\Delta_0^{1/2})$, by the definition of the modular operator, and because $D(\Delta_0^{1/2}) \subseteq D(\Delta_0^{1/4})$ by the Spectral Theorem.

In the following we consider the spaces $\mathfrak{M}\,, \mathcal{H}\,, \mathfrak{M}_*$ ordered by their positive cones $\mathfrak{M}_+\,, \mathcal{H}^+\,, \mathfrak{M}_{*+}$. We will denote by $\sigma(\mathfrak{M}, \mathfrak{M}_*)$ the weak*-topology of $\mathfrak{M}$, by $\sigma(\mathfrak{M}_*, \mathfrak{M})$ the weak-topology of $\mathfrak{M}_*$ and by $\sigma(\mathcal{H}, \mathcal{H})$ the weak-topology of $\mathcal{H}$.

Proposition 2.22. *The above maps are bounded, positivity preserving injections with norm dense range. Moreover we have*

i) i_0 is the dual map of i_{0*} and $j_0 = i_{0*} \circ i_0$;

ii) i_0 is an order isomorphism between the order-intervals $[0, 1_A]$ in $\mathfrak{M}$ and $[0, \xi_0]$ in $\mathcal{H}$;

iii) i_{0*} is an order isomorphism between the order-intervals $[0, \xi_0]$ in $\mathcal{H}$ and $[0, \omega_0]$ in $\mathfrak{M}_*$;

iv) the map i_0 is $\sigma(\mathfrak{M}, \mathfrak{M}_*) - \sigma(\mathcal{H}, \mathcal{H})$-continuous

v) the map i_{0*} is $\sigma(\mathcal{H}, \mathcal{H}) - \sigma(\mathfrak{M}_*, \mathfrak{M})$-continuous

vi) the map j_0 is $\sigma(\mathfrak{M}, \mathfrak{M}_*) - \sigma(\mathfrak{M}_*, \mathfrak{M})$-continuous.

In particular, item ii) tells us how to identify the algebra $\mathfrak{M}$ in the Hilbert space $\mathcal{H}$: for example, an element $\xi \in \mathcal{H}^+$ is of the form $\Delta_0^{1/4} x\xi_0$ for some

$x \geq 0$ if and only if $0 \leq \xi \leq k\xi_0$ for some $k \geq 0$. Moreover, the algebra norm can be read from the order structure of the positive cone:

$$\|x\|_{\mathfrak{M}} = \inf\{k \in [0, +\infty) : 0 \leq \xi \leq k\xi_0\}\,.$$

Example 2.23. (Symmetric embedding on type I factors) Consider on the type I factor $\mathcal{B}(H)$, the normal state $\omega(x) := \mathrm{Tr}(\rho x)$ associated to a positive, trace-class operator $\rho \in \mathcal{B}(H)$ and the Hilbert-Schmidt standard form considered in Example 2.19. It is easy to verify that $\Delta^{1/4}\xi = \rho^{1/4}\xi\rho^{-1/4}$ for all $\xi \in D(\Delta^{1/4})$ so that, since the cyclic vector is $\xi_\rho = \rho^{1/2}$, we have $\Delta^{1/4}(x\xi_\rho) = \Delta^{1/4}(x\rho^{1/2}) = \rho^{1/4}x\rho^{1/4}$ for all $x \in \mathcal{B}(H)$. It is then clear why the symmetric embedding i_0 carries a positive element x of the von Neumann algebra into a positive element $i_0(x)$ of the standard Hilbert space. The isomorphism in item ii) of the above proposition reduces, in this case, to the fact that for a positive bounded operator x on H and some $k \geq 0$, $\rho^{1/4}x\rho^{1/4} \leq k\rho^{1/2}$ is equivalent to $x \leq k \cdot 1_{\mathcal{B}(H)}$.

Since $\mathfrak{M}\xi_0 \subseteq D(\Delta_0^{1/2}) \subseteq D(\Delta_0^{1/4})$, for any $x \in \mathfrak{M}$ we have

$$\begin{aligned}\|i_0(x)\|^2_{\mathcal{H}} &= (\Delta_0^{1/4}x\xi_0|\,\Delta_0^{1/4}x\xi_0)_{\mathcal{H}} = (\Delta_0^{1/2}x\xi_0|\,x\xi_0)_{\mathcal{H}} = (J_0x^*\xi_0|\,x\xi_0)_{\mathcal{H}} \\ &= \langle j_0(x), x\rangle \leq \|x^*\|_{\mathfrak{M}} \cdot \|j_0(x)\|_{\mathfrak{M}_*} = \|x\|_{\mathfrak{M}} \cdot \|j_0(x)\|_{\mathfrak{M}_*}\,.\end{aligned}$$

This may suggest that these embeddings form the skeleton of a *symmetric*, complex interpolation system among the spaces $\mathfrak{M}$, $\mathcal{H}$, $\mathfrak{M}_*$. This is in fact the case and it is the starting point for the construction of *noncommutative L^p-spaces* (see for example [H2], [Ko], [Te]). We refer to Sections 5 and 6 of Quanhua Xu's Lectures in this volume for a detailed exposition of this matter. In particular we extrapolate the following result from [Te], which we will need later on.

Proposition 2.24. *(Noncommutative interpolation) Let $(\mathfrak{M}, \mathcal{H}, \mathcal{H}^+, J)$ be a standard form of a von Neumann algebra $\mathfrak{M}$, $\xi_0 \in \mathcal{H}^+$ a cyclic and separating vector and i_0, i_{0*} and j_0 the associated symmetric embeddings of $\mathfrak{M}$ into $\mathcal{H}$, $\mathcal{H}$ into $\mathfrak{M}_*$ and $\mathfrak{M}$ into $\mathfrak{M}_*$, respectively.*
Let $T_1 : \mathfrak{M}_* \to \mathfrak{M}_*$ be a map such that

$$T_1(j_0(\mathfrak{M})) \subseteq j_0(\mathfrak{M})\,, \qquad T_1(i_{0*}(\mathcal{H})) \subseteq i_{0*}(\mathcal{H}).$$

Denote by $T_\infty : \mathfrak{M} \to \mathfrak{M}$ and $T_2 : \mathcal{H} \to \mathcal{H}$ be the maps determined by

$$T_1 \circ j_0 = j_0 \circ T_\infty\,, \qquad T_1 \circ i_{0*} = i_{0*} \circ T_2\,.$$

Then, if T_1 and T_∞ are bounded with norm M_1 and M_∞, respectively, then T_2 is bounded with norm less than $M_1^{1/2} \cdot M_\infty^{1/2}$

$$\|T_2\xi\|^2_{\mathcal{H}} \leq M_1 \cdot M_\infty \|\xi\||^2_{\mathcal{H}} \qquad \xi \in \mathcal{H}\,. \tag{2.12}$$

In particular, if T_1 and T_∞ are contractive then T_2 is contractive too.

2.3 KMS-symmetric Maps and Semigroups on C* and von Neumann Algebras

In this section we introduce one of the main object of our investigation: *KMS-symmetric semigroups on C* and von Neumann algebras* and, in particular, *KMS-symmetric, positive and Markovian semigroups.* In the von Neumann algebra case and with respect to the modular automorphism group, this class of semigroups was introduced in [Cip1], [GL1,2]. KMS-symmetric positive and Markovian semigroups were introduced in [Cip2]. *The consideration of KMS-symmetric semigroups on C* algebras, which are not necessarily positive or Markovian, is a novelty.*

Markovian semigroups, symmetric with respect to traces, were introduced by L. Gross [G1],[G2] to study physical Hamiltonians of Boson and Fermion systems. A general theory of Dirichlet forms on algebras endowed with reasonable traces was developed by S.Albeverio and R.Hoegh-Krohn [AHK1,2] and later studied by J.M.Lindsay and E.B.Davies [DL1,2] and by J.L.Sauvageot [S2,3].

In a commutative situation, a map Φ, or a semigroup of them, on the C*-algebra $C_0(X)$ can be extended to the von Neumann algebra $L^\infty(X,m)$, its predual $L^1(X,m)$ and the standard Hilbert space $L^2(X,m)$, for *any* finite Radon measure m on X with respect to which Φ is *symmetric*:

$$\int_X \Phi(f)\cdot g\,dm = \int_X f\cdot\Phi(g)\,dm \qquad f,g\in C_0(X)\,.$$

These extensions, considered mainly for positive, or Markovian, maps and semigroups, are of great value for constructing and studying symmetric Markov processes (see [FOT]) and interacting particle systems (see [Lig]).

In this section we show how such an extension program can be carried out on any C*-algebra, provided a suitable *symmetry* holds true with respect to *KMS-states* (see [BR2]). States in this class, introduced by the physicists R. Kubo [Kub], D.C. Martin and J. Schwinger [MS], and identified mathematically by R. Haag, N.M. Hugenoltz and M. Winnink [HHW], are fundamental for representing equilibria of quantum systems of infinite degrees of freedom and thermal reservoirs (see [BR2], [Sew], [KFGV]). The symmetry condition we introduce is a generalization of the detailed balance condition (see [Al], [D1] and [KFGV]).

Unless otherwise stated, maps $(\Phi, D(\Phi))$ on a C-algebra A will always be considered real, in the sense that their domain $D(\Phi)$ is an involutive subspace of A and $\Phi(a^*) = \Phi(a)^*$ for all a in $D(\Phi)$. For simplicity, we will work with unital C*-algebras. Otherwise, one may add a unit to A or consider A embedded into its (unital) enveloping von Neumann algebra A^{**}.*

Definition 2.25. (**Positive and Markovian semigroups**) A map $\Phi : A \to A$ on a C*-algebra A is said to be

i) *positive* if $\Phi(A_+) \subseteq A_+$;

ii) *Markovian* if it is positive and $\Phi(a) \leq 1_A$ whenever $a = a^*$ and $a \leq 1_A$;

iii) *completely positive* (resp. *completely Markovian*), if for every $n \in \mathbb{N}^*$ the matricial extension

$$\Phi \otimes I_n : \mathrm{M}_n(A) \to \mathrm{M}_n(A) \qquad (\Phi \otimes I_n)[a_{ij}]_{i,j=1}^n := [\Phi(a_{ij})]_{i,j=1}^n$$

is positive (resp. Markovian) on the C*-algebra $\mathrm{M}_n(A) = A \otimes \mathrm{M}_n(\mathbb{C})$ of $n \times n$-matrices with entries in A.

iv) A *one-parameter semigroup* $\{\Phi_t : t \geq 0\}$ on A is said to be *positive* (resp. *completely positive, Markovian, completely Markovian*) provided Φ_t is positive (resp completely positive, Markovian, completely Markovian) for all $t \geq 0$.

Since an element a of A is in the closed unit ball ($\|a\| \leq 1$) if and only if the element $\begin{pmatrix} 1_A & a \\ a^* & 1_A \end{pmatrix}$ is positive in $\mathrm{M}_2(A)$, one sees that *completely Markovian semigroups are just completely positive contraction semigroups.* This class of semigroups, often called *dynamical semigroups* in the literature, is of special importance for application to Quantum Open Systems [D1] and Quantum Probability. We refer to Philippe Biane's Lectures in this volume for the important connection between Markovian semigroups and stochastic processes in noncommutative spaces.

The structure of generators of σ-weakly continuous, completely Markovian semigroups on von Neumann algebras, symmetric with respect to traces will be carefully studied in Chapter 4.

Example 2.26. (Structure of norm continuous, completely positive semigroups) Uniform continuity forces the semigroup to have a bounded generator $L : A \to A$ (see [BR1 Proposition 3.1.1]):

$$\Phi_t = \sum_{n \geq 0} \frac{t^n}{n!} L^n \,, \qquad L^n(a) := L(L(\ldots L(a)))\,, \quad a \in A\,.$$

Suppose A is acting on the Hilbert space h and $\{\Phi_t : t \geq 0\}$ is norm continuous and completely positive. Then, by a theorem due G. Lindblad [Lin] and V. Gorini-A. Kossakowsi-E.C.G. Sudarsan [GKS], for matrices, and to E. Christensen-D. E. Evans [CE] for general C*-algebras, the generator L may be represented as

$$L(a) = i[H, a] + (Ra + aR) - \phi(a)\,,$$

where $H = H^*$ is a self-adjoint operator on h belonging to the σ-weak closure $\mathfrak{M} \subseteq B(h)$ of A, $\phi : A \to \mathfrak{M}$ is a completely positive map and $R = L(1_A) - \phi(1_A)$. Moreover, combining this result with the fundamental Stinespring theorem [Sti] (see Appendix 7.3), one obtains the general form of the generator of a norm continuous, σ-weakly continuous, completely positive, identity preserving semigroup on a von Neumann algebra $\mathfrak{M} \subseteq B(h)$:

$$L(a) = i[H, a] + \sum_{k\in I} y_k^* y_k a - 2y_k^* a y_k + a y_k^* y_k$$

where $\{y_k \in B(h) : k \in I\}$ is a family such that the operator $\sum_{k\in I} y_k^* y_k$ is bounded and $\sum_{k\in I} y_k^* a y_k \in \mathfrak{M}$ for all $a \in \mathfrak{M}$. Operators L of the above type are called *Lindblad generators*. The structure of generators of strongly continuous Markovian semigroups which are symmetric with respect to a semifinite faithful trace will be investigated in Chapter 4.

To introduce the second main ingredient of this section, we recall that, for a strongly (resp. σ-weakly) continuous group of automorphisms $\alpha := \{\alpha_t : t \in \mathbb{R}\}$ of a C* (resp. von Neumann) algebra A, we denote by A_α the norm (resp. σ-weakly) dense, α-invariant *-subalgebra of α-analytic elements of A (see Appendix 7.3).

On a finite dimensional C*-algebra, say $A = M_n(\mathbb{C})$, any automorphism group appears as

$$\alpha_t(a) = e^{itH} a e^{-itH} \qquad a \in A$$

for a self-adjoint matrix H. It is easy to see, using the cyclicity of the trace, that the state

$$\omega(a) = \mathrm{Trace}(e^{-\beta H} a)/\mathrm{Trace}(e^{-\beta H})$$

satisfies the relation

$$\omega(ba) = \omega(a\alpha_{i\beta}(b)) \qquad a, b \in A.$$

Moreover, ω is the unique state with this property and it may be thought of as the equilibrium state of a finite quantum system, whose time evolution is governed by the automorphism group.
States of the above type still exist in infinite dimensional situations, where, for example, A may be the C*-algebra $\mathcal{K}(h)$ of all compact operators on an infinite dimensional Hilbert space h. This, however, forces the dynamics to be generated by a Hamiltonian H with discrete spectrum. To avoid this restriction, one may considers the above relation between ω and α as the starting point for isolating a rich class of states. The only drawback involved in this point of view is that one has to abandon the idea of representing states in this class in the above simple way, i.e. by the density matrix $e^{-\beta H}/\mathrm{Trace}(e^{-\beta H})$.

Definition 2.27. (**KMS-states**) Let $\alpha := \{\alpha_t : t \in \mathbb{R}\}$ be a strongly continuous group of automorphisms of a C*-algebra A and $\beta \in \mathbb{R}$. A state ω is said to be a (α, β)-KMS state if it is α-invariant and if the following *KMS-condition* holds true:

$$\omega(a\alpha_{i\beta}(b)) = \omega(ba) \tag{2.13}$$

for all a, b in a norm dense, α-invariant *-subalgebra of A_α. If A is a von Neumann algebra and $\alpha := \{\alpha_t : t \in \mathbb{R}\}$ is a $\sigma(\mathfrak{M}, \mathfrak{M}_*)$-continuous group of automorphisms, a state ω is said to be a (α, β)-KMS state if ω is α-invariant, normal and the KMS-condition above holds true for all a, b in a $\sigma(\mathfrak{M}, \mathfrak{M}_*)$-dense, α-invariant *-subalgebra of A_α. KMS states corresponding to $\beta = 0$ are just the traces over A.

These states describe equilibria of quantum statistical systems, whose physical observables are represented by elements of A, corresponding to the time evolution represented by the automorphisms group $\{\alpha_t : t \in \mathbb{R}\}$ (see [BR2]). The parameter β, sometimes called the *inverse temerature*, is proportional to $h/2\pi T$, where T is the absolute temperature and h Planck's constant.

The KMS-condition above can be restated in a form similar to the modular condition in Theorem 2.8, independent of the consideration of a norm dense, α-invariant *-subalgebras of A_α.

Proposition 2.28. *(***KMS condition***)([BR2 Proposition 5.3.7]) Let $\alpha := \{\alpha_t : t \in \mathbb{R}\}$ be a strongly (resp. σ-weakly) continuous group of automorphisms of a C^* (resp. von Neumann) algebra A, $\beta \in \mathbb{R}$ and ω a state on A (normal in the von Neumann algebra case).*
Define D_β to be the domain $\{z \in \mathbb{C} : 0 < \mathrm{Im} z < \beta\}$ for $\beta \geq 0$ and $\{z \in \mathbb{C} : \beta < \mathrm{Im} z < 0\}$ for $\beta \leq 0$ and let $\overline{D_\beta}$ be the closure of D_β if $\beta \neq 0$ and $\overline{D_\beta} = \mathbb{R}$ for $\beta = 0$.
The following conditions are equivalent:

i) ω is a (α, β)-KMS state;

ii) for any pair $a, b \in A$, there exists a bounded, continuous function $F_{a,b} : \overline{D_\beta} \longrightarrow A$, which is analytic in D_β and such that

$$F_{a,b}(t) = \omega(a\alpha_t(b))\,, \qquad F_{a,b}(t + i\beta) = \omega(\alpha_t(b)a) \qquad t \in \mathbb{R}\,. \tag{2.14}$$

Furthermore, if the above conditions are satisfied, then the following bound holds true

$$|F_{a,b}(z)| \leq \|a\| \cdot \|b\| \qquad z \in \overline{D_\beta}\,.$$

Finally, for $a \in A\,, b \in A_\alpha$, the function $F_{a,b}$ is the restriction to $\overline{D_\beta}$ of the entire function $z \mapsto \omega(a\alpha_z(b))$.

A faithful normal state ω on a von Neumann algebra $\mathfrak{M}$ is a $(\sigma, -1)$-KMS state with respect to the modular automorphism group $\sigma^\omega : \mathbb{R} \to \mathrm{Aut}(\mathfrak{M})$ of the pair $(\mathfrak{M}, \omega)$ (see Definition 2.7).

Example 2.29. (KMS-states on CAR C*-algebras) Let $\mathfrak{h}_0$ be a pre-Hilbert space and $\mathfrak{h}$ its completion. Then there exists, a unique up to *-isomorphism, C*-algebra $\mathfrak{A}(\mathfrak{h})$ generated by a family $\{a(f) \in B(\mathfrak{h}) : f \in \mathfrak{h}_0\}$ of bounded operators satisfying

i) $\mathfrak{h}_0 \ni f \to a(f)$ is antilinear;
ii) $a(f)a(g) + a(g)a(f) = 0\,, \qquad f, g \in \mathfrak{h}_0\,;$
iii) $a(f)a(g)^* + a(g)^*a(f) = (f|g) \cdot \mathbb{I}_{\mathfrak{h}}\,, \qquad f, g \in \mathfrak{h}_0\,.$

The C*-algebra $\mathfrak{A}(\mathfrak{h})$ is called the CAR algebra over the Hilbert space $\mathfrak{h}$ or the algebra of canonical anti-commutation relations. It represents the algebra of physical observables of quantum mechanical systems obeying Fermi-Dirac statistics. Given a self-adjoint operator H on $\mathfrak{h}$, the map $\alpha : \mathbb{R} \to \mathrm{Aut}(\mathfrak{A}(\mathfrak{h}))$ defined by

$$\alpha_t(a(f)) := a(e^{itH} f)\,, \qquad \alpha_t(a^*(f)) := a^*(e^{itH} f) \qquad f \in \mathfrak{h}_0$$

defines a strongly continuous automorphism group of the CAR algebra, called Bogoliubov transformations (see [BR2]). Clearly, if $\mathfrak{h}_0$ is a dense set of analytic vectors for H then the *-algebra generated by the family $\{a(f) \in B(\mathfrak{h}) : f \in \mathfrak{h}_0\}$ is a dense, α-invariant *-sub-algebra of $\mathfrak{A}(\mathfrak{h})$ consisting of analytic vectors for the automorphisms group. For a fixed $\beta \in \mathbb{R}$, the $(\alpha\,,\beta)$-KMS-condition for a given state ω requires, in particular, that

$$\omega(a^*(f)a(g)) = \omega(a(g)a^*(e^{-\beta H} f)) \qquad f, g \in \mathfrak{h}_0\,.$$

Since, by the canonical anti-commutation relations,

$$a(g)a^*\left(e^{-\beta H} f\right) = (g|e^{-\beta H} f) \cdot \mathbb{I}_{\mathfrak{h}} - a^*(e^{-\beta H} f)a(g)\,,$$

we should have

$$\omega(a^*((\mathbb{I}_{\mathfrak{h}} + e^{-\beta H})f)a(g)) = (g|e^{-\beta H} f)$$

and then

$$\omega(a^*(f)a(g)) = \left(g|\, e^{-\beta H}(I + e^{-\beta H})^{-1} f\right) \qquad f, g \in \mathfrak{h}_0\,.$$

This formula determines, through the CAR relations, a state ω_β over $\mathfrak{A}(\mathfrak{h})$ which is called the gauge-invariant, quasi-free state associated to H and β. It is the unique $(\alpha\,,\beta)$-KMS state over $\mathfrak{A}(\mathfrak{h})$ (see [BR2 Section 5.3]).
Into this framework falls the "Ideal Fermi Gas" where $\mathfrak{h} := L^2(\mathbb{R}^d\,, \mathrm{dx})$, $\mathfrak{h}_0$ is the space of rapidly decreasing functions, $H := -H_0 - \mu \cdot I$, H_0 denoting the Laplacian operator on $\mathbb{R}^d$, and $\mu \in \mathbb{R}$.

Example 2.30. (KMS-states on CCR C*-algebras) Given a complex pre-Hilbert space $\mathfrak{h}_0$ with Hilbert space completion $\mathfrak{h}$, there exists a unique up to *-isomorphism, C*-algebra $\mathfrak{A}(\mathfrak{h}_0)$ generated by a family $\{W(f) \in B(\mathfrak{h}) : f \in \mathfrak{h}_0\}$ of unitary operators satisfying

i) $W(-f) = W(f)^* \qquad f \in \mathfrak{h}_0\,;$
ii) $W(f)W(g) = e^{-i\mathrm{Im}(f|g)}W(g)W(f) \qquad f, g \in \mathfrak{h}_0\,.$

This is Weyl's form of the canonical commutation relations CCR, describing quantum mechanical systems, possibly having an unbounded number of particles, obeying Bose-Einstein statistics. The unitaries $W(f)$ are called Weyl operators.

Consider a self-adjoint, positive operator H on $\mathfrak{h}$, not having zero as an eigenvalue and such that $e^{itH}\mathfrak{h}_0 \subseteq \mathfrak{h}_0$ for all $t \in \mathbb{R}$ and $\mathfrak{h}_0 \subseteq \mathrm{Dom}(e^{-\beta H}(I - e^{-\beta H})^{-1})$ for some $\beta > 0$. The *gauge invariant, quasi-free state over* $\mathfrak{U}(\mathfrak{h}_0)$ determined by H and $\beta > 0$ is given by

$$\omega(W(f)) := e^{-\frac{1}{4}\left(f\,\middle|\,(I+e^{-\beta H})(I-e^{-\beta H})^{-1}f\right)}\,, \qquad f \in \mathfrak{h}_0\,.$$

The operator H also specifies the group of automorphisms through the Bogoliubov transformations of $\mathfrak{U}(\mathfrak{h}_0)$:

$$\alpha_t(W(f)) := W(e^{itH}f)\,, \qquad f \in \mathfrak{h}_0 \quad t \in \mathbb{R}\,.$$

Although this is not a strongly continuous automorphism group of $\mathfrak{U}(\mathfrak{h}_0)$, it is easy to check that it leaves the quasi-free state ω invariant, it defines a group of σ-weakly-continuous automorphisms $\{\widehat{\alpha}_t : t \in \mathbb{R}\}$ of the von Neumann algebra $\mathfrak{M}_\omega := \pi_\omega(\mathfrak{U}(\mathfrak{h}_0))''$ in the GNS representation $(\pi_\omega\,, \mathcal{H}_\omega)$ of ω. This weak extension is indeed a σ-weakly-continuous group of automorphisms and one checks that the weak extension $\widehat{\omega}$ is a $(\widehat{\alpha}\,, \beta)$-KMS state on $\mathfrak{M}_\omega$. Phase transitions occur for these systems, accommodating, for example, the phenomena of Bose-Einstein condensation (see [BR2]).

We now define the class of semigroups, we are interested in these lectures. As already mentioned above, the condition we introduce generalizes the symmetry condition of the commutative or tracial cases introduced in [AHK1]. In the particular case of a von Neumann algebra, and with respect to the modular automorphisms group, it was introduced in [Cip] [GL1,2]. It is a generalization of the *detailed balance condition* of the type considered in the theory of Quantum Open Systems (see [D1], [GKS]). We notice, in particular, that it applies to dynamical semigroups and KMS states on C*-algebras.

Definition 2.31. (**KMS-symmetry and KMS-duality**) Let $\alpha := \{\alpha_t : t \in \mathbb{R}\}$ be a strongly continuous group of automorphisms of a C*-algebra A and ω be a fixed (α, β)-KMS state for some $\beta \in \mathbb{R}$. A bounded map $\Phi : A \to A$ is said to be (α, β)-*KMS symmetric with respect to* ω if

$$\omega\Big(b\Phi(a)\Big) = \omega\Big(\alpha_{-\frac{i\beta}{2}}(a)\Phi(\alpha_{+\frac{i\beta}{2}}(b))\Big) \tag{2.15}$$

for all a, b in a norm dense, α-invariant *-subalgebra B of A_α. A strongly continuous semigroup $\{\Phi_t : t \geq 0\}$ on A is said to be (α, β)-*KMS symmetric* *with respect to* ω if Φ_t is (α, β)-KMS symmetric with respect to ω for all $t \geq 0$. In the von Neumann algebra case, ω is assumed to be normal, maps and semigroups to be σ-weakly continuous and the subalgebra B has to be σ-weakly dense. Two maps $\Phi_1 , \Phi_2 : A \to A$ satisfying the condition

$$\omega\Big(b\Phi_1(a)\Big) = \omega\Big(\alpha_{-\frac{i\beta}{2}}(a)\Phi_2(\alpha_{+\frac{i\beta}{2}}(b))\Big)$$

for all a, b in a norm dense, α-invariant *-subalgebra B of A_α will be said to be in (α, β)-*KMS duality with respect to* ω.

In the von Neumann algebra case the duality condition above was introduced in [AC] to fully generalize the notion of *conditional expectation* and it was generalized in [Petz] for a weight in place of a state. In the von Neumann algebra case this condition plays a distinctive role in Quantum Communication Processes as described in [OP].

Notice that if in the above definition $\beta = 0$, then ω is necessarily a tracial state and (2.15) simplifies to

$$\omega(\Phi(a)b) = \omega(a\Phi(b)) \qquad a, b \in A\,. \tag{2.16}$$

Maps satisfying the above symmetry condition with respect to traces on C^* or von Neumann algebras, were considered in [G1], [AHK1], [S2], [DL1].
Notice also that, for a general $(\alpha\,, \beta)$-KMS state ω, if the maps Φ commutes with the automorphism group α then, using the KMS-condition (2.14), one easily checks that the KMS-symmetry (2.15) is equivalent to the condition (2.16). This symmetry condition, introduced in [KFGV] as the *quantum detailed balance* condition (but also referred to as *GNS-symmetry*) plays a role in the theory of Quantum Open Systems.
The essential difference between KMS-symmetry and the quantum detailed balance condition is that, as opposed to the former, only the latter forces the map Φ *to commute with the automorphism group*. More explicitly, if a map Φ satisfies (2.16) with respect to the (α, β)-KMS state ω then it commutes with α and satisfies (2.15) too (see [Cip1] for the proof and [FU] for several examples of this fact).

In the framework of the *dynamical approach to equilibrium*, given a dynamical system $\alpha := \{\alpha_t : t \in \mathbb{R}\}$ on A, one would like to find, for each fixed phase of the system represented by the (α, β)-KMS state ω, an ergodic, identity preserving, positive semigroup $\mathbf{\Phi} = \{\Phi_t : t \geq 0\}$ on A, having ω as a unique, invariant state. In other words, one requires that

$$\omega(\Phi_t(a)) = \omega(a) \qquad a \in A\,, \quad t \geq 0\,,$$

and also that, for all states ω' on A

$$\lim_{t \to 0} \omega' \circ \Phi_t = \omega\,,$$

the convergence taking place in weak*-topology of A^*. *If a phase transition occurs, these requirements are incompatible with the commutativity between the semigroup and the automorphism group, i.e. between the dissipative dynamics and the time evolution of the system. In that case, in fact, all equilibria of the system, being in particular α-invariant states, are $\mathbf{\Phi}$-invariant too, in contrast to the required ergodicity.*

Notice also that, when Φ is the identity map then, using the α-invariance of ω only, one may check that the identity (2.15) reduce to the KMS condition (2.14):

$$\omega(ba) = \omega\Big(\alpha_{-\frac{i\beta}{2}}(a)\alpha_{+\frac{i\beta}{2}}(b)\Big) = \omega\Big(a\alpha_{+i\beta}(b)\Big)\,.$$

In other words, an (α,β)- KMS symmetric continuous semigroup $\{\Phi_t : t \ge 0\}$ on A represents a one parameter deformation of the $(\alpha\,,\beta)$-KMS condition for ω.

Example 2.32. (KMS-symmetric, norm continuous, completely Markovian semigroups) We have seen, in Example 2.26, the general form of the Lindblad generator L of a completely Markovian, identity preserving, norm continuous, σ-weakly continuous semigroup on a von Neumann algebra $\mathfrak{M}$:

$$L(a) = i[H,a] + \sum_{i\in I} y_i^* y_i a - 2y_i^* a y_i + a y_i^* y_i\,,$$

where $\sum_{k\in I} y_i^* y_i$ has to converge in $\mathfrak{M}$ and $\sum_{i\in I} y_i^* a y_i \in \mathfrak{M}$ for all $a \in \mathfrak{M}$. Suppose that $(\mathfrak{M}\,,\mathcal{H}\,,\mathcal{H}^+\,,\mathcal{J})$ is a standard form of $\mathfrak{M}$ and $\xi_0 \in \mathcal{H}^+$ is the vector representing a fixed normal state ω_0 on it. Assume I to be a finite index and the operator coefficients $\{y_i : i \in I\}$ as well as H to be entire analytic with respect to the modular group $\{\sigma_t : t \in \mathbb{R}\}$ of ω_0. Notice that, since L is bounded, the series

$$\Phi_t = \sum_{n\ge 0} \frac{t^n}{n!} L^n$$

is norm convergent and the ω_0-KMS symmetry of L would imply the ω_0-KMS symmetry of Φ_t, which in turn would be a ω_0-KMS symmetric, norm continuous, completely Markovian semigroup on $\mathfrak{M}$. In this respect it has been proved in [P3] that under the assumption

$$\sum_{i\in I} x_i J_0 x_i J_0 = \sum_{i\in I} x_i^* J_0 x_i^* J_0\,,$$

L is ω_0-KMS symmetric if and only if the following identity holds true

$$H = \sum_{i\in I} \int_{\mathbb{R}} \sigma_t(x_k^* \sigma_{-i/2}(x_k) - \sigma_{i/2}(x_k^*) x_k) f_0(t)\, dt\,,$$

for $x_i := \sigma_{i/4}(y_i)$ $i \in I$ and $f_0(t) := 1/\cosh(2\pi t)$ $t \in \mathbb{R}$. Moreover, a complete characterization has been recently achieved in [FU1 Theorem 7.3] in the case when $\mathfrak{M}$ is a type I factor $B(h)$. Using the Hilbert-Schmidt standard form of Example 2.19 where the state ω_0 is represented by a positive, trace class operator $\rho \in B(h)$, $\omega_0(x) = \mathrm{Trace}(\rho x)$, setting

$$G := -\frac{1}{2}\sum_{k\in I} y_k^* y_k - iH\,,$$

one has that the ω_0-KMS symmetry of L is equivalent to the following conditions

$$\rho^{1/2}G^* = G\rho^{1/2} + ic\rho^{1/2}$$
$$\rho^{1/2}y_k^* = \sum_{l\in I} u_{kl}y_l\rho^{1/2} \qquad k \in I$$

for some $c \in \mathbb{R}$ and some unitary matrix $[u_{kl}]_{k,l=1}^n \in M_n(\mathbb{C})$, n being the cardinality of the index set I.

Using the notation of Proposition 2.28, we are going to see that KMS-symmetry may be expressed, alternatively in a way which does not refer to a specific dense, invariant *-subalgebra of analytic elements. For simplicity, we state and prove this result for C*-algebras only, leaving the reader to adapt the details to the von Neumann algebra situation.

Proposition 2.33. *Let $\alpha := \{\alpha_t : t \in \mathbb{R}\}$ be a strongly continuous group of automorphisms of a C*-algebra A and ω a $(\alpha\,,\beta)$-KMS state for some $\beta \in \mathbb{R}$. Then, for a bounded map $\Phi : A \to A$, the following conditions are equivalent:*

i) Φ is (α,β)-KMS symmetric with respect to ω;

ii) for any pair $a, b \in A$, there exists a bounded, continuous function $F_{a,b} : \overline{D_\beta} \longrightarrow A$ which is analytic in D_β and such that, for all $t \in \mathbb{R}$,

$$F_{a,b}(t) = \omega\big(\alpha_{-\frac{t}{2}}(a)\Phi(\alpha_{+\frac{t}{2}}(b))\big)\,, \quad F_{a,b}(t+i\beta) = \omega\big(\alpha_{+\frac{t}{2}}(b)\Phi(\alpha_{-\frac{t}{2}}(a))\big)\,. \tag{2.17}$$

Furthermore, if the above conditions are satisfied, then the function $F_{a,b}$ is bounded on $\overline{D_\beta}$ and

$$|F_{a,b}(z)| \le \|\Phi\| \cdot \|a\| \cdot \|b\|\,, \qquad z \in \overline{D_\beta}\,.$$

Finally, for $a \in A\,, b \in A_\alpha$, the function $F_{a,b}$ is the restriction to $\overline{D_\beta}$ of the entire function

$$G_{a,b}(z) := \omega\big(\alpha_{-\frac{z}{2}}(a)\Phi(\alpha_{+\frac{z}{2}}(b))\big)\,, \qquad z \in \mathbb{C}\,.$$

Proof. Assuming i) and denoting by $B \subseteq A_\alpha$ the subalgebra occurring in Definition 2.31, consider, for a fixed pair $a, b \in B$, the function

$$F_{a,b}(z) := \omega\big(\alpha_{-\frac{z}{2}}(a)\Phi(\alpha_{+\frac{z}{2}}(b))\big)\,, \qquad z\in\mathbb{C}\,.$$

Then $F_{a,b}$ is an entire function and, using the (α,β)-KMS symmetry, we have, for any $t\in\mathbb{R}$,

$$\begin{aligned}F_{a,b}(t) &= \omega\big(\alpha_{-\frac{t}{2}}(a)\Phi(\alpha_{+\frac{t}{2}}(b))\big)\,,\\ F_{a,b}(t+i\beta) &= \omega\big(\alpha_{-\frac{t+i\beta}{2}}(b)\Phi(\alpha_{+\frac{t+i\beta}{2}}(a))\big)\\ &= \omega\big(\alpha_{-\frac{i\beta}{2}}(\alpha_{-\frac{t}{2}}(a))\Phi(\alpha_{+\frac{i\beta}{2}}(\alpha_{+\frac{t}{2}}(b)))\big)\\ &= \omega\big(\alpha_{+\frac{t}{2}}(b)\Phi(\alpha_{-\frac{t}{2}}(a))\big)\,.\end{aligned}$$

As the map $z\mapsto\alpha_z(b)$ is analytic, it follows that the functions $[0,\beta]\ni s\mapsto\|\alpha_{\pm\frac{is}{2}}(b)\|$ are continuous, hence they are bounded and $M_\pm := \sup\{\|\alpha_{\pm\frac{is}{2}}(b)\|: s\in[0,\beta]\}$ are finite. We then have, for all $t+is\in\overline{D_\beta}$,

$$\begin{aligned}|F_{a,b}(t+is)| &= \big|\omega\big(\alpha_{-\frac{t}{2}}(\alpha_{-\frac{is}{2}}(a))\Phi(\alpha_{+\frac{t}{2}}(\alpha_{+\frac{is}{2}}(b)))\big)\big| \le \|\Phi\|\cdot M_-\cdot M_+\,,\\ |F_{a,b}(t)| &\le \|\Phi\|\cdot\|a\|\cdot\|b\|\\ |F_{a,b}(t+i\beta)| &\le \|\Phi\|\cdot\|a\|\cdot\|b\|\,.\end{aligned}$$

Applying the Three-Line Theorem [BR2 Proposition 5.3.5], we finally get the bound

$$\sup_{z\in\overline{D_\beta}}|F_{a,b}(z)| \le \max\big\{\sup_{t\in\mathbb{R}}|F_{a,b}(t)| \quad ; \quad \sup_{t\in\mathbb{R}}|F_{a,b}(t+i\beta)|\big\}\le \|\Phi\|\cdot\|a\|\cdot\|b\|\,.$$

For general $a,b\in A$ one proceeds by approximation, choosing sequences $\{a_n\in B : n\ge 1\}$ and $\{b_n\in B : n\ge 1\}$, norm convergent to a and b, respectively, and uniformly bounded with $\|a_n\|\le\|a\|$, $\|b_n\|\le\|b\|$ for $n,m\ge 1$. For z belonging to the boundary lines of $\overline{D_\beta}$, we have

$$\begin{aligned}&|F_{a_n,b_n}(z) - F_{a_m,b_m}(z)|\\ &\le \max\big\{\sup_{t\in\mathbb{R}}|F_{a_n,b_n}(t) - F_{a_m,b_m}(t)|\,;\ \sup_{t\in\mathbb{R}}|F_{a_n,b_n}((t+i\beta))\\ &\qquad - F_{a_m,b_m}(t)(t+i\beta)|\big\}\\ &= \max\big\{\sup_{t\in\mathbb{R}}|\omega\big(\alpha_{-\frac{t}{2}}(a_n)\Phi(\alpha_{+\frac{t}{2}}(b_n))\big) - \omega\big(\alpha_{-\frac{t}{2}}(a_m)\Phi(\alpha_{+\frac{t}{2}}(b_m))\big)| \quad ;\\ &\qquad \sup_{t\in\mathbb{R}}|\omega\big(\alpha_{+\frac{t}{2}}(b_n)\Phi(\alpha_{-\frac{t}{2}}(a_n))\big) - \omega\big(\alpha_{+\frac{t}{2}}(b_m)\Phi(\alpha_{-\frac{t}{2}}(a_m))\big)|\big\}\\ &\le \|\Phi\|\Big(\|a_n-a_m\|\cdot\|b\| + \|a\|\cdot\|b_n-b_m\|\Big)\,.\end{aligned}$$

This shows that $\{F_{a_n,b_n} : n\ge 1\}$ is a uniformly Cauchy sequence of bounded, continuous functions on the boundary of the closed strip $\overline{D_\beta}$, hence, by the Three-Line Theorem again, it is a Cauchy sequence of bounded, continuous functions on the whole closed strip. Its limit function $F_{a,b}$ is then a bounded, continuous function on $\overline{D_\beta}$, which is analytic on D_β and satisfies

$$\begin{aligned} F_{a,b}(t) &= \lim_{n\to\infty} \omega\big(\alpha_{-\frac{t}{2}}(a_n)\Phi(\alpha_{+\frac{t}{2}}(b_n))\big) \\ &= \omega\big(\alpha_{-\frac{t}{2}}(a)\Phi(\alpha_{+\frac{t}{2}}(b))\big) \qquad t\in\mathbb{R}\,, \\ F_{a,b}(t+i\beta) &= \lim_{n\to\infty} \omega\big(\alpha_{+\frac{t}{2}}(b)\Phi(\alpha_{-\frac{t}{2}}(a_n))\big) \\ &= \omega\big(\alpha_{+\frac{t}{2}}(b_n)\Phi(\alpha_{-\frac{t}{2}}(a))\big) \qquad t\in\mathbb{R}\,, \\ \sup_{z\in\overline{D_\beta}} |F_{a,b}(z)| &\le \|\Phi\|\cdot\|a\|\cdot\|b\|\,. \end{aligned}$$

Conversely, assume condition ii) and define the function

$$G_{a,b}(z) := \omega\big(\alpha_{-\frac{z}{2}}(a)\Phi(\alpha_{+\frac{z}{2}}(b))\big)\,,$$

for a fixed pair $a, b \in B$. Then $G_{a,b}$ is an entire function such that $G_{a,b}(t) = F_{a,b}(t)$ for any $t \in \mathbb{R}$. Being analytic within the open strip, the functions $G_{a,b}$ and $F_{a,b}$ have to coincide there and then on the whole closed strip $\overline{D_\beta}$, so that

$$F_{a,b}(z) = \omega\big(\alpha_{-\frac{z}{2}}(a)\Phi(\alpha_{+\frac{z}{2}}(b))\big) \qquad z\in\overline{D_\beta}\,.$$

In particular, by (2.18), we have the desired identity

$$\omega\Big(\alpha_{-\frac{i\beta}{2}}(a)\Phi(\alpha_{+\frac{i\beta}{2}}(b))\Big) = G_{a,b}(+i\beta) = F_{a,b}(+i\beta) = \omega(b\Phi(a))\,.$$

Corollary 2.34. *The (α,β)-KMS symmetry of a map $\Phi : A \to A$ with respect to a (α,β)-KMS state ω holds true with respect to a specific dense, α-invariant *-subalgebra of α-analytic elements if and only if it holds true on the whole of A_α.*

Remark 2.35. The above result allows the derivation of alternative forms of the KMS symmetry, for example the following one:

$$\omega\big(\Phi(a)\alpha_{+\frac{i\beta}{2}}(b)\big) = \omega\big(\alpha_{-\frac{i\beta}{2}}(a)\Phi(b)\big) \qquad a,b\in A_\alpha\,. \tag{2.18}$$

In fact, by Corollary 2.34 we may consider the KMS symmetry (2.15) to hold on A_α. Applying the KMS condition for ω to both sides of (2.15) we get (2.18) because $\alpha_{+\frac{i\beta}{2}}$ *is bijective on* A_α, the inverse being the map $\alpha_{-\frac{i\beta}{2}}$ (see Appendix 7.3). Using the KMS condition on the right hand side of (2.18), we get our last form of the KMS symmetry:

$$\omega(\Phi(a)\alpha_{+\frac{i\beta}{2}}(b)) = \omega(\Phi(b)\alpha_{+\frac{i\beta}{2}}(a)) \qquad a,b\in A_\alpha\,. \tag{2.19}$$

Hence, the KMS-symmetry reduces to the symmetry of the bilinear form $(a,b) \mapsto \omega(\Phi(a)\alpha_{+\frac{i\beta}{2}}(b))$ on A_α. There is a difference among these formulations of the KMS-symmetry which forces one to prefer (2.15) as the true definition. While, as a consequence of Proposition 2.33, (2.15) holds true for a specific dense, α-invariant *-subalgebra B of A_α if and only if it holds true for all of them, the last two forms of the KMS property are equivalent to (2.15) when they are given, as above, on the whole algebra A_α. This is because not only $\alpha_t(A_\alpha) = A_\alpha$ for all $t \in \mathbb{R}$, but also $\alpha_z(A_\alpha) = A_\alpha$ for all $z \in \mathbb{C}$. This property is not shared by a generic dense, α-invariant *-subalgebra B of analytic elements.

The first relevant consequence of the KMS-symmetry is that it allows to study maps and semigroups in GNS-representation $(\pi_\omega, \mathcal{H}_\omega, \xi_\omega)$ of the KMS-state ω. This is based on the following result.

Lemma 2.36. *Let $\{\alpha_t : t \in \mathbb{R}\}$ be a strongly continuous group of automorphisms of a C^*-algebra A and ω be a fixed (α, β)-KMS state for some $\beta \in \mathbb{R}$. Then a map $\Phi : A \to A$ which is (α, β)-KMS symmetric with respect to ω leaves globally invariant the kernel* $\ker(\pi_\omega)$ *of the GNS-representation of ω. With the obvious assumptions, the same occurs in the von Neumann algebra case too.*

Proof. As $\ker \pi_\omega = \{a \in A : \omega(a^*a) = 0\}$, $\ker \pi_\omega$ is clearly α-invariant. Assuming $a \in \ker \pi_\omega$, we then have $\alpha_t(a) \in \ker \pi_\omega$ for all $t \in \mathbb{R}$. By condition (2.18), the α-invariance of ω and by the Cauchy-Schwarz inequality, we have, for a fixed $b \in A$ and all $t \in \mathbb{R}$,

$$\begin{aligned} |F_{a,b}(t)|^2 &\le \omega\big(\alpha_{-\frac{t}{2}}(a)^*\alpha_{-\frac{t}{2}}(a)\big) \cdot \omega\big(\Phi(\alpha_{+\frac{t}{2}}(b))^*\Phi(\alpha_{+\frac{t}{2}}(b))\big) \\ &= \omega(a^*a) \cdot \omega\big(\Phi(\alpha_{+\frac{t}{2}}(b))^*\Phi(\alpha_{+\frac{t}{2}}(b))\big) = 0\,. \end{aligned}$$

Being analytic, $F_{a,b}$ vanishes identically, so that, again by condition (2.18),

$$\omega\big(b\Phi(a)\big) = F_{a,b}(+i\beta) = 0\,.$$

Choosing $b = \Phi(a)^*$ we finally have $\Phi(a) \in \ker \pi_\omega$.

Proposition 2.37. *(Weak extension of the KMS-symmetry maps) Let $\alpha := \{\alpha_t : t \in \mathbb{R}\}$ be a strongly continuous group of automorphisms of a C^*-algebra A and ω be a fixed (α, β)-KMS state for some $\beta \in \mathbb{R}$. Let $(\pi_\omega, \mathcal{H}_\omega, \xi_\omega)$ be the corresponding GNS-representation, $\hat\omega$ the normal extension of ω to $\mathfrak{M} := \pi_\omega(A)''$ and $\hat\alpha := \{\hat\alpha_t : t \in \mathbb{R}\}$ the unique σ-weakly continuous group of automorphisms of $\mathfrak{M}$ such that*

$$\hat\alpha_t(\pi_\omega(a)) = \pi_\omega(\alpha_t(a))\,, \qquad a \in A \quad t \in \mathbb{R}\,, \tag{2.20}$$

with respect to which $\hat\omega$ is a $(\hat\alpha, \beta)$-KMS state (see [BR2 Corollary 5.3.4]).

Suppose that $\Phi : A \to A$ is a $(\alpha\,, \beta)$-KMS symmetric map. Then there exists a unique σ-weakly continuous map $\hat\Phi : \mathfrak{M} \to \mathfrak{M}$ determined by

$$\hat\Phi(\pi_\omega(a)) = \pi_\omega(\Phi(a)) \qquad a \in A\,. \tag{2.21}$$

This extension is $\hat{\omega}$-KMS symmetric in the sense that

$$\hat{\omega}\Big(\hat{\Phi}(x)\hat{\sigma}_{-\frac{i}{2}}(y)\Big) = \hat{\omega}\Big(\hat{\sigma}_{+\frac{i}{2}}(x)\hat{\Phi}(y)\Big) \tag{2.22}$$

for all x, y in a σ-weakly dense, $\hat{\sigma}$-invariant *-subalgebra of $\mathfrak{M}$. Moreover, $\|\hat{\Phi}\| \le \|\Phi\|$ and if Φ is positive then $\hat{\Phi}$ is positive too.

Proof. By Lemma 2.36, formula (2.21) validly determines a unique, σ-weakly densely defined map $(\hat{\Phi}, D(\hat{\Phi}))$ on $\mathfrak{M}$, its domain being $D(\hat{\Phi}) := \pi_\omega(A) \subset \mathfrak{M}$. By Corollary 2.34, we may suppose the KMS symmetry of ω satisfied on the whole algebra of analytic elements A_α. As the modular group $\widehat{\sigma}_t$ of the normal extension $\widehat{\omega}$ of the $(\alpha\,, \beta)$-KMS state ω coincides with the group $\widehat{\alpha}_{-\beta t}$ (see [BR2 Corollary 5.3.4] and the discussion after [BR2 Definition 5.3.1]), the $\widehat{\omega}$-KMS symmetry condition (2.22) follows directly from (2.18) and it is satisfied on the σ-weakly dense, $\widehat{\sigma}$-invariant *-subalgebra $\pi_\omega(A_\alpha) \subseteq \mathfrak{M}$.
For the sake of simplicity, we shall assume from now on that π_ω is faithful, so that $\ker \pi_\omega = \{0\}$. In particular, we shall identify elements a of A with their images $\pi_\omega(a)$ in $\mathfrak{M}$ so that $A \subseteq \mathfrak{M}$ and $D(\widehat{\Phi}) = A$.
To extend the map $\widehat{\Phi}$ to the whole von Neumann algebra $\mathfrak{M}$, we start by noticing that it is bounded on its domain:

$$\|\widehat{\Phi}(a)\| \le \|\Phi\| \cdot \|a\| \qquad \forall\, a \in A \subseteq \mathfrak{M}\,.$$

We now proceed to show that the $\widehat{\omega}$-KMS symmetry condition (2.22) implies the map $(\hat{\Phi}, D(\hat{\Phi}))$ is σ-weakly closable on $\mathfrak{M}$. In fact, let $\{x_i : i \in I\} \subset A$ be a net in its domain, σ-weakly converging to zero, for which the net $\{\hat{\Phi}(x_i) : i \in I\} \subset \mathfrak{M}$ is σ-weakly convergent to some $z \in \mathfrak{M}$. Then by (2.22)

$$\begin{aligned}
\widehat{\omega}\Big(z\widehat{\sigma}_{-\frac{i}{2}}(y)\Big) &= \lim_{i\in I} \widehat{\omega}\Big(\widehat{\Phi}(x_i)\,\widehat{\sigma}_{-\frac{i}{2}}(y)\Big) \\
&= \lim_{i\in I} \widehat{\omega}\Big(\widehat{\sigma}_{+\frac{i}{2}}(x_i)\widehat{\Phi}(y)\Big) \\
&= \lim_{i\in I} \big(\xi_{\widehat{\omega}}\big|\Delta_{\widehat{\omega}}^{-\frac{1}{2}} x_i \Delta_{\widehat{\omega}}^{+\frac{1}{2}} \widehat{\Phi}(y)\xi_{\widehat{\omega}}\big) \\
&= \lim_{i\in I} \big(\xi_{\widehat{\omega}}\big|x_i \Delta_{\widehat{\omega}}^{+\frac{1}{2}} \widehat{\Phi}(y)\xi_{\widehat{\omega}}\big) \\
&= 0
\end{aligned} \tag{2.23}$$

for any $y \in A_\alpha$. Choosing $y = \widehat{\sigma}_{+\frac{i}{2}}(x)$, we have $\widehat{\omega}(zx) = 0$ for all $x \in A_\alpha$. Since A_α is σ-weakly dense in $\mathfrak{M}$ we get $z = 0$, thus proving $\widehat{\Phi}$ to be σ-weakly closable. To show that (2.21) determines a σ-weakly continuous map, defined everywhere on $\mathfrak{M}$, we are left to prove that the σ-weak closure of $(\hat{\Phi}, D(\hat{\Phi}))$ is σ-weakly continuous. This will be a consequence of the Closed Graph Theorem, once we show that the closure of $(\hat{\Phi}, D(\hat{\Phi}))$ is everywhere defined. Let $x \in \mathfrak{M}$ be a generic, fixed vector and choose a net $\{x_i : i \in I\}$ $\subset A$ σ-weakly converging to it. The boundedness of the map $\widehat{\Phi}$ implies that $\{\widehat{\Phi}(x_i) : i \in I\}$ is bounded in $\mathfrak{M}$ so that it is, by the Banach-Alaoglu Theorem,

a σ-weakly relatively compact set. Possibly considering a suitable subnet, we deduce that $\{\widehat{\Phi}(x_i) : i \in I\}$ is σ-weakly convergent in $\mathfrak{M}$, so that x is in the domain of the closure of the map $(\widehat{\Phi}, D(\widehat{\Phi}))$.
To extend the bound $\|\widehat{\Phi}(x)\| \leq \|\Phi\| \cdot \|x\|$ from x in A to the whole von Neumann algebra, consider x in the unit ball of $\mathfrak{M}$. By Kaplanski's density theorem [BR1 Theorem 2.4.16], there exists a net $\{x_i : i \in I\}$ in the unit ball of A, which is σ-strongly*, hence σ-weakly, convergent to x. Since $\widehat{\Phi}$ is σ-weakly continuous, for every normal functional $\tau \in \mathfrak{M}_*$ we then have

$$|\langle \tau\,, \widehat{\Phi}(x)\rangle| = |\lim_{i\in I} |\langle \tau\,, \widehat{\Phi}(x_i)\rangle \leq \|\tau\|_{\mathfrak{M}_*} |\liminf_{i\in I} \|\Phi\| \cdot \|x_i\|_{\mathfrak{M}} = \|\tau\|_{\mathfrak{M}_*} \cdot \|\Phi\|\,,$$

thus $\|\widehat{\Phi}(x)\| \leq \|\Phi\|$. Since this holds true for all x in the unit ball of $\mathfrak{M}$, we get the desired bound.

We now proceed to show that if $\Phi : A \to A$ is a positive map then $\widehat{\Phi} : \mathfrak{M} \to \mathfrak{M}$ is positive too. Fix an element $x \in \mathfrak{M}_+$ and consider, by Kaplansky's Density Theorem, a net $\{x_i : i \in I\}$ in A, σ-strongly* convergent to it in $\mathfrak{M}$. Since convergent nets are bounded, by [T2 Chapter II Lemma 2.5] we have $x_i \to x$ strongly* and hence strongly. Applying [T2 Chapter II Theorem 4.7], we have $|x_i| \to x$ strongly and, by [T2 Chapter Proposition 4.1], $|x_i| \to x$ in the strong* topology too. Using again [T2 Chapter II Lemma 2.5] we have that $|x_i| \to x$ in the σ-strong* topology and then σ-weakly too. By the σ-weak continuity of the map $\widehat{\Phi}$, we get $\widehat{\Phi}(|x_i|) \to \widehat{\Phi}(x)$ σ-weakly in $\mathfrak{M}_+$. Since the positive cone $\mathfrak{M}_+$ is σ-weakly closed, we get $\widehat{\Phi}(x) \in \mathfrak{M}_+$.

With the hypotheses of the previous theorem we have the following

Corollary 2.38. *(Duality relation of KMS-symmetric maps) The map $\widehat{\Phi}_*$: $\mathfrak{M}_* \to \mathfrak{M}_*$ determined by restricting to the pre-dual space $\mathfrak{M}_*$ the adjoint map $\Phi^* : \mathfrak{M}^* \to \mathfrak{M}^*$ satisfies the duality relation*

$$\hat{\Phi}_* \circ j_{\widehat{\omega}} = j_{\widehat{\omega}} \circ \hat{\Phi}\,, \tag{2.24}$$

where $j_{\widehat{\omega}} : \mathfrak{M} \to \mathfrak{M}_*$ is the symmetric embedding determined by $\widehat{\omega}$. Moreover, if Φ is positive then $\widehat{\Phi}_*$ is positive and if Φ is Markovian then $\widehat{\Phi}_*$ is Markovian in the following sense $\widehat{\Phi}_*(\widehat{\omega}) \leq \widehat{\omega}$, or, more explicitly,

$$\widehat{\omega}(\widehat{\Phi}(a)) \leq \widehat{\omega}(a) \qquad a \in \mathfrak{M}_+.$$

Proof. Denoting by $\xi_{\widehat{\omega}}$ the cyclic vector representing the state $\widehat{\omega}$ and by $\Delta_{\widehat{\omega}}\,, J_{\widehat{\omega}}$ the associated modular operators, we have $J_{\widehat{\omega}}\xi_{\widehat{\omega}} = \xi_{\widehat{\omega}}$ and $\Delta^z_{\widehat{\omega}}\xi_{\widehat{\omega}} = \xi_{\widehat{\omega}}$ for all $z \in \mathbb{C}$.
To prove the duality relation (2.24), recall that $\widehat{\sigma}_z(x) = \Delta^{iz}_{\widehat{\omega}} x \Delta^{-iz}_{\widehat{\omega}}$ for all complex numbers z and all analytic vectors x (see for instance the discussion following [BR1 Corollary 2.5.24]). From the $\widehat{\omega}$-KMS symmetry (2.22), the definition of $j_{\widehat{\omega}}$ (see Definition 2.21 iii)) and the properties of the modular

operators, it follows that, for all x and y in the subalgebra $\mathfrak{M}_{\widehat{\sigma}} \subseteq \mathfrak{M}$ of analytic elements of the modular group, we have

$$\begin{aligned}
\left(\xi_{\widehat{\omega}}\middle|\widehat{\Phi}(x)\widehat{\sigma}_{-\frac{i}{2}}(y)\xi_{\widehat{\omega}}\right) &= \left(\xi_{\widehat{\omega}}\middle|\widehat{\sigma}_{+\frac{i}{2}}(x)\widehat{\Phi}(y)\xi_{\widehat{\omega}}\right) \\
\left(\xi_{\widehat{\omega}}\middle|\widehat{\Phi}(x)\Delta_{\widehat{\omega}}^{\frac{1}{2}}y\Delta_{\widehat{\omega}}^{-\frac{1}{2}}\xi_{\widehat{\omega}}\right) &= \left(\xi_{\widehat{\omega}}\middle|\Delta_{\widehat{\omega}}^{-\frac{1}{2}}x\Delta_{\widehat{\omega}}^{\frac{1}{2}}\widehat{\Phi}(y)\xi_{\widehat{\omega}}\right) \\
\left(\xi_{\widehat{\omega}}\middle|\widehat{\Phi}(x)\Delta_{\widehat{\omega}}^{\frac{1}{2}}y\xi_{\widehat{\omega}}\right) &= \left(\xi_{\widehat{\omega}}\middle|x\Delta_{\widehat{\omega}}^{\frac{1}{2}}\widehat{\Phi}(y)\xi_{\widehat{\omega}}\right) \\
\left(\xi_{\widehat{\omega}}\middle|\widehat{\Phi}(x)J_{\widehat{\omega}}y^*\xi_{\widehat{\omega}}\right) &= \left(\xi_{\widehat{\omega}}\middle|xJ_{\widehat{\omega}}\widehat{\Phi}(y)^*\xi_{\widehat{\omega}}\right) \\
\left(\xi_{\widehat{\omega}}\middle|\widehat{\Phi}(x)J_{\widehat{\omega}}y^*J_{\widehat{\omega}}\xi_{\widehat{\omega}}\right) &= \left(\xi_{\widehat{\omega}}\middle|xJ_{\widehat{\omega}}\widehat{\Phi}(y)^*J_{\widehat{\omega}}\xi_{\widehat{\omega}}\right) \\
\left(\xi_{\widehat{\omega}}\middle|J_{\widehat{\omega}}y^*J_{\widehat{\omega}}\widehat{\Phi}(x)\xi_{\widehat{\omega}}\right) &= \left(\xi_{\widehat{\omega}}\middle|J_{\widehat{\omega}}\widehat{\Phi}(y)^*J_{\widehat{\omega}}x\xi_{\widehat{\omega}}\right) \\
\left(J_{\widehat{\omega}}yJ_{\widehat{\omega}}\xi_{\widehat{\omega}}\middle|\widehat{\Phi}(x)\xi_{\widehat{\omega}}\right) &= \left(J_{\widehat{\omega}}\widehat{\Phi}(y)J_{\widehat{\omega}}\xi_{\widehat{\omega}}\middle|x\xi_{\widehat{\omega}}\right) \\
\left(J_{\widehat{\omega}}y\xi_{\widehat{\omega}}\middle|\widehat{\Phi}(x)\xi_{\widehat{\omega}}\right) &= \left(J_{\widehat{\omega}}\widehat{\Phi}(y)\xi_{\widehat{\omega}}\middle|x\xi_{\widehat{\omega}}\right) \\
\langle j_{\widehat{\omega}}(\widehat{\Phi}(x))\,, y\rangle &= \langle j_{\widehat{\omega}}(x)\,, \widehat{\Phi}(y)\rangle\,.
\end{aligned}$$

Since $\mathfrak{M}_{\widehat{\sigma}}$ is σ-weakly dense in $\mathfrak{M}$, we get the duality relation on the whole of $\mathfrak{M}$. The statements concerning positivity and Markovianity follow directly from the order properties of the symmetric embedding $j_{\widehat{\omega}}$ stated in Proposition 2.23.

The next result shows that not only single maps but also KMS symmetric, *continuous* semigroups may be extended to the von Neumann algebra associated to the GNS representation.

Theorem 2.39. *(Weak extension of KMS-symmetric continuous semigroups) Let $\alpha := \{\alpha_t : t \in \mathbb{R}\}$ be a strongly continuous group of automorphisms of a C^*-algebra A and ω be a fixed (α, β)-KMS state for some $\beta \in \mathbb{R}$. Let $(\pi_\omega, \mathcal{H}_\omega, \xi_\omega)$ be the corresponding GNS-representation, $\widehat{\omega}$ the normal extension of ω to $\mathfrak{M} := \pi_\omega(A)''$ and $\widehat{\alpha} := \{\widehat{\alpha}_t : t \in \mathbb{R}\}$ the induced σ-weakly continuous group of automorphisms of $\mathfrak{M}$.*

Suppose that $\{\Phi_t : t \geq 0\}$ is a strongly continuous semigroups on A, $(\alpha\,, \beta)$-KMS symmetric with respect to ω. Then there exists a unique σ-weakly continuous semigroup $\{\widehat{\Phi}_t : t \geq 0\}$ on $\mathfrak{M}$ determined by

$$\widehat{\Phi}_t(\pi_\omega(a)) = \pi_\omega(\Phi_t(a)) \quad a \in A\,, \qquad t \geq 0\,. \tag{2.25}$$

This extension is $\widehat{\omega}$-KMS symmetric in the sense that

$$\hat{\omega}\left(\widehat{\Phi}_t(x)\widehat{\sigma}_{-\frac{i}{2}}(y)\right) = \widehat{\omega}\left(\widehat{\sigma}_{+\frac{i}{2}}(x)\widehat{\Phi}_t(y)\right) \qquad t \geq 0\,, \tag{2.26}$$

for all x, y in a σ-weakly dense, $\widehat{\sigma}$-invariant *-subalgebra of $\mathfrak{M}$. Moreover, if $\{\Phi_t : t \geq 0\}$ is positive, completely positive, Markovian or completely Markovian then $\{\widehat{\Phi}_t : t \geq 0\}$ shares the same properties.

Proof. Applying Proposition 2.37 to each individual map of the family, we get a semigroup $\{\widehat{\Phi}_t : t \geq 0\}$ of σ-weakly continuous maps on $\mathfrak{M}$. What is left to prove is its σ-weak continuity as a semigroup. This is in fact equivalent to the weak, and hence to the strong continuity of the semigroup of $\sigma(\mathfrak{M}_*, \mathfrak{M})$-continuous maps $\{\widehat{\Phi}_{t*} : t \geq 0\}$ on the predual space $\mathfrak{M}_*$, defined using Corollary 2.38 and satisfying (2.24). Hence, by definition, we have that $\|\widehat{\Phi}_{t*}\| = \|\widehat{\Phi}_t\|$. Since, moreover, $\{\Phi_t : t \geq 0\}$ is a strongly continuous semigroup, there exist constants $M > 0$, $\gamma \in \mathbb{R}$ such that $\|\widehat{\Phi}_t\| \leq \|\Phi_t\| \leq M \cdot e^{\gamma t}$ (see [BR1 Proposition 3.1.3]). This gives the bound

$$\begin{aligned}\|\widehat{\Phi}_{t*}(\tau) - \tau\| &\leq \|\widehat{\Phi}_{t*}(\tau) - \widehat{\Phi}_{t*}(\tau')\| + \|\widehat{\Phi}_{t*}(\tau') - \tau'\| + \|\tau' - \tau\| \\ &\leq \|\widehat{\Phi}_{t*}\| \cdot \|\tau - \tau'\| + \|\widehat{\Phi}_{t*}(\tau') - \tau'\| + \|\tau' - \tau\| \\ &\leq (1 + M \cdot e^{\gamma t}) \cdot \|\tau - \tau'\| + \|\widehat{\Phi}_t(\tau') - \tau'\|\end{aligned}$$

for any $\tau, \tau' \in \mathfrak{M}_*$, by which it is enough to verify the strong continuity of $\{\widehat{\Phi}_{t*} : t \geq 0\}$ on a norm dense subspace of $\mathfrak{M}_*$. Since $\pi_\omega(A)$ is, by definition, $\sigma(\mathfrak{M}, \mathfrak{M}_*)$-dense in $\mathfrak{M}$ and the symmetric embedding $j_{\widehat{\omega}} : \mathfrak{M} \to \mathfrak{M}_*$ has norm dense range (Proposition 2.23), it is enough to prove strong continuity on $j_{\widehat{\omega}}(\pi_\omega(A))$. By (2.24) one has $\widehat{\Phi}_{t*} \circ j_{\widehat{\omega}} = j_{\widehat{\omega}} \circ \widehat{\Phi}_t$ for all $t \geq 0$, so that on $j_{\widehat{\omega}}(\pi_\omega(A))$ the restriction of $\widehat{\Phi}_{t*}$ acts as

$$\widehat{\Phi}_{t*}(j_{\widehat{\omega}}(\pi_\omega(a))) = j_\omega(\pi_\omega(\Phi_t(a)))\,.$$

The strong continuity of $\{\widehat{\Phi}_{t*} : t \geq 0\}$ on $j_{\widehat{\omega}}(\pi_\omega(A))$ then follows from that of $\{\Phi_t : t \geq 0\}$ on A. The proofs of the stated order properties follow easily from the order properties of the symmetric embeddings listed in Proposition 2.23.

Notice that the strongly continuous semigroup on the predual space $\mathfrak{M}_*$ considered in the proof of the previous result, and determined by the relation

$$\widehat{\Phi}_{t*} \circ j_{\widehat{\omega}} = j_{\widehat{\omega}} \circ \widehat{\Phi}_t \qquad t \geq 0\,,$$

is *Markovian with respect to* $\widehat{\omega}$ in the sense that

$$\widehat{\Phi}_{t*}(\widehat{\omega}) \leq \widehat{\omega} \qquad \forall\, t \geq 0\,,$$

or, more explicitly,

$$\widehat{\omega}(\widehat{\Phi}_t(a)) \leq \widehat{\omega}(a) \qquad \forall\, a \in \mathfrak{M}_+\,, \quad \forall\, t \geq 0\,.$$

2.4 Markovian Semigroups on Standard Forms of von Neumann Algebras

So far we have succeeded in extending maps and semigroups, which are KMS symmetric with respect to a KMS state ω, from a C*-algebra to the von Neumann algebra and to its predual space generated by the GNS representation $(\pi_\omega, \mathcal{H}_\omega, \xi_\omega)$. Our next task is to perform a further extension to the Hilbert space $\mathcal{H}_\omega$, in such a way as to keep, when they hold, *positivity* and *Markovianity*. Notice that, while the presence of the standard cone $\mathcal{H}_\omega^+$ makes obvious the formulation of positivity for maps on $\mathcal{H}_\omega$, the notion of Markovianity has to be introduced.

To simplify notations, but also for the sake of generality, we start byworking in the standard form $(\mathfrak{M}, \mathcal{H}, \mathcal{H}^+, \mathcal{J})$ of a von Neumann algebra $\mathfrak{M}$, on which a fixed normal state ω_0 is considered. We shall denote by $\xi_0 \in \mathcal{H}^+$ the positive, cyclic and separating vector representing it: $\omega_0(\cdot) = (\xi_0| \cdot \xi_0)$. Fundamental for us will be, in particular, the continuity and the order properties of the symmetric embeddings i_0, j_0 associated to ω_0, introduced in Section 2.2.

Unless otherwise stated, maps T on $\mathcal{H}$ are always assumed to be real, in the sense that $T(\mathcal{H}^J) \subseteq \mathcal{H}^J$.

Definition 2.40. (**Positive and Markovian semigroups on Hilbert spaces of standard forms**) Let $(\mathfrak{M}, \mathcal{H}, \mathcal{H}^+, \mathcal{J})$ be a standard form of the von Neumann algebra $\mathfrak{M}$ and $\xi_0 \in \mathcal{H}^+$ the vector representing a fixed normal state ω_0 on it. A map $T : \mathcal{H} \to \mathcal{H}$ is said to be

i) *positive* if $T(\mathcal{H}^+) \subseteq \mathcal{H}^+$;

ii) *Markovian with respect to* ξ_0 if it is positive and $T\xi_0 \leq \xi_0$;

iii) *completely positive* (resp. *completely Markovian*) if, for every $n \in \mathbb{N}^*$, the map

$$T \otimes I_n : \mathcal{H} \otimes M_n(\mathbb{C}) \to \mathcal{H} \otimes M_n(\mathbb{C}) \qquad (T \times I_n)[\xi_{ij}]_{i,j=1}^n = [T\xi_{ij}]_{i,j=1}^n$$

is positive (resp. Markovian) on the Hilbert space $\mathcal{H} \otimes M_n(\mathbb{C})$ of the standard form of $\mathfrak{M} \otimes M_n(\mathbb{C})$ (in the tensor product of Hilbert spaces $\mathcal{H} \otimes M_n(\mathbb{C})$, the factor $M_n(\mathbb{C})$ and its scalar product is understood as the Hilbert -Schmidt standard form of the von Neumann algebra $M_n(\mathbb{C})$; the cyclic vector representing the normalized trace being the suitable multiple of the identity matrix).

iv) a semigroup $\{T_t : t \geq 0\}$ on $\mathcal{H}$ is said to be *positive (resp. Markovian, completely positive, completely Markovian)* if T_t is positive (resp. Markovian, completely positive, completely Markovian) for all $t \geq 0$.

It is easy to check that T is Markovian with respect to ξ_0 if and only if it leaves globally invariant the order interval $[0,\xi_0]\subset\mathcal{H}^+$:

$$0\le\xi\le\xi_0\quad\Rightarrow\quad 0\le T\xi\le\xi_0\,.$$

Notice that, while the notion of positive map on $\mathcal{H}$ deals with the structure of ordered Hilbert space only, Markovianity depends upon the choice of a cyclic vector $\xi_0\in\mathcal{H}^+$.

Given a positive semigroup $\{T_t : t\ge 0\}$ on $\mathcal{H}$ and a number $\gamma\ge 0$, vectors $\eta\in\mathcal{H}^+$ such that

$$e^{-t\gamma}T_t\eta\le\eta\qquad\forall\, t\ge 0$$

are called γ-*excessive*, so that the semigroup is Markovian with respect to ξ_0 if and only if this vector is 0-excessive with respect to it.
In the commutative case, where $\mathfrak{M}=L^\infty(X,\mu)$, $\mathcal{H}=L^2(X,\mu)$ and $\mathcal{H}^+=L^2_+(X,\mu)$ is the cone of positive, square summable functions with respect to a positive Radon measure μ on X, positivity has the usual meaning. Then, as long as the measure is finite, and one considers as cyclic vector the constant function $\xi_0=1$, both positivity and Markovianity in the above sense reduce to well known classical notions (see [FOT] for example). However, even in this commutative setting, the above definition makes it possible to consider as Markovian a wider class of semigroups than those which can be treated by the classical definition.

Example 2.41. (Markovianity of Schrödinger semigroups with respect to a ground-state) Consider, for example, the semigroup e^{-tH} on $L^2(\mathbb{R}^n\,,dx)$ generated by a Schrödinger operator $H=-\mathrm{div}\circ\mathrm{grad}+V$ associated to a nice potential function V. By the uniqueness of the Beurling-Deny-Le Jan decomposition (see Example 4.19 below), these semigroups are positivity preserving and not Markovian in the classical sense, unless the potential is positive. However, if H admits a *unique ground-state* ϕ_0, i.e. the bottom $-\gamma$ of its spectrum is an eigenvalue of multiplicity one, then the corresponding normalized eigenvector ϕ_0 is strictly positive and γ-excessive. This is the case, for example, when for some $\lambda\le 0$ the negative part $(V-\lambda)_-$ of the function $V-\lambda$ belongs to the space $L^{\frac{n}{2}}(\mathbb{R}^n\,,dx)$. In the case when $\gamma\le 0$, e^{-tH} is then Markovian with respect to ϕ_0 in the above sense. Notice that the associated normal state ω_0 gives the distribution of the position of the particle of the quantum system described by H in its ground-state.

Example 2.42. (Stability of Markovianity under subordination of semigroups) Let $U:G\to\mathcal{B}(\mathcal{H})$ be a strongly continuous representation of a locally compact abelian group G leaving the positive cone globally invariant: $U(g)\mathcal{H}^+=\mathcal{H}^+$ for all $g\in G$. Suppose that $\{\mu_t : t\ge 0\}$ is a symmetric convolution semigroup of probabilities on G. The subordinate semigroup

$$T_t\xi:=\int_G\mu_t(dg)U(g)\xi\qquad\xi\in\mathcal{H}$$

is a strongly continuous, symmetric, contractive and positivity preserving semigroup. It is also (completely) Markovian with respect to any cyclic vector $\xi_0 \in \mathcal{H}^+$ left invariant by the representation. This applies, in particular, to cases in which the representation is given by the modular automorphism group of any faithful, normal state on $\mathfrak{M}$. Consider, for example, the case where

$$G = \mathbb{R} \qquad \mu_t(dx) := (4\pi t)^{-1/2} e^{-x^2/4t}\, dx\,, \quad t > 0\,, \quad \mu_0 := \delta_0$$

and $U(t) = \Delta_0^{it}$ where Δ_0 is the modular operator corresponding to a cyclic vector $\xi_0 \in \mathcal{H}^+$. Then we have

$$T_t = e^{-t|\log \Delta_0|^2} \qquad t \geq 0\,.$$

Other example of this construction are discussed in [Cip1 Chapter 3].

Notice that, while the definition of positive map on the Hilbert space of a standard form only depends upon the order structure of the Hilbert space, Markovianity is a property deeply connected with the behavior of the map at the algebra level. The next result will show that Markovian maps and semigroups on $\mathcal{H}$ are exactly those which extend to normal, positive contractive maps on the von Neumann algebra $\mathfrak{M}$ and to weakly continuous, positive, contractive maps on the predual $\mathfrak{M}_*$.

Proposition 2.43. *Let $\Phi : \mathfrak{M} \to \mathfrak{M}$ be a (real) linear map on the von Neumann algebra $\mathfrak{M}$. Then the following properties are equivalent:*

i) Φ is ω_0-KMS symmetric

$$\omega(\Phi(x)\sigma_{-\frac{i}{2}}(y)) = \omega(\sigma_{+\frac{i}{2}}(x)\Phi(y)) \qquad x, y \in \mathfrak{M}_\sigma\,;$$

ii) the densely defined linear map $T : D(T) \to \mathcal{H}$ on the Hilbert space $\mathcal{H}$, given by

$$T \circ i_0 = i_0 \circ \Phi\,, \qquad D(T) := i_0(\mathfrak{M}_\sigma)\,,$$

is symmetric

$$(T\xi|\,\eta) = (\xi|\,T\eta) \qquad \xi\,, \eta \in D(T)\,;$$

iii) the densely defined linear map $\Phi_* : D(\Phi_*) \to \mathfrak{M}_*$, on the predual space $\mathfrak{M}_*$, given by

$$\Phi_* \circ j_0 = j_0 \circ \Phi\,, \qquad D(\Phi_*) := j_0(\mathfrak{M}_\sigma)\,,$$

is in duality with Φ:

$$\langle \Phi_*(j_0(x))|y\rangle = \langle j_0(x)|\Phi(y)\rangle \qquad x, y \in \mathfrak{M}\,.$$

Suppose that the previous symmetry conditions hold true. Then *iv)* Φ *,* T *and* Φ_* *are bounded maps and* Φ *is* $\sigma(\mathfrak{M}, \mathfrak{M}_*)$*-continuous;*

v) the Markovianity of Φ*,* T *and* Φ_* *are equivalent.*

Proof. Notice first that, by Proposition 2.23, $D(T)$ is norm dense in $\mathcal{H}$ because $\mathfrak{M}_\sigma$ is $\sigma(\mathfrak{M}\,,\mathfrak{M}_*)$-dense in $\mathfrak{M}$ and i_0 is $\sigma(\mathfrak{M}\,,\mathfrak{M}_*)-\sigma(\mathcal{H}\,,\mathcal{H})$ continuous with dense range.
Analogously, $D(\Phi_*)$ is $\sigma(\mathfrak{M}_*\,,\mathfrak{M})$ dense in $\mathfrak{M}_*$ because, $\mathfrak{M}_\sigma$ is $\sigma(\mathfrak{M}\,\mathfrak{M}_*)$-dense in $\mathfrak{M}$ and j_0 is $\sigma(\mathfrak{M}_*\,\mathfrak{M}) - \sigma(\mathfrak{M}\,\mathfrak{M}_*)$ continuous with dense range. Since for all $x, y \in \mathfrak{M}_\sigma$ we have

$$\omega(\Phi(x)\sigma_{-\frac{i}{2}}(y)) = (\xi_0|\,\Phi(x)\Delta_0^{\frac{1}{2}}y\xi_0) = (i_0(\Phi(x^*))|\,i_0(y)) = (Ti_0(x^*)|\,i_0(y))$$

and

$$\omega(\sigma_{\frac{i}{2}}(x)\Phi(y)) = (\xi_0|\,x\Delta_0^{+\frac{1}{2}}\Phi(y)\xi_0) = (i_0(x^*)|\,i_0(\Phi(y))) = (i_0(x^*)|\,Ti_0(y))\,,$$

the ω_0-KMS symmetry of Φ and the symmetry of T are equivalent. Analogously, as for all $x, y \in \mathfrak{M}_\sigma$ we have

$$\begin{aligned}\omega(\Phi(x)\sigma_{-\frac{i}{2}}(y)) &= (\xi_0|\,\Phi(x)\Delta_0^{\frac{1}{2}}y\xi_0) = (\xi_0|\,\Phi(x)Jy^*J\xi_0) \\ &= (Jy\xi_0|\,\Phi(x)\xi_0) = \langle j_0(\Phi(x))|\,y\rangle\end{aligned}$$

and

$$\omega(\sigma_{\frac{i}{2}}(x)\Phi(y)) = (\xi_0|\,x\Delta_0^{+\frac{1}{2}}\Phi(y)\xi_0) = (\xi_0|\,xJ\Phi(y)^*J\xi_0) = \langle j_0(x)|\,\Phi(y)\rangle\,,$$

the ω_0-KMS symmetry of Φ and the duality between the maps Φ and Φ_* are also equivalent properties.
Suppose now that one of the above conditions holds true. By the duality relation with Φ_*, the map Φ has a densely defined adjoint map, and hence is $\sigma(\mathfrak{M}\,,\mathfrak{M}_*)$-closable. As it is also everywhere defined, it is $\sigma(\mathfrak{M}\,,\mathfrak{M}_*)$ and norm continuous. Consequently, the map Φ_* is $\sigma(\mathfrak{M}_*\,,\mathfrak{M})$ and norm continuous. The boundedness of T follows from the interpolation bound (2.12) (see Proposition 2.24).
The last statement concerning the equivalence between Markovianity of Φ, T and Φ_* easily follows from the order properties of the symmetric injections (see Proposition 2.22).

The following is the main result of this section: *the class of strongly continuous, symmetric semigroups on the Hilbert space* $\mathcal{H}$ *which are Markovian with respect to* ξ_0*, the class* ω_0*-KMS symmetric,* $\sigma(\mathfrak{M}, \mathfrak{M}_*)$*-continuous Markovian semigroups on the von Neumann algebra* $\mathfrak{M}$ *and the class of* ω_0*-Markovian, strongly continuous semigroups on the predual space* $\mathfrak{M}_*$ *are in one to one correspondence.*

Theorem 2.44. *Let $(\mathfrak{M}, \mathcal{H}, \mathcal{H}^+, \mathcal{J})$ be a standard form of the von Neumann algebra $\mathfrak{M}$, and $\xi_0 \in \mathcal{H}^+$ be a cyclic vector representing a fixed normal state ω_0 on it.*

i) Let $\{\Phi_t : t \geq 0\}$ be a ω_0-KMS symmetric, $\sigma(\mathfrak{M}, \mathfrak{M}_*)$-continuous semigroup on $\mathfrak{M}$. Then the relation

$$T_t \circ i_0 = i_0 \circ \Phi_t$$

induces a strongly continuous semigroup on the Hilbert space $\mathcal{H}$; analogously, the relation

$$\Phi_{*t} \circ j_0 = j_0 \circ \Phi_t$$

induces a strongly continuous semigroup on the predual space $\mathfrak{M}_*$.

ii) Suppose that $\{T_t : t \geq 0\}$ is a symmetric, strongly continuous semigroup on $\mathcal{H}$, Markovian with respect to ξ_0. Then the relation

$$T_t \circ i_0 = i_0 \circ \Phi_t$$

induces a ω_0-KMS symmetric, $\sigma(\mathfrak{M}, \mathfrak{M}_*)$-continuous, Markovian semigroup on $\mathfrak{M}$; analogously, the relation

$$\Phi_{*t} \circ i_{0*} = i_{0*} \circ T_t$$

induces a strongly continuous semigroup on the predual space $\mathfrak{M}_*$.

Moreover, positivity, complete positivity, Markovianity and complete Markovianity, are properties shared by all or none of the above semigroups.

Proof. A direct application of Proposition 2.43 verifies both the correct definition of semigroups of continuous maps on the spaces $\mathcal{H}$ and $\mathfrak{M}_*$, in item i), and on the spaces $\mathfrak{M}$ and $\mathfrak{M}_*$, in item ii), and their order properties. The proof of the continuity with respect to the parameter t is straightforward and is left to the reader.

2.5 Ergodic, Positive Semigroups

A classical result, due to G. Frobenius and O. Perron, states that the eigenvalue $\|a\|$ of a hermitian irreducible $a \in M_n(\mathbb{C})$, with nonnegative entries is simple and there exists an associated eigenvector with nonnegative coordinates. This uniqueness result has been extended by L. Gross [G1], in an infinite dimensional setting, to symmetric, positive operators acting on Hilbert spaces of type $L^2(X, m)$, where positivity has the usual pointwise meaning. The same author also extended the result in the noncommutative setting, for positive operators acting on the Segal standard form $L^2(\mathfrak{M}, \tau)$ of a finite von Neumann algebra $\mathfrak{M}$ (see [Se]). In this framework the author

discussed existence and uniqueness of ground-states of physical Hamiltonians for Boson and Fermion systems in Quantum Field Theory (see also [F]).
In this section we illustrate how to extend the uniqueness result to positive operators acting on Hilbert spaces of standard forms $(\mathfrak{M}\,,\mathcal{H}\,,\mathcal{H}^+\,,\mathcal{J})$ of von Neumann algebras $\mathfrak{M}$.

Let us recall that a closed sub-cone $F \subseteq \mathcal{H}^+$ is called a *face* of $\mathcal{H}^+$ if it is *hereditary*, in the sense that

$$\xi \in \mathcal{F}\,, \quad \eta \in \mathcal{H}^+\,, \quad \eta \leq \xi \qquad \Rightarrow \qquad \eta \in \mathcal{F}\,.$$

A face is proper if it is different from the trivial ones: $\{0\}$ and $\mathcal{H}^+$ (see [Co1]).

Definition 2.45. (Ergodic maps and semigroups) A positive map $T:\mathcal{H}\to\mathcal{H}$ is said to be

i) *ergodic* if for all $\xi\,,\eta \in \mathcal{H}^+$, $\xi\,,\eta \neq 0$, there exists $n \in \mathbb{N}^*$ such that $(\xi|\,T^n\eta) > 0$;

ii) *indecomposable* if it leaves invariant no proper faces of $\mathcal{H}^+$, i.e. for a face $\mathcal{F} \subseteq \mathcal{H}^+$, if $T(\mathcal{F}) \subseteq \mathcal{F}$ then necessarily $\mathcal{F} = \{0\}$ or $\mathcal{F} = \mathcal{H}^+$.

A positive semigroup $\{T_t : t \geq 0\}$ on $\mathcal{H}$ is said to be

iii) *ergodic* if for all $\xi\,,\eta \in \mathcal{H}^+$, $\xi\,,\eta \neq 0$, there exists $t > 0$ such that $(\xi|\,T_t\eta) > 0$;

iv) *indecomposable* if T_t is indecomposable for some $t > 0$.

Example 2.46. (Faces of positive cones of commutative von Neumann algebras) In a cone like $L^2_+(X,m)$, the subcone $\mathcal{F}_B$ of all positive functions vanishing on the complement of a Borel set $B \subseteq X$ of positive measure is a face, and all of them arise in this way.

Faces of the self-polar cone $\mathcal{H}^+$ are in one-to-one correspondence with projections of the von Neumann algebra $\mathfrak{M}$ (see [Co1]). In fact, setting $P_e := eJeJ$ for projections $e \in \mathrm{Proj}(\mathfrak{M})$, one has that

$$\mathcal{F} = P_e(\mathcal{H}^+)$$

is a face and all of them can described in this way.

Theorem 2.47. *(Ergodicity of positive maps and semigroups [Cip3]) Let $T:\mathcal{H}\to\mathcal{H}$ be a symmetric, positive map.*

The following properties are equivalent:

i) $\|T\|$ is a simple eigenvalue and there exists a corresponding cyclic eigenvector in $\mathcal{H}^+$;

ii) T is indecomposable;

iii) T commutes with no proper projection P_e, $e \in \mathrm{Proj}(\mathfrak{M})$;

iv) T is ergodic.

Corollary 2.48. *(Ergodicity of positive semigroups [Cip3]) Let $\{T_t : t \geq 0\}$ be a strongly continuous, positive, symmetric semigroup on $\mathcal{H}$, and let $\inf \sigma(H)$ be the infimum of the spectrum of its self-adjoint generator H.*

The following properties are equivalent:

i) $\inf \sigma(H)$ is a simple eigenvalue and there exists a corresponding cyclic eigenvector in $\mathcal{H}^+$;

ii) $\{T_t : t \geq 0\}$ is indecomposable;

iii) $\{T_t : t \geq 0\}$ is ergodic.

We will meet later, in Example 2.58 and in Corollary 3.4, examples of ergodic semigroups. Non ergodic Markovian semigroups will appear naturally in the geometric setting of Chapter 5 (see Remark 5.13).

2.6 Dirichlet Forms and KMS-symmetric, Markovian Semigroups

A classical result due to A. Beurling and J. Deny characterizes Markovian semigroups on Hilbert spaces of square integrable functions, in terms of a contraction property of the quadratic forms associated to their generators, with respect to projections onto a suitable convex set.
In this section we will prove an extension of that result in the framework of standard forms of von Neumann algebras. This part is taken from [Cip1]. See also [GL1,2] for a development of the theory in the framework of Haagerup L^p-spaces.

In this section we consider a strongly continuous, symmetric semigroup $\{T_t : t \geq 0\}$ on the Hilbert space $\mathcal{H}$ of a standard form. We will denote by $(H, D(H))$ its self-adjoint generator and by $(\mathcal{E}, \mathcal{F})$ the associated closed quadratic form. It will be useful to regard the quadratic form as a lower semicontinuous, convex functional

$$\mathcal{E} : \mathcal{H} \to (-\infty, +\infty] \qquad \text{so that} \qquad \mathcal{F} := \{\xi \in \mathcal{H} : \mathcal{E}[\xi] < +\infty\}\,.$$

The quadratic form will be assumed to be J-real in the sense that

$$\mathcal{E}[J\xi] = \mathcal{E}[\xi] \qquad \xi \in \mathcal{H}$$

and bounded from below in the sense that for, some $\beta \in \mathbb{R}$,

$$\mathcal{E}[\xi] \geq \beta \|\xi\|^2 \qquad \xi \in \mathcal{H}\,.$$

The domain $\mathcal{F}$ is then a J-invariant linear manifold, and it can be shown that $\mathcal{E}$ is determined by its restriction to the J-real part $\mathcal{F}^J := \mathcal{F} \cap \mathcal{H}^J$ of its domain. Notice that the hermitian, sesquilinear form, defined by polarization,

$$\mathcal{E} : \mathcal{F} \times \mathcal{F} \to \mathbb{C} \quad \mathcal{E}(\xi, \eta) = \frac{1}{4}\{\mathcal{E}[\xi+\eta] - \mathcal{E}[\xi-\eta] + i\mathcal{E}[\xi+i\eta] - i\mathcal{E}[\xi-i\eta]\} \quad \xi, \eta \in \mathcal{F},$$

allows us to re-construct the quadratic form as $\mathcal{E}[\xi] = \mathcal{E}(\xi, \xi)$. As the lower semicontinuity of the quadratic form is equivalent to its closedness, the scalar products on the domain $\mathcal{F}$

$$(\xi|\eta)_\lambda := \mathcal{E}(\xi, \eta) + \lambda(\xi|\eta) \qquad \xi \in \mathcal{F}, \lambda > -\beta.$$

define a family of Hilbert structures with equivalent norms given by $\|\xi\|^2_\lambda = (\xi|\xi)_\lambda$.

To motivate the introduction of the tools needed for the characterizations alluded to above, let us briefly review the commutative case. There, a Beurling-Deny criterion (see [BD2], [Den]) characterizes Markovian semigroups as those corresponding to quadratic forms which do not increase their values under the nonlinear map $u \mapsto u \wedge 1$:

$$\mathcal{E}[u \wedge 1] \leq \mathcal{E}[u],$$

i.e. in terms of so called Dirichlet forms.
To extend this criterion to the noncommutative setting, where, essentially, the cone $L^2_+(X, \mu)$ in $L^2(X, \mu)$ is replaced by the self-polar cone $\mathcal{H}^+$ in $\mathcal{H}$, one is tempted to replace the constant function 1 by a cyclic vector $\xi_0 \in \mathcal{H}^+$ and interprets $\xi \wedge \xi_0$ as $\inf(\xi, \xi_0)$, i.e. in terms of a lattice operation. However $(\mathcal{H}, \mathcal{H}^+)$ is not a vector lattice apart from the commutative case (see [Io]).
The way to bypass these difficulties can be found by noticing that, in the commutative case, the function $u \wedge 1$ is the projection of $u \in L^2_\mathbb{R}(X, \mu)$ onto the closed convex set

$$1 - L^2_\mathbb{R}(X, \mu) = \{v \in L^2_\mathbb{R}(X, \mu) : v \leq 1\}.$$

Definition 2.49. Let us denote by $\mathrm{Proj}(\xi, C)$ the projection of the vector $\xi \in \mathcal{H}^J$ onto the closed convex set $C \subseteq \mathcal{H}^J$. Then define, for $\xi, \eta \in \mathcal{H}^J$

$$\xi \vee \eta := \mathrm{Proj}(\xi, \eta + C) \qquad \text{and} \qquad \xi \wedge \eta := \mathrm{Proj}(\xi, \eta - C).$$

We list below, omitting the proof (see [Cip1], [Io]), the main properties of these nonlinear operations.

Lemma 2.50. *Let $\xi, \eta \in \mathcal{H}^J$. The following properties hold:*

i) if $\sup(\xi, \eta)$ *(resp.* $\inf(\xi, \eta)$*) exists then* $\sup(\xi, \eta) = \xi \vee \eta$ *(resp.* $\inf(\xi, \eta) = \xi \wedge \eta$*);*

ii) $\xi \vee 0 = \xi_+$, $\xi \wedge 0 = \xi_-$;

iii) $\xi \vee \eta = \eta + (\xi - \eta)_+$ *and* $\xi \wedge \eta = \eta - (\xi - \eta)_-$;

iv) $\xi \vee \eta = \eta \vee \xi$ *and* $\xi \wedge \eta = \eta \wedge \xi$;

v) $\xi \vee \eta + \xi \wedge \eta = \xi + \eta$ *and* $\xi \vee \eta - \xi \wedge \eta = |\xi - \eta|$;

vi) $\|\xi \vee \eta\|^2 + \|\xi \wedge \eta\|^2 = \|\xi\|^2 + \|\eta\|^2$.

We may now define the main object of a noncommutative potential theory.

Definition 2.51. (Markovian and Dirichlet forms) Let $(\mathfrak{M}, \mathcal{H}, \mathcal{H}^+, J)$ be a standard form of a von Neumann algebra $\mathfrak{M}$ and $\xi_0 \in \mathcal{H}^+$ a cyclic and separating vector.
A J-real quadratic form $\mathcal{E} : \mathcal{H} \to (-\infty, +\infty]$ is said to be *Markovian* with respect to ξ_0 if

$$\mathcal{E}[\xi \wedge \xi_0] \leq \mathcal{E}[\xi] \qquad \forall \xi \in \mathcal{H}^J . \tag{2.27}$$

A closed Markovian form is called a Dirichlet form.

In particular, if $\mathcal{E}$ is Markovian and $\mathcal{E}[\xi]$ is finite then $\mathcal{E}[\xi \wedge \xi_0]$ is finite too. In other words, under the Hilbertian projection $\xi \mapsto \xi \wedge \xi_0$, the value of the quadratic form does not increase. As noticed above, this definition reduces to the usual one in the commutative setting. We are going to see that in any standard form, Dirichlet forms represent an infinitesimal characterization of strongly continuous, symmetric Markovian semigroups.

Theorem 2.52. *(Characterization of Markovian semigroups by Dirichlet forms) Let $(\mathfrak{M}, \mathcal{H}, \mathcal{H}^+, J)$ be a standard form of a von Neumann algebra $\mathfrak{M}$ and $\xi_0 \in \mathcal{H}^+$ a cyclic vector. Let $\{T_t : t \geq 0\}$ be a J-real, symmetric, contractive, strongly continuous semigroup on the Hilbert space $\mathcal{H}$ and $\mathcal{E} : \mathcal{H} \to [0, +\infty]$ the associated J-real, closed quadratic form. The following properties are equivalent*

i) $\{T_t : t \geq 0\}$ *is Markovian with respect to* ξ_0;

ii) $\mathcal{E}$ *is a Dirichlet form with respect to* ξ_0.

Proof. Let us denote by C the closed convex set $\xi_0 - \mathcal{H}^+$ and by ξ_C the projection onto C of a vector $\xi \in \mathcal{H}^J$. Assume property i) and consider $\xi \in \mathcal{H}^J$. Since $\xi_C \in C$ by definition and $T_t \xi_C \in C$ by hypothesis, the properties of Hilbertian projections then imply that $(\xi - \xi_C | T_t \xi_C - \xi_C) \leq 0$ for all $t > 0$. In terms of the bounded, positive quadratic forms $\mathcal{E}^t[\cdot] := t^{-1}((I - T_t) \cdot |\cdot)$, this can be written as follows: $\mathcal{E}^t[\xi_C] \leq \mathcal{E}^t(\xi, \xi_C)$. By the Cauchy-Schwarz inequality we get $\mathcal{E}^t[\xi_C] \leq \mathcal{E}^t[\xi]$ for all $t > 0$ and by the Spectral Theorem, letting $t \to 0$, we obtain $\mathcal{E}[\xi_C] \leq \mathcal{E}[\xi]$.
To prove the converse we start noticing that Markovianity of the semigroup is equivalent to Markovianity of its resolvent family $\{R_\lambda : \lambda > 0\}$ defined through $R_\lambda = \int_0^\infty e^{-\lambda t} T_t \, dt$ for all $\lambda > 0$: specifically $\lambda R_\lambda C \subseteq C$ for all $\lambda > 0$. In one direction this follows from the convexity of the set $C = \xi - \mathcal{H}^+$ and the

fact that the measures $\lambda e^{-\lambda t}\,dt$ are probabilities. The opposite implication comes from the well known representation $T_t = \lim_{n\to\infty}\big(\frac{n}{t}R_{\frac{n}{t}}\big)^n$.
To show that if $\xi \in C$ then $\overline{\xi} := \lambda R_\lambda \xi \in C$, consider the functional $F : \mathcal{H} \to [0,\infty]$ defined by

$$F(\eta) := \lambda^{-1}\mathcal{E}[\eta] + \|\eta - \xi\|^2 .$$

By the Spectral Theorem one sees

$$F(\eta) - F(\overline{\xi}) = \|(\lambda R_\lambda)^{-1/2}(\eta - \overline{\xi})\|^2 ,$$

so that $\overline{\xi}$ is the unique minimizer of F. The definition of $\overline{\xi}_C$ as the nearest point to $\overline{\xi}$ in C and the assumption $\xi \in C$ imply $\|\overline{\xi}_C - \xi\| \le \|\overline{\xi} - \xi\|$. Since by assumption $\mathcal{E}[\overline{\xi}_C] \le \mathcal{E}[\overline{\xi}]$ we then have

$$F(\overline{\xi}_C) = \lambda^{-1}\mathcal{E}[\overline{\xi}_C] + \|\overline{\xi}_C - \xi\|^2 \le \lambda^{-1}\mathcal{E}[\overline{\xi}] + \|\overline{\xi} - \xi\|^2 \le F(\overline{\xi}) .$$

By uniqueness of the minimizer, $\overline{\xi}_C = \overline{\xi}$ which means $\overline{\xi} \in C$.

Our second characterization concerns positive semigroups. Apart from its independent interest, it will provide an intermediate tool for proving Markovianity. The result generalizes the so called “second Beurling-Deny criterion” (see [BD2], [Den]).

Theorem 2.53. *(Quadratic form characterization of positive semigroups) Let $(\mathfrak{M},\ \mathcal{H},\mathcal{H}^+,J)$ be a standard form of the von Neumann algebra $\mathfrak{M}$. Let $\{T_t : t \ge 0\}$ be a J-real, symmetric, strongly continuous, semigroup on the Hilbert space $\mathcal{H}$ and $\mathcal{E} : \mathcal{H} \to (-\infty,+\infty]$ the associated J-real, closed quadratic form. The following properties are equivalent*

i) $\{T_t : t \ge 0\}$ is positive;

ii) $\mathcal{E}[|\xi|] \le \mathcal{E}[\xi]$ for all $\xi \in \mathcal{H}^J$. In particular if $\xi \in \mathcal{F}^J$ than $|\xi| \in \mathcal{F}^J$;

iii) $\xi \in \mathcal{F}^j$ implies $\xi_+, \xi_- \in \mathcal{F}$ and $\mathcal{E}(\xi_+, \xi_-) \le 0$.

Proof. Assuming the property i), the following identity

$$\mathcal{E}^t[\xi_+ - \xi_-] - \mathcal{E}^t[\xi_+ + \xi_-] = 4(\xi_+|T_t\xi_-) - 4(\xi_+|\xi_-) = 4(\xi_+|T_t\xi_-)$$

establishes property ii) for the family of bounded quadratic forms $\mathcal{E}^t$ depending on $t > 0$. Letting t approach zero we get the property ii) for $\mathcal{E}$. To prove the converse we still go via positivity of the resolvent, this property being equivalent to positivity of the semigroup by reasoning similar to that used in the previous theorem and based on convexity.
To prove that for each sufficiently large λ we have $R_\lambda(\mathcal{H}^+) \subseteq \mathcal{H}^+$, notice that the resolvent map R_λ may be seen as the adjoint $I^* : \mathcal{H} \to \mathcal{F}$ of the embedding $I : \mathcal{F} \to \mathcal{H}$ when the domain $\mathcal{F}$ is endowed with the graph norm $\|\cdot\|_\lambda$. Let ξ be in $R_\lambda(\mathcal{H}^+)$. To prove that $\xi \in \mathcal{H}^+$ we will show that $\xi = |\xi|$. Since by the Spectral Theorem $R_\lambda(\mathcal{H}) \subseteq \mathcal{F}$, we have that $\xi \in \mathcal{F}^J$. Hence by

hypothesis ii) we have $|\xi| \in \mathcal{F}^J$ and $\||\xi|\|_\lambda \leq \|\xi\|_\lambda$. Suppose that $\eta \in \mathcal{H}^+$ is such that $\xi = R_\lambda \eta = I^* \eta$. Then

$$(|\xi| \,|\, \xi)_\lambda = (|\xi| \,|\, I^*\eta)_\lambda = (|\xi| \,|\, \eta) \geq |(\xi \,|\, \eta)| = |(\xi \,|\, I^*\eta)_\lambda| = \|\xi\|^2_\lambda ,$$

so that by the Cauchy-Schwarz inequality we obtain

$$\|\xi\|^2_\lambda \leq (|\xi| \,|\, \xi)_\lambda \leq \| \, |\xi| \, \|_\lambda \cdot \|\xi\|_\lambda \leq \|\xi\|^2_\lambda$$

and thus $|\xi| = \xi$. The equivalence between ii) and iii) easily follows from the identities $2\xi_\pm = |\xi| \pm \xi$ and $\mathcal{E}[|\xi|] - \mathcal{E}[\xi] = \mathcal{E}[\xi_+ + \xi_-] - \mathcal{E}[\xi_+ - \xi_-] = 4\mathcal{E}(\xi_+, \xi_-)$.

The application of the criterion in Theorem 2.53 above is frequently simplified by the following situation.

Theorem 2.54. *Let $\mathcal{E} : \mathcal{H} \to (-\infty, +\infty]$ be a non-negative, J-real closed quadratic form such that*

- *i) $\mathcal{E}$ is non-negative,*
- *ii) $\xi_0 \in \mathcal{F}$ and $\mathcal{E}(\xi_0, \xi) \geq 0$ for all $\xi \in \mathcal{F} \cap \mathcal{H}^+$,*
- *iii) $\mathcal{E}[|\xi|] \leq \mathcal{E}[\xi] \qquad \forall\, \xi \in \mathcal{H}^J$.*

Then $\mathcal{E}$ is a Dirichlet form with respect to ξ_0.

Proof. Since, by hypothesis i), $\xi_0 \in \mathcal{F}$ and, by Lemma 2.27 iii), $\xi \wedge \xi_0 = \xi_0 - (\xi - \xi_0)_-$, the Markovianity property $\mathcal{E}[\xi \wedge \xi_0] \leq \mathcal{E}[\xi]$ of $\mathcal{E}$ can re-written as follows:

$$\begin{aligned}
\mathcal{E}[\xi_0 - (\xi - \xi_0)_-] &\leq \mathcal{E}[\xi_0 + (\xi - \xi_0)] \\
\mathcal{E}[\xi_0] - 2\mathcal{E}(\xi_0, (\xi - \xi_0)_-) + \mathcal{E}[(\xi - \xi_0)_-] &\leq \mathcal{E}[\xi_0] - 2\mathcal{E}(\xi_0, \xi - \xi_0) + \mathcal{E}[\xi - \xi_0] \\
-2\mathcal{E}(\xi_0, (\xi - \xi_0)_+) &\leq \mathcal{E}[\xi - \xi_0] - \mathcal{E}[(\xi - \xi_0)_+] \,.
\end{aligned}$$

Since by hypothesis ii) the left hand side of the last inequality is negative, to prove the result it is enough to show that the right hand side is positive, i.e. $\mathcal{E}[\eta_+] \leq \mathcal{E}[\eta]$ for all $\eta \in \mathcal{H}^J$, or even

$$\mathcal{E}[\eta_+] \leq \mathcal{E}[\eta_+] + \mathcal{E}[\eta_-] - 2\mathcal{E}(\eta_+, \eta_-) \,.$$

This follows by assumptions i), iii) and the equivalence in Theorem 2.30 between statement ii) and iii).

Example 2.55. (Bounded Dirichlet forms) Let $(\mathfrak{M}, \mathcal{H}, \mathcal{H}^+, J)$ be a standard form of the von Neumann algebra $\mathfrak{M}$ and $\xi_0 \in \mathcal{H}^+$ a cyclic vector. Consider, for a set of elements $a_k \in \mathfrak{M}$ and positive numbers $\mu_k, \nu_k > 0\,, \quad k = 1, \ldots, n\,,$ the operators

$$d_k : \mathcal{H} \to \mathcal{H} \qquad d_k := i(\mu_k a_k - \nu_k j(a_k^*)) \,,$$

the quadratic form

$$\mathcal{E}[\xi] := \sum_{k=1}^{n} \|d_k\xi\|^2$$

and its associated symmetric, contractive semigroup $\{T_t : t \geq 0\}$. Then we have

- i) $\mathcal{E}$ is J-real if and only if

$$\sum_{k=1}^{n} [\mu_k^2 a_k^* a_k - \nu_k^2 a_k a_k^*] \in \mathfrak{M} \cap \mathfrak{M}' \,;$$

- ii) if $\mathcal{E}$ is J-real then $\{T_t : t \geq 0\}$ is positive;
- iii) if $\mathcal{E}$ is J-real then $\mathcal{E}$ is ξ_0-Markovian if and only if

$$\sum_{k=1}^{n} [\mu_k^2 a_k^* a_k - \mu_k\nu_k(a_k j(a_k) + a_k^* j(a_k^*)) + \nu_k^2 a_k a_k^*]\xi_0 \in \mathcal{H}^+ \,;$$

- iv) $\{T_t : t \geq 0\}$ is conservative ($T_t\xi_0 = \xi_0$ for all $t \geq 0$) if and only if the numbers $(\mu_k/\nu_k)^2$, $k = 1, \ldots, n$, are eigenvalues of the modular operator Δ_{ξ_0}, corresponding the eigenvectors $a_k\xi_0$. In particular, this is the case when $\mu_k = \nu_k$ for all $k = 1, \ldots, n$ and the elements a_k belongs to the *centralizer* of the state $\omega_0(\cdot) = (\xi_0| \cdot \xi_0)$ associated to ξ_0,

$$\mathfrak{M}_{\omega_0} := \{x \in \mathfrak{M} : \omega_0(xy) = \omega_0(yx) \quad \forall\, y \in \mathfrak{M}\} \,.$$

To verify i) notice that

$$\mathcal{E}[\xi] = \sum_{k=1}^{n} \big(\xi|(\mu_k a_k^* - \nu_k j(a_k))(\mu_k a_k - \nu_k j(a_k^*))\xi\big)$$

and

$$\mathcal{E}[J\xi] = \sum_{k=1}^{n} \big(\xi|(\nu_k a_k - \mu_k j(a_k^*))(\nu_k^* a_k - \mu_k j(a_k))\xi\big) \,,$$

so that $\mathcal{E}$ is J-real if and only if

$$\sum_{k=1}^{n} \nu_k^2(a_k a_k^* + j(a_k^* a_k)) = \sum_{k=1}^{n} \mu_k^2(a_k^* a_k + j(a_k a_k^*)) \,.$$

Rearranging this last equation as $\sum_{k=1}^{n}[\mu_k^2 a_k^* a_k - \nu_k^2 a_k a_k^*] = j(\sum_{k=1}^{n}[\mu_k^2 a_k^* a_k - \nu_k^2 a_k a_k^*])$ we get the desired condition in item i), as $a = j(a)$ for $a \in \mathfrak{M}$ if and only if a belongs to the *center* $\mathfrak{M} \cap \mathfrak{M}'$ of $\mathfrak{M}$.

Assuming $\mathcal{E}$ to be J-real, to prove the positivity property of the semigroup, we are going to verify condition iii) in Theorem 2.53. Let $\xi_\pm \in \mathcal{H}^+$ be two positive orthogonal vectors. Denote by $s'_\pm \in \mathfrak{M}'$ the support projection in $\mathfrak{M}'$ of the vectors $\xi_\pm$: these are, by definition, the projection onto the closure of the subspaces $\mathfrak{M}'\xi_\pm$ (see [Ara]). Since s'_+ and s'_- are orthogonal, $s'_+s'_- = s'_-s'_+ = 0$, and they commute with the operators $a_1 \ldots, a_n \in \mathfrak{M}$ we have

$$\begin{aligned}\mathcal{E}(\xi_+,\xi_-) &= \sum_{k=1}^n ((\mu_k a_k - \nu_k j(a_k^*))\xi_+ | \mu_k(a_k - \nu_k j(a_k^*))\xi_-) \\ &= -\sum_{k=1}^n \mu_k\nu_k((a_k j(a_k) + a_k^* j(a_k^*))\xi_+|\xi_-) \\ &\le 0\end{aligned}$$

by Proposition 2.13 iv).

Assuming $\mathcal{E}$ to be J-real, to prove Markovianity of $\mathcal{E}$, we may use Theorem 2.54: since the form is nonnegative by construction, and condition iii) of Theorem 2.54 is satisfied, by the above calculation and by Theorem 2.53, what is left to be shown is that ξ_0 is *excessive* for $\mathcal{E}$: $\mathcal{E}(\xi,\xi_0) \ge 0$ for all $\xi \in \mathcal{H}^+$ (in this case the form domain coincides with the whole of $\mathcal{H}$). A direct calculation gives

$$\begin{aligned}\mathcal{E}(\xi,\xi_0) &= \sum_{k=1}^n (\xi|d_k^* d_k \xi_0) \\ &= \left(\xi \Big| \sum_{k=1}^n [\mu_k^2 a_k^* a_k - \mu_k\nu_k(a_k j(a_k) + a_k^* j(a_k^*)) + \nu_k^2 j(a_k a_k^*)]\xi_0\right).\end{aligned}$$

Since $\mathcal{H}^+$ is self-dual, the vector ξ_0 is excessive for $\mathcal{E}$ if and only if the vector $\sum_{k=1}^n [\mu_k^2 a_k^* a_k - \mu_k\nu_k(a_k j(a_k) + a_k^* j(a_k^*)) + \nu_k^2 a_k a_k^*]\xi_0$ is in $\mathcal{H}^+$.

Conservativity of the semigroup generated by $\mathcal{E}$ is clearly equivalent to the fact that ξ_0 belongs to the kernel of the generator and then, by the Spectral Theorem, to $\mathcal{E}[\xi_0] = 0$. This means that $d_k\xi_0 = 0$ for all $k = 1,\ldots,n$. By the definition of the operators d_k this happens if and only if

$$\mu_k a_k \xi_0 = \nu_k j(a_k^*)\xi_0 \qquad k = 1,\ldots,n\,.$$

Using the properties of the modular operators, we may re-write this equation in the form

$$\mu_k a_k \xi_0 = \nu_k j(a_k^*)\xi_0 = \nu_k J a_k^* \xi_0 = \nu_k J J \Delta_{\xi_0}^{1/2} a_k \xi_0 = \nu_k \Delta_{\xi_0}^{1/2} a_k \xi_0\,,$$

from which the statement in item iv) above follows. When all the coefficients a_k belong to the centralizer of ω_0, they strongly commute with the modular operator Δ_{ξ_0} and the last equation simplifies as follows

$$\mu_k a_k \xi_0 = \nu_k \Delta_{\xi_0}^{1/2} a_k \xi_0 = \nu_k a_k \Delta_{\xi_0}^{1/2} \xi_0 = \nu_k a_k \xi_0\,.$$

This is verified if and only if $\mu_k = \nu_k$ for all $k = 1, \ldots, n$.

Notice that, in this example, the generator H has the form

$$H = \sum_{k=1}^{n} \mu_k^2 a_k^* a_k - \mu_k \nu_k (a_k j(a_k) + a_k^* j(a_k^*)) + \nu_k^2 j(a_k a_k^*) ,$$

similar to that of the *Lindblad generator* of a dynamical, uniformly continuous semigroup (see Example 2.26). The similarity is even more evident if, beside the (say left) action of $\mathfrak{M}$ on $\mathcal{H}$ considered so far,

$$\mathcal{H} \times \mathfrak{M} \ni (\xi, x) \mapsto \xi x \in \mathcal{H} ,$$

we also consider the right one, defined by

$$\mathcal{H} \times \mathfrak{M} \ni (\xi, x) \mapsto \xi x := j(x^*)\xi = Jx^* J\xi \in \mathcal{H} .$$

Using this action, we have in fact that

$$H\xi = \sum_{k=1}^{n} \mu_k^2 a_k^* a_k \xi - \mu_k \nu_k (a_k \xi a_k^* + a_k^* \xi a_k) + \nu_k^2 \xi a_k a_k^* .$$

Notice, moreover, that the maps $d_k : \mathcal{H} \to \mathcal{H}$, by which we constructed the Dirichlet form $\mathcal{E}$ are *covariant derivations* with respect to the bi-module action above. In fact, considering the derivations of $\mathfrak{M}$ given by

$$\delta_b : \mathfrak{M} \to \mathfrak{M} \qquad \delta_b(a) := i[b, a] = i(ba - ab) \qquad a, b \in \mathfrak{M} ,$$

the following *Leibniz rules* hold true:

$$d_k(a\xi) = \delta_{\mu_i a_i}(a)\xi + a d_k(\xi) , \qquad d_k(\xi a) = d_k(\xi) a + \xi \delta_{\nu_i a_i}(a) .$$

Compare this with Chapter 5, equation 5.9. In the tracial case constructions similar to those above have been considered in [GIS] to generate non symmetric Dirichlet forms and non symmetric Markovian semigroups.

Example 2.56. (An unbounded Dirichlet form) Let $(a, D(a))$ be a self-adjoint operator, affiliated to the von Neumann algebra $\mathfrak{M}$, and consider the operator defined by

$$d_a : D(d_a) \to \mathcal{H} \qquad d_a := i(a - j(a)) , \qquad D(d_a) := D(a) \cap JD(a) ,$$

together with the positive, J-real quadratic form

$$\mathcal{E}[\xi] := \|d_a \xi\|^2 , \qquad \mathcal{F} = D(d_a) .$$

Notice that, since a and $j(a)$ commute strongly, the operator d_a and the quadratic form $\mathcal{E}$ are closable on the domain $\mathcal{F} = D(d_a)$. We are going to show that *if a is affiliated to the centralizer $\mathfrak{M}_{\omega_0}$ then $\mathcal{E}$ is Markovian.* This will be done by a monotone approximation procedure. By Haagerup's representation lemma (see [H1]), for each fixed vector $\xi \in \mathcal{H}$ there exists a unique, positive, bounded Borel measure ν supported on $\mathrm{Sp}(a) \times \mathrm{Sp}(a)$ such that

$$\int_{\mathrm{Sp}(a)\times\mathrm{Sp}(a)} f(s)g(t)\,\nu(ds,dt) = (\xi|\, f(a)j(g(a))\xi)$$

for continuous functions f and g on the spectrum $\mathrm{Sp}(a) \subseteq \mathbb{R}$ of a. Using this measure we have the following representation

$$\mathcal{E}[\xi] = \int_{\mathrm{Sp}(a)\times\mathrm{Sp}(a)} |s-t|^2\,\nu(ds,dt)\,.$$

Consider the sequence $\{f_n \in C_b(\mathbb{R}) : n \in \mathbb{N}^*\}$ of bounded, continuous functions defined by $f_n(t) = t$ for $t \in [-n, +n]$, while $f_n(t) = n \cdot \mathrm{sgn}(t)$ otherwise, and the sequence of bounded quadratic forms:

$$\mathcal{E}_n[\xi] = \|f_n(a)\xi - \xi f_n(a)\|^2\,.$$

Since $f_n(a) \in \mathfrak{M}_{\omega_0}$, by the previous example, we have that *the*$\mathcal{E}_n$ are Dirichlet forms. Using the measure ν we may represent these forms as follows:

$$\mathcal{E}_n[\xi] = \int_{\mathrm{Sp}(a)\times\mathrm{Sp}(a)} |f_n(s)-f_n(t)|^2\,\nu(ds,dt)\,.$$

Since, as is easy to verify, $|f_n(s)-f_n(t)| \le |f_{n+1}(s)-f_{n+1}(t)|$ for all $(s,t) \in \mathbb{R}^2$ and $n \in \mathbb{N}^*$, we have that the quadratic form $\mathcal{E}$ is monotone the limit of the sequence of Dirichlet forms $\mathcal{E}_n$:

$$\mathcal{E}[\xi] = \sup_n \mathcal{E}_n[\xi] \qquad \forall\, \xi \in \mathcal{H}.$$

Markovianity of $\mathcal{E}$ follows from the Markovianity of the approximating forms $\mathcal{E}_n$. The closure of $\mathcal{E}$ is then closed and Markovian, so that it is a Dirichlet form.

Example 2.57. (Quantum Ornstein-Uhlenbeck semigroup, Quantum Brownian motion, Birth-and-Death process) We describe here the construction of a Dirichlet form on a type I factor von Neumann algebra $\mathcal{B}(h)$ which generates a Markovian semigroup of those types appearing in quantum optics (see [D1]).

Let us consider, on the Hilbert space $h := l^2(\mathbb{N})$, the von Neumann algebra $\mathcal{B}(h)$ and its Hilbert-Schmidt standard form

$$(\mathcal{B}(h)\,, \mathcal{L}^2(h)\,, \mathcal{L}^2_+(h)\,, J)$$

discussed in Example 2.17. Let $\{e_n : n \geq 0\} \subset h$ be the canonical Hilbert basis, and denote by $|\, e_m\rangle\langle e_n|$, $n, m \geq 0$, the partial isometries, having $\mathbb{C}e_n$ has initial space and $\mathbb{C}e_m$ as final one.

For a pair of fixed parameters $\mu > \lambda > 0$, set $\nu := \lambda^2/\mu^2$ and let

$$\phi_\nu(x) := \mathrm{Tr}(\rho_\nu x) \qquad x \in \mathcal{B}(h)\,,$$

the normal state on $\mathcal{B}(h)$ represented by the trace-class operator

$$\rho_\nu := (1-\nu)\sum_{n\geq 0} \nu^n |e_n\rangle\langle e_n|\,.$$

The associated cyclic vector ξ_ν in $\mathcal{L}^2_+(h)$ is then given by

$$\xi_\nu = \rho_\nu^{1/2} = (1-\nu)^{1/2}\sum_{n\geq 0} \nu^{n/2}|e_n\rangle\langle e_n|\,,$$

so that $\phi_\nu(x) = \langle \xi_\nu |\, x\xi_\nu\rangle$. The *creation* and *annihilation operators* a^* and a on h are defined by

$$a^* e_n := \sqrt{n+1}e_{n+1}\,, \qquad a e_n := \begin{cases} \sqrt{n}e_{n-1} & \text{if } n > 0; \\ 0 & \text{if } n = 0. \end{cases}$$

They are adjoint to one another on their common domain

$$D(a) = D(a^*) = \Big\{ e \in h : \sum_{n\geq 0} \sqrt{n}|\langle e|\, e_n\rangle|^2 < \infty \Big\}\,,$$

and satisfy the *Canonical Commutation Relation*

$$a\,a^* - a^* a = I\,.$$

The quadratic form given by

$$\mathcal{E}[\xi] := \|\mu a\xi - \lambda\xi a^*\|^2 + \|\mu a\xi^* - \lambda\xi^* a^*\|^2$$

is well defined on the dense subspace of $\mathcal{L}^2(h)$ defined as

$$D(\mathcal{E}) := \text{linear span}\{|\, e_m\rangle\langle e_n|\,, n, m \geq 0\}\,.$$

In fact, it is easy to check that for $\xi \in D(\mathcal{E})$, the operators $a\xi$, $a^*\xi$, ξa and ξa^* are bounded. It is then possible to prove that the closure of $(\mathcal{E}\,, D(\mathcal{E}))$ is a Dirichlet form with respect to ξ_ν, generating the so called *quantum Ornstein-Uhlenbeck* Markovian semigroup (see [CFL]).

Moreover, it is easy to check that $\mathcal{E}$ vanishes only on the multiples of the vector ξ_ν, so that, by Corollary 2.48, the associated *quantum Ornstein-Uhlenbeck* semigroup is *ergodic*. In [CFL] it was shown also that, the semigroup has the

Feller property, in the sense that it leaves invariant the algebra of compact operators $\mathcal{K}(h)$, and on this C*-algebra the semigroup is strongly continuous.

This example exhibits one of the characteristic features of *Noncommutative or Quantum Probability*, namely, the possibility of accommodating different classical processes in a single quantum process. *This point is illustrated in Philippe Biane's Lectures in this volume.*
In fact, the quantum Ornstein-Uhlenbeck semigroup leaves different *maximal abelian subalgebras* of $\mathcal{B}(h)$ globally invariant ([Ped 2.8]): reducing it to a suitable pair of them, one may obtain, for example, the semigroups of the *classical Ornstein-Uhlenbeck* and *Birth-and-Death processes* (see [CFL]).

When $\lambda = \mu$, the role of the invariant state ϕ_ν has to be played by the normal, semifinite trace τ on $\mathcal{B}(h)$. However, even in this case, using the theory developed by [AHK1] (see Chapter 4), it is possible to prove that the closure of the quadratic form

$$\mathcal{E}[\xi] := \|a\xi - \xi a^*\|^2 + \|a\xi^* - \xi^* a^*\|^2 \qquad \xi \in D(\mathcal{E})$$

is a Dirichlet form. The associated τ-symmetric Markovian semigroup on $\mathcal{B}(h)$ may be *dilated* by a *Quantum Stochastic processes*, known as *Quantum Brownian motion*. On a suitable, invariant, maximal abelian subalgebra, the dynamical semigroup reduces to the *heat semigroup* of a classical *Brownian motion* (see [CFL]).
A whole family of Quantum Ornstein-Uhlenbeck semigroups, Markovian with respect to suitable quasi-free states on the CCR algebra, has been introduced and deeply investigated in [KP].

We would like to illustrate now a construction due to Y.M. Park [P1,3] which, though similar to that of Example 2.55, is better suited for applications to Quantum Statistical Mechanics (see Chapter 3).

Definition 2.58. (Admissible functions) Let us denote by I_λ, the strip

$$I_\lambda := \{z \in \mathbb{C} : |\mathrm{Im} z| \le \lambda\} \qquad \lambda > 0\,,$$

and consider the subspace $\mathfrak{M}_\lambda$ of elements $x \in \mathfrak{M}$ for which the map $\mathbb{R} \ni t \mapsto \sigma_t(x) \in \mathfrak{M}$ can be extended to an analytic map in a domain containing the strip I_λ.
An analytic function $f : D \to \mathbb{C}$, defined in a domain D containing the strip $I_{1/4}$, is called *admissible* if the following properties hold true:

- i) $f(t) \ge 0$ for all $t \in \mathbb{R}$,
- ii) $f(t + i/4) + f(t - i/4) \ge 0$, for all $t \in \mathbb{R}$
- iii) there exist $M > 0$ and $p > 1$, such that the bound

$$|f(t + is)| \le M(1 + |t|)^{-p}$$

holds uniformly for $s \in [-1/4\,, +1/4]$.

For example, the function

$$f(t) := \sqrt{\frac{2}{\pi}} \int_{\mathbb{R}} (e^{k/4t} + e^{-k/4})^{-1} e^{-k^2/2} e^{-itk}\, dk \qquad t \in \mathbb{R}\,,$$

is admissible for all $p > 1$. We will also consider the function $f_0 : \mathbb{R} \to \mathbb{R}$ given by

$$f_0(t) := \frac{1}{\cosh(2\pi t)} = 2(e^{2\pi t} + e^{-2\pi t})^{-1} \qquad t \in \mathbb{R}\,.$$

This function, which plays a distinguished role in the proof of the Tomita-Takesaki Theorem (see [Br2], [T1], [V]), is *almost admissible* in the sense that it has an analytic extension to the interior of $I_{1/4}$, denoted f_0 again, and, on the boundary of $I_{1/4}$, it is a distribution satisfying

$$f_0(t + i/4) + f_0(t - i/4) = \delta(t)\,.$$

Admissible functions will play the role of *coefficients* for the class of Dirichlet forms we are going to discuss.

Proposition 2.59. *([P1,3]) Let* $(\mathfrak{M}, \mathcal{H}, \mathcal{H}^+, J)$ *be a standard form of the von Neumann algebra* $\mathfrak{M}$ *and* $\xi_0 \in \mathcal{H}^+$ *a cyclic vector. Consider* $x \in \mathfrak{M}_{1/4}$*, and let* f *represent an admissible function or equal the function* f_0*. Then the quadratic form* $\mathcal{E} : \mathcal{H} \to [0, +\infty)$*, defined by*

$$\mathcal{E}[\xi] := \int_{\mathbb{R}} \|(\sigma_{t-i/4}(x) - j(\sigma_{t-i/4}(x^*)))\xi\|^2 f(t)\, dt \qquad \xi \in \mathcal{H}\,, \tag{2.28}$$

is a Dirichlet form.

Proof. In this proof, for the sake of clarity, we will denote the scalar product in $\mathcal{H}$ *by angle brackets* $\langle \cdot | \cdot \rangle$. We will consider the case $f = f_0$ only. The proof in case of admissible functions is similar. Notice that, by the assumption $x \in \mathfrak{M}_{1/4}$, we have (see Appendix 7.3)

$$\sigma_{t-i/4}(x) = \sigma_t(\sigma_{-i/4}(x)) \qquad t \in \mathbb{R}\,, \tag{2.29}$$

so that

$$\|\sigma_{t-i/4}(x)\| = \|\sigma_{-i/4}(x)\| \qquad t \in \mathbb{R}$$

and $\mathcal{E}$ is well defined on the whole $\mathcal{H}$, as f_0 is integrable. To apply Theorem 2.53, we are going to verify the property appearing there in item iii). Consider two orthogonal, positive elements $\xi_\pm \in \mathcal{H}^+$, and decompose $\mathcal{E}(\xi_+ | \xi_-)$ as follows:

$$\mathcal{E}(\xi_+ | \xi_-) = \mathcal{E}_1(\xi_+ | \xi_-) + \mathcal{E}_2(\xi_+ | \xi_-) + \mathcal{E}_1^*(\xi_+ | \xi_-) + \mathcal{E}_2^*(\xi_+ | \xi_-)\,, \tag{2.30}$$

where

$$\mathcal{E}_1(\xi_+|\,\xi_-) := \int_{\mathbb{R}} \Big(\langle \sigma_{t-i/4}(x)\xi_+ |\, \sigma_{t-i/4}(x)\xi_- \rangle + \langle \sigma_{t-i/4}(x^*)\xi_- |\, \sigma_{t-i/4}(x^*)\xi_+ \rangle \Big) f_0(t)dt \,, \tag{2.31}$$

$$\mathcal{E}_2(\xi_+|\,\xi_-) := -\int_{\mathbb{R}} \Big(\langle \sigma_{t-i/4}(x)\xi_+ |\, j(\sigma_{t-i/4}(x^*))\xi_- \rangle + \langle j(\sigma_{t-i/4}(x^*))\xi_+ |\, \sigma_{t-i/4}(x)\xi_- \rangle \Big) f_0(t)dt \,, \tag{2.32}$$

and $\mathcal{E}_1^*(\xi_+|\,\xi_-)$, $\mathcal{E}_2^*(\xi_+|\,\xi_-)$ are obtained from $\mathcal{E}_1(\xi_+|\,\xi_-)$, $\mathcal{E}_2(\xi_+|\,\xi_-)$, respectively, replacing x by x^*. Reasoning as in Example 2.55, we get

$$\mathcal{E}_1(\xi_+|\,\xi_-) = \mathcal{E}_1^*(\xi_+|\,\xi_-) = 0$$

as ξ_+ and ξ_- have orthogonal support projection in $\mathfrak{M}'$ and $\sigma_{t-i/4}(x)\,, \sigma_{t-i/4}(x^*) \in \mathfrak{M}$. To evaluate the second and fourth part in expression 2.30, notice that

$$\sigma_{t-i/4}(x)^* = \sigma_{t+i/4}(x^*)\,, \qquad j(\sigma_{t+i/4}(x)^*) = \sigma_{t-i/4}(j(x))\,.$$

We then have

$$\mathcal{E}_2(\xi_+|\,\xi_-) = -\int_{\mathbb{R}} \Big(\langle \xi_+ |\, \sigma_{t+i/4}(x^*j(x^*))\xi_- \rangle + \langle \xi_+ |\, \sigma_{t-i/4}(xj(x))\xi_- \rangle \Big) f_0(t)dt \,, \tag{2.33}$$

$$\mathcal{E}_2^*(\xi_+|\,\xi_-) = -\int_{\mathbb{R}} \Big(\langle \xi_+ |\, \sigma_{t+i/4}(xj(x))\xi_- \rangle + \langle \xi_+ |\, \sigma_{t-i/4}(x^*j(x^*))\xi_- \rangle \Big) f_0(t)dt \,, \tag{2.34}$$

$$\mathcal{E}(\xi_+|\,\xi_-) = -\int_{\mathbb{R}} \Big(\langle \xi_+ |\, (\sigma_{i/4} + \sigma_{-i/4})(\sigma_t(xj(x) + x^*j(x^*)))\xi_- \rangle \Big) f_0(t)dt \,. \tag{2.35}$$

Setting

$$I_0(y) := \int_{\mathbb{R}} \sigma_t(y) f_0(t)\, dt \qquad y \in \mathfrak{M}\,,$$

we may re-write (2.35) as follows:

$$\mathcal{E}(\xi_+|\,\xi_-) = -\langle \xi_+ |\, (\sigma_{i/4} + \sigma_{-i/4})(I_0(xj(x) + x^*j(x^*)))\xi_- \rangle \,. \tag{2.36}$$

Notice that, in the formulas above, the modular automorphism group is understood to act, not only on $\mathfrak{M}$, but on the whole algebra $B(\mathcal{H})$ of bounded operators on $\mathcal{H}$. It may be shown (see [P1,3], [Br2 Theorem 2.5.14], [T1 Lemma 3.10], [V Lemma 4.1]) that

$$I_0\big((\sigma_{i/4}+\sigma_{-i/4})(y)\big) = y \qquad \forall\, y \in B(\mathcal{H})\,.$$

By Proposition 2.13 iv), we then have

$$\mathcal{E}(\xi_+|\,\xi_-) = -\langle \xi_+|\,(xj(x)+x^*j(x^*))\xi_-\rangle \le 0\,. \tag{2.37}$$

Applying Theorem 2.53, the semigroup generated by $\mathcal{E}$ is positive, and that the following contraction property holds true:

$$\mathcal{E}[|\xi|] \le \mathcal{E}[\xi] \qquad \xi \in \mathcal{H}\,.$$

As $\mathcal{E}$ is, by construction, nonnegative, applying Theorem 2.54, we then have that $\mathcal{E}$ is a Dirichlet form, provided we verify it vanishes on ξ_0. This follows from the identities

$$\begin{aligned}
&(\sigma_{t-i/4}(x) - j(\sigma_{t-i/4}(x^*)))\xi_0 \\
&\quad = \Delta^{it+1/4}x\Delta^{-it-1/4}\xi_0 - J\Delta^{it+1/4}x^*\Delta^{-it-1/4}J\xi_0 \\
&\quad = i_0(\sigma_t(x)) - J(i_0(\sigma_t(x^*))) \\
&\quad = i_0(\sigma_t(x)) - J(i_0(\sigma_t(x)^*)) \\
&\quad = i_0(\sigma_t(x)) - i_0(\sigma_t(x)) \\
&\quad = 0\,.
\end{aligned}$$

Applying *essentially* the construction above, we describe next a class of Dirichlet forms on the CCR and CAR algebras, studied in [BKP1,2]. The corresponding semigroups are $\widehat{\omega}$-KMS-symmetric with respect to the normal extensions $\widehat{\omega}$ of the quasi-free KMS-states ω introduced in Example 2.29 and Example 2.30.

Example 2.60. (Dirichlet forms and quasi-free states on CAR algebras) Within the framework of Example 2.29, let $(\pi_\omega\,, \mathcal{H}_\omega\,\xi_\omega)$ be the GNS-representation of the CAR algebra $\mathfrak{U}(\mathfrak{h}_0)$ with respect to the quasi-free state ω, defined by the Hamiltonian operator H at the inverse temperature β. Strengthening, the previous assumptions made on $\mathfrak{h}_0$, i.e. assuming that

- $\mathfrak{h}_0$ is a dense subspace of analytic elements for the unitary group $\mathbb{R} \ni t \mapsto e^{itH}$,
- $e^{izH}\xi \in \mathfrak{h}_0$ for all $\xi \in \mathfrak{h}_0$ and $z \in \mathbb{C}$,

one obtains that, for $f \in \mathfrak{h}_0$, $a(f)$ is entire analytic with respect to the modular group of ω.

The construction of Proposition 2.59 will be, in this particular situation, modified so ad to take into account the natural $\mathbb{Z}_2$-grading, given by the involutive, *-automorphism

$$\gamma : \mathfrak{U}(\mathfrak{h}_0) \to \mathfrak{U}(\mathfrak{h}_0) \qquad \gamma(a(f)) := -a(f) \qquad f \in \mathfrak{h}_0\,.$$

As γ leaves ω invariant, by Proposition 2.16, there exists a positive, unitary operator $U_\gamma : \mathcal{H}_\omega \to \mathcal{H}_\omega$, such that $\gamma(x) = U_\gamma x U_\gamma^{-1}$, $x \in \mathfrak{M}_\omega$, $U_\gamma \xi_\omega = \xi_\omega$ and $U_\gamma^2 = I$. It is easy to check that $U_\gamma x \xi_\omega = \gamma(x)\xi_\omega$ for all $x \in \mathfrak{M}_\omega$.

Consider now a complete, orthonormal system $\{g_k : k \geq 1\} \subset \mathfrak{h}_0$ and an admissible function f, normalized so to have integral one over $\mathbb{R}$. The quadratic form $\mathcal{E} : \mathcal{H}_\omega \to [0, +\infty]$

$$\mathcal{E}[\xi] := \sum_{k\geq 1} \int_{\mathbb{R}} \|(\sigma_{t-i/4}(a(g_k)) - j(\sigma_{t-i/4}(a^*(g_k))))U_\gamma \xi\|^2 f(t)\, dt \qquad \xi \in \mathcal{H}_\omega\,, \tag{2.38}$$

is then a Dirichlet form and the associated Markovian semigroup commutes with the symmetry γ. It can also be shown that the semigroup is independent of the choices of the orthonormal basis so that, in particular, it commutes with the modular group. Moreover, the semigroup is ergodic and independent of the choice of the normalized admissible function.
This construction applies, for example, to the "Ideal Fermi Gas" where $\mathfrak{h} := L^2(\mathbb{R}^d\,, \mathrm{dx})$, $\mathfrak{h}_0$ is the subspace of functions having compactly supported Fourier transform, $H := -H_0 - \mu \cdot I$, H_0 denoting the Laplacian operator on $\mathbb{R}^d$, $\mu \in \mathbb{R}$ and $\beta > 0$.

Example 2.61. (Dirichlet forms and quasi-free states on CCR algebras) As in Example 2.30, let $(\pi_\omega\,, \mathcal{H}_\omega\, \xi_\omega)$ be the GNS-representation of the CCR C*-algebra $\mathfrak{U}(\mathfrak{h}_0)$ with respect to the quasi-free state ω, defined by the Hamiltonian operator H and by the inverse temperature $\beta > 0$. Denote by

$$W_\omega(f) := \pi_\omega(W(f)) \qquad f \in \mathfrak{h}_0\,,$$

the Weyl operators in the GNS-representation. As the functions $\mathbb{R} \ni t \mapsto \omega(W(tf))$ are continuous, for any fixed $f \in \mathfrak{h}_0$, the state ω is *regular* and the unitary groups $\mathbb{R} \ni t \mapsto W_\omega(tf)$ are strongly continuous (see [BR2 5.2.3]). Denote by $\Phi_\omega(f)$ their self-adjoint generators

$$W_\omega(tf) = e^{it\Phi_\omega(f)} \qquad t \in \mathbb{R}\,,$$

and define the annihilation and creation operators as follows

$$\begin{aligned} a_\omega(f) &:= \frac{\Phi_\omega(f) + i\Phi_\omega(if)}{\sqrt{2}}\,, \\ a^*_\omega(f) &:= \frac{\Phi_\omega(f) - i\Phi_\omega(if)}{\sqrt{2}}\,. \end{aligned} \tag{2.39}$$

These are densely defined, closed operators, adjoint to one another, satisfying the *Canonical Commutation Relations.* Strengthening again, the standing assumptions made on $\mathfrak{h}_0$, exactly as we did in Example 2.59, one may verify that

- the subspace $\mathfrak{M}_\sigma\xi_\omega$ is dense in the Hilbert space $\mathcal{H}_\omega$,
- the functions $\mathbb{R} \ni t \to \sigma_t(a(f))\xi$ and $\mathbb{R} \ni t \to \sigma_t(a^*(f))\xi$ admit entire analytic extensions for all $f \in \mathfrak{h}_0$, $\xi \in \mathfrak{M}_\sigma\xi_\omega$
- on vectors in $\mathfrak{M}_\sigma\xi_\omega$, these analytic extensions are given by

$$\sigma_z(a(f)) = a(e^{izH}f) \qquad \sigma_z(a^*(f)) = a^*(e^{i\overline{z}H}f) \qquad f \in \mathfrak{h}_0 .$$

Consider now a complete, orthonormal system $\{g_k : k \geq 1\} \subset \mathfrak{h}_0$ and a normalized admissible function f. The quadratic form $\mathcal{E} : \mathcal{H}_\omega \to [0, +\infty]$

$$\mathcal{E}[\xi] := \sum_{k\geq 1} \int_{\mathbb{R}} \|(\sigma_{t-i/4}(a(g_k)) - j(\sigma_{t-i/4}(a^*(g_k))))\xi\|^2 f(t)\, dt \qquad \xi \in \mathcal{H}_\omega \tag{2.40}$$

is then a Dirichlet form which is independent of the choice of orthonormal basis and the normalized, admissible function. Moreover, the corresponding semigroup is ergodic.

This construction applies, for example, to the "Ideal Bose Gas" where $\mathfrak{h} := L^2(\mathbb{R}^d, \mathrm{dx})$, $\mathfrak{h}_0$ is the subspace of functions having compactly supported Fourier transform, $H := -H_0 + \mu \cdot I$, H_0 denoting the Laplacian operator on $\mathbb{R}^d$, $\mu > 0$ and $\beta > 0$.

3 Dirichlet Forms in Quantum Statistical Mechanics

In this section we apply the theory developed so far to the construction of Dirichlet forms in the framework of Quantum Statistical Mechanics. We illustrate here a construction due to Y.M. Park [P1], [P2]. The reader may consult the work of A. Majewski-B. Zegarlinski [MZ1,2] and A. Majewski-R. Olkiewicz-B. Zegarlinski [MOZ], for alternative approaches based on generalized conditional expectations.

The problem to face is the *dynamical approach to equilibrium*. Consider a time evolution of a quantum system, hence a continuous group of automorphisms $\{\alpha_t : t \in \mathbb{R}\}$ of a C* or von Neumann algebra A. At any fixed inverse temperature β, the set of (α, β)-KMS states, representing the equilibria of the dynamical system, are the solution of the KMS equation. For each fixed (α, β)-KMS state, one would like to construct a dissipative dynamics, hence a continuous semigroup $\{\Phi_t : t \geq 0\}$ on A, ergodic and and admitting ω as the unique invariant state. In this section a partial answer to this problem will be provided, through an L^2 approach based on the construction of a suitable Dirichlet form. The discussion of the commutative case may be found in [Lig] while constructions of semigroups in the framework of Quantum Statistical Mechanics may found in [Mat1], [Mat2], [Mat3].

3.1 Quantum Spin Systems

Let us describe now briefly the quantum spin system and their dynamics (see [BR2 6.2] for a detailed exposition). Let $\mathbb{Z}^d$ be the $d \geq 1$ dimensional lattice space, whose sites are occupied by spins $\frac{1}{2}$ particles. The observables at site $x \in \mathbb{Z}^d$ are elements of the algebra

$$A_{\{x\}} := M_2(\mathbb{C}) .$$

The algebra of observables confined in the finite region $X \subset \mathbb{Z}^d$, given by

$$A_X := \bigotimes_{x \in X} A_{\{x\}} ,$$

is then the full matrix algebra $M_{2^{|X|}}(\mathbb{C})$, where $|X|$ denotes the cardinality of a set X. Let us denote by $\mathcal{L}$ the class (ordered by inclusion) of all finite subsets of $\mathbb{Z}^d$. When $L_1 , L_2 \in \mathcal{L}$ are disjoint regions, $L_1 \cap L_2 = \emptyset$, then

$$A_{L_1 \cup L_2} = A_{L_1} \otimes A_{L_2} .$$

On the other hand, if $L_1 \subseteq L_2$ and 1_{L_2} denotes the unit of A_{L_2}, the algebra A_{L_1} is identified with the subalgebra $A_{L_1} \otimes 1_{L_2}$ of $A_{L_1 \cup L_2}$. The normed *algebra* of all *local observables* is given by

$$A_0 := \bigcup_{X \in \mathcal{L}} A_X ,$$

while the *quasi-local* C*-algebra A is the norm completion of the local algebra A_0.

The mutual influence of spins confined to finite regions is represented by an *interaction*, i.e. a family $\Phi := \{\Phi_X : X \in \mathcal{L}\}$ of self-adjoint elements $\Phi_X \in A_X$. The bounded derivation

$$A_X \ni a \mapsto i\big[\Phi_Y , a\big] \qquad a \in A ,$$

generates a uniformly continuous group of automorphisms of A, representing the time evolution of the observables subject to the influence of the particles confined to Y. In order to take into account simultaneously the mutual influences among particles in different regions, one may hope that a superposition of these bounded derivations may give rise to a closable derivation $(\delta, D(\delta))$ on A, provided the interaction is sufficiently moderate. There are various conditions on the strength of an interaction providing derivations generating continuous groups of automorphisms of A. The following classical result, applicable to interactions for which the many body forces are negligible in an appropriate sense, is not the most general, as far as the problem of the existence of the dynamics is concerned. It implies, however, the existence of a *finite group velocity* for the dynamics of the systems, which will be used in the sequel to construct the Dirichlet form generating the Markovian approach to the equilibrium. We will denote by $D(X)$ the diameter of a set X.

Theorem 3.1. *([BR2 Theorem 6.2.4, 6.2.11], [LR]) Consider, on the quasi-local C^*-algebra A, an interactions satisfying, for a fixed $\lambda > 0$,*

$$\|\Phi\|_\lambda := \sup_{x\in\mathbb{Z}^d} \sum_{x\in X\in\mathcal{L}} |X| 4^{|X|} e^{\lambda D(X)} \|\Phi_X\| < +\infty\,. \tag{3.1}$$

Then, setting

$$D(\delta) := A_0 \qquad \delta(a) := \sum_{X\cap Y\neq\emptyset} i\big[\Phi_Y, a\big] \qquad a\in A_X\,,\quad X\in\mathcal{L}\,, \tag{3.2}$$

a closable derivation is correctly defined. Its closure generates a strongly continuous group $\alpha^\Phi := \{\alpha^\Phi_t : t\in\mathbb{R}\}$ of automorphisms of A, satisfying the following properties
i) analyticity: the time evolutions $\mathbb{R}\ni t\to\alpha^\Phi_t(a)$ of local observables $a\in A_0$, admit analytic extensions to domains containing the strip I_{β_0}, where $\beta_0 := \frac{\lambda}{2\|\Phi\|_\lambda}$;
ii) finite group velocity: denoting by $d(x,X)$ distance of the site $x\in\mathbb{Z}^d$ from the region $X\in\mathcal{L}$, we have for all $a\in A_{\{x\}}\,, b\in A_X\,, t\in\mathbb{R}$

$$\|[\alpha^\Phi_t(a), b]\| \le 2\|a\|\cdot\|b\|\cdot|X|\cdot e^{-\left(\lambda d(x,X))-2|t|\|\Phi\|_\lambda\right)}\,. \tag{3.3}$$

Example 3.2. (Ising and Heisenberg models) Suppose that, in addition to an external potential, represented by a one-body interaction, particles may influence each other only through a two-body interaction. This means that $\Phi(X) = 0$ whenever $|X|\ge 3$, so that the norms $\|\Phi\|_\lambda$ in (3.1) are finite if and only if

$$\sup_{x\in\mathbb{Z}^d}\|\Phi(\{x\})\| < +\infty\,, \qquad \sup_{x\in\mathbb{Z}^d}\sum_{y\in\mathbb{Z}^d} e^{\lambda|x-y|}\|\Phi(\{x,y\})\| < +\infty\,.$$

These are just uniform bounds on the energy of the particles occupying the sites of the lattice. In case Φ is translationally invariant, this reduces to

$$\sum_{y\in\mathbb{Z}^d} e^{\lambda|y|}\|\Phi(\{0,y\})\| < +\infty\,.$$

Using the *Pauli's matrices* $\sigma^x_j\in A_{\{x\}}$, $j = 0,1,2,3$, at a fixed site $x\in\mathbb{Z}^d$:

$$\sigma^x_0 = \begin{pmatrix}1&0\\0&1\end{pmatrix} \qquad \sigma^x_1 = \begin{pmatrix}0&1\\1&0\end{pmatrix} \qquad \sigma^x_2 = \begin{pmatrix}0&-i\\i&0\end{pmatrix} \qquad \sigma^x_3 = \begin{pmatrix}1&0\\0&-1\end{pmatrix}\,,$$

one may choose, for example,

$$\Phi(\{0\}) := h\sigma_3^0\,, \qquad \Phi(\{0,x\}) := \sum_{i=1}^{3} J_i(x)\sigma_i^0\sigma_i^x\,,$$

with $h \in \mathbb{R}$ and

$$\sum_{i=1}^{3}\sum_{x\in\mathbb{Z}^d} e^{\lambda|x|}|J_i(x)| < +\infty\,.$$

These choices are referred to as the *anisotropic Heisenberg model* when $J_i \neq 0$ and $J_i \neq J_j$ for some pair i,j; the *isotropic Heisenberg model* when $J_1 = J_2 = J_3 \neq 0$; the $X - Y$ *model* when $J_i \neq 0$, $i = 1,2$ but $J_3 = 0$; the *Ising model* when $J_1 = J_2 = 0$.

3.2 Markovian Approach to Equilibrium

Let ω be a (α^Φ, β)-KMS-state at inverse temperature $\beta > 0$, corresponding to the evolution $\{\alpha_t^\Phi : t \in \mathbb{R}\}$, hence to the interaction Φ satisfying the assumption of the previous theorem. Let $(\pi_\omega, \mathcal{H}_\omega, \xi_\omega)$ be the GNS representations of the state ω, $\mathfrak{M}$ the von Neumann algebra $\pi_\omega(A)''$ and $(\mathfrak{M}, \mathcal{H}_\omega, \mathcal{H}_\omega^+, J_\omega)$ the corresponding standard form.

The normal extension of ω to $\mathfrak{M}$ is a $(\widehat{\alpha}^{\mathbf{\Phi}}, \beta)$-KMS-state w.r.t. the normal extension $\{\widehat{\alpha}_t^\Phi : t \in \mathbb{R}\}$ of the time evolution on A. Hence the modular group $\{\sigma_t : t \in \mathbb{R}\}$ of the cyclic vector ξ_ω coincides with $\{\widehat{\alpha}^\Phi_{-\beta t} : t \in \mathbb{R}\}$. This implies, in particular, that the time evolutions of the local observables in $\mathfrak{M}$ admit analytic extensions to domains containing the strip $I_{\beta_0/\beta}$:

$$\pi_\omega(A_0) \subset \mathfrak{M}_{\beta_0/\beta}\,.$$

To construct a Dirichlet form on the GNS Hilbert space $\mathcal{H}_\omega$, we first apply Proposition 2.59 with f a fixed admissible function, or with $f = f_0$.
Denote by $\mathcal{E}_{x,j}$ the quadratic forms associated to the self-adjoint elements $a_j^x := \pi_\omega(\sigma_j^x)$:

$$\mathcal{E}_{x,j}[\xi] = \int_{\mathbb{R}} \|(\sigma_{t-i/4}(a_j^x) - j(\sigma_{t-i/4}(a_j^x)))\xi\|^2\, f(t)dt\,. \tag{3.4}$$

Notice that, by Proposition 2.59, these forms are correctly defined, and in fact completely Dirichlet forms, provided the ratio β_0/β is greater than $1/2$.

Theorem 3.3. *Let Φ be an interaction on the quasi-local algebra A satisfying the bound (3.1), for a fixed $\lambda > 0$. Suppose that ω is a (α^Φ, β)-KMS-state* *corresponding to the evolution* $\{\alpha_t^{\Phi} : t \in \mathbb{R}\}$ *at an inverse temperature* $\beta > 0$ *satisfying*

$$\beta < \frac{\lambda}{\|\Phi\|_\lambda} \,. \tag{3.5}$$

Then, for any p-admissible function f *with* $p > d+1$ *and for* $f = f_0$*, the quadratic functional*

$$\mathcal{E} : \mathcal{H}_\omega \to [0, +\infty] \qquad \mathcal{E}[\xi] := \sum_{x\in\mathbb{Z}^d} \sum_{j=0}^{3} \mathcal{E}_{x,j}[\xi] \tag{3.6}$$

is a completely Dirichlet form on $\mathcal{H}_\omega$*, with respect to the cyclic vector* ξ_ω *representing* ω*.*

Proof. The condition $\beta < \frac{\lambda}{\|\Phi\|_\lambda}$ guarantees that $\beta_0/\beta > \frac{1}{2}$, so that the self-adjoint, local elements $\{a_j^x : x \in \mathbb{Z}^d, j = 0,1,2,3\}$ belong to $\mathfrak{M}_{1/2}$. By Proposition 2.59, the quadratic forms $\mathcal{E}_{x,j}$ are completely Dirichlet forms. As the functional $\mathcal{E}$ is defined as the supremum of bounded, completely Dirichlet forms, it shares with them the completely Markovian property. What we have to prove is that $\mathcal{E}$ is densely defined. We will show that $\mathcal{E}$ is finite on the symmetric embedding in $\mathcal{H}_\omega$ of the local algebra $\pi_\omega(A_0)$.
By the boundedness of the symmetric embeddings, see Proposition 2.22, one has $\|i_\omega(b)\| \le \|b\|$, for all $b \in \mathfrak{M}$. We have for all $b \in \mathfrak{M}$, $a = a^* \in \mathfrak{M}_{1/2}$

$$\|(\sigma_{t-i/4}(a) - j(\sigma_{t-i/4}(a)))i_\omega(b)\| = \|i_\omega([\sigma_t(a), b])\| \le \|[\sigma_t(a), b]\| \,,$$

and then

$$\mathcal{E}[i_\omega(b)] \le \sum_{j=0}^{3} \sum_{x\in\mathbb{Z}^d} \int_{\mathbb{R}} \|[\sigma_t(a_j^x), b]\|^2 f(t)\, dt \qquad b \in \mathfrak{M} \,. \tag{3.7}$$

Assume now that $b \in \pi_\omega(A_0)$, or, more precisely, that $b \in \pi_\omega(A_X)$ for some fixed $X \in \mathcal{L}$. For each fixed index $j = 0,1,2,3$, let us split the sum over $x \in \mathbb{Z}^d$, in the right hand side of (3.7) as follows:

$$\sum_{x\in\mathbb{Z}^d} \int_{\mathbb{R}} \|[\sigma_t(a_j^x), b]\|^2 f(t)\, dt = I_j^1 + I_j^2 \tag{3.8}$$

where

$$I_j^1 := \sum_{N\in\mathbb{N}} \sum_{d(x,X)=N} \int_{|t|\le \frac{N\beta_0}{2}} \|[\sigma_t(a_j^x), b]\|^2 f(t)\, dt \,,$$

$$I_j^2 := \sum_{N\in\mathbb{N}} \sum_{d(x,X)=N} \int_{|t|> \frac{N\beta_0}{2}} \|[\sigma_t(a_j^x), b]\|^2 f(t)\, dt \,.$$

By Theorem 3.1 ii), and in particular the bound (3.3), if $b = \pi_\omega(c)$ for some $c \in A_X$, as Pauli matrices have unit norm, we have

$$\begin{aligned} \|[\sigma_t(a_j^x), b]\| &= \|[\sigma_t(\pi_\omega(\sigma_j^x)), \pi_\omega(c)]\| = \|[\pi_\omega(\alpha^\Phi_{-\beta t}(\sigma_j^x)), \pi_\omega(c)]\| \\ &\leq \|[\alpha^\Phi_{-\beta t}(\sigma_j^x), c]\| \\ &\leq 2 \cdot \|c\| \cdot |X| \cdot e^{-\left(\lambda d(x,X)) - 2|t| \|\Phi\|_\lambda\right)} \qquad t \in \mathbb{R}\,, \end{aligned} \tag{3.9}$$

Since on the d-dimensional square lattice $\mathbb{Z}^d$ the following bound holds true

$$\sharp\{x \in \mathbb{Z}^d : d(x,X) = N\} \simeq N^{d-1} \qquad N \to \infty\,,$$

using (3.9) we have that

$$\begin{aligned} I_j^1 &\leq 4 \cdot \|c\|^2 \cdot |X|^2 \sum_{N\in\mathbb{N}} \sum_{d(x,X)=N} \int_{|t| \leq \frac{N\beta_0}{2}} e^{-2\left(\lambda N - 2|t| \|\Phi\|_\lambda\right)} f(t) dt \\ &\leq 4 \cdot \|c\|^2 \cdot |X|^2 \cdot \Big(\int_\mathbb{R} f(t) dt\Big) \sum_{N\in\mathbb{N}} \sum_{d(x,X)=N} e^{-N\lambda} < +\infty\,. \end{aligned} \tag{3.10}$$

Since $\|[\sigma_t(a_j^x), b]\| \leq 2\|b\|$ for all $t \in \mathbb{R}$ and $j = 0, 1, 2, 3$, in case $f = f_0$, the decay properties of f_0 imply that I_j^2 is finite. In case of a general p-admissible function

$$f(t) \leq M \cdot (1 + |t|)^{-p} \qquad t \in \mathbb{R}$$

for some $M > 0$ and $p > d + 1$, so that we still have

$$\begin{aligned} I_j^2 &\leq 4 \cdot \|b\|^2 \cdot M \cdot \sum_{N\in\mathbb{N}} \sum_{d(x,X)=N} \int_{|t| > \frac{N\beta_0}{2}} (1 + |t|)^{-p} dt \\ &\leq 4 \cdot \|b\|^2 \cdot M \cdot \sum_{N\in\mathbb{N}} \sum_{d(x,X)=N} \Big(\frac{2}{p-1}\Big)\Big(1 + \frac{N\beta_0}{2}\Big)^{1-p} < +\infty\,. \end{aligned} \tag{3.11}$$

Corollary 3.4. *([P2 Theorem 2.1]) Under the assumptions of Theorem 3.3 the following properties are equivalent:*

i) ω is an extremal (α^Φ, β)-KMS-state;

ii) ω is a factor state;

iii) the Markovian semigroup $\{T_t : t \geq 0\}$ is ergodic.

Proof. The equivalence between properties i) and ii) is a well known property of KMS-states and may be found, for example, in [BR2 Theorem 5.3.30]. Before establishing the equivalence between properties ii) and iii), notice first that, the subspace $\mathcal{K}_\omega \subseteq \mathcal{H}_\omega$, where the Dirichlet form (3.6) is vanishing, coincides both with the subspace where the associated semigroup acts as the identity

$$\{\xi \in \mathcal{H}_\omega : T_t\xi = \xi\,, t \geq 0\}\,,$$

as well as with the eigenspace of the generator H corresponding to the eigenvalue zero

$$\{\xi \in \mathcal{H}_\omega : H\xi = 0\} .$$

Notice also that, since the involutive algebra generated by the Pauli matrices $\{\sigma_j^x : x \in \mathbb{Z}^d , j = 0, 1, 2, 3\}$, is norm dense in the quasi-local C*-algebra A, the involutive algebra generated by $\{\pi_\omega(\sigma_j^x) : x \in \mathbb{Z}^d , j = 0, 1, 2, 3\}$ is σ-weakly dense in the von Neumann algebra $\mathfrak{M}$. By a more general result, due Y.M. Park [P2 Theorem 2.1], the structure of the Dirichlet form (3.6) is such that its vanishing subspace is precisely

$$\mathcal{K}_\omega = \overline{\mathcal{Z}(\mathfrak{M})\xi_\omega} ,$$

i.e. the closure of the symmetric image in $\mathcal{H}_\omega$ of the center $\mathcal{Z}(\mathfrak{M}) := \mathfrak{M} \cap \mathfrak{M}'$ of the algebra $\mathfrak{M}$. Suppose now that ω is a factor state, so that $\mathcal{Z}(\mathfrak{M}) = \mathbb{C} \cdot 1_{\mathfrak{M}}$. Then the eigenvector ξ_ω is simple and, by Corollary 2.48, the semigroup is ergodic. Conversely, if the semigroup is ergodic, Corollary 2.48 implies that ξ_ω is simple, so that the center $\mathcal{Z}(\mathfrak{M})$ is trivial and ω is a factor state.

4 Dirichlet Forms and Differential Calculus on C*-algebras

In this chapter we show that, on algebras endowed with semi-finite traces, Dirichlet forms are in one-to-one correspondence with differential calculi. On one hand this correspondence provides a tool to construct Markovian semigroups symmetric with respect to traces. On the other hand this allows to analyze Dirichlet spaces from a geometric point of view. The meaning of this correspondence will be clarified through several examples in this chapter. The correspondence will be fundamental to prove the geometric applications of the last two chapters of these notes.

4.1 Dirichlet Forms and Markovian Semigroups with Respect to Traces

Our aim, in this section, is to show that *any regular Dirichlet form on a C*-algebra A endowed with a reasonable trace gives rise to a first order differential calculus on A*. The matter of this section is taken from [CS1]. Under the stronger hypothesis that the domain of the self-adjoint generator associated to the Dirichlet form contains a dense sub-algebra, it was previously proved in [S2,3]. The use of derivation in the construction of unbounded Dirichlet forms was also considered in [DL2] and [GIS].

Let A be a C*-algebra and τ a densely defined, faithful, semi-finite, lower semi-continuous trace on it. When τ is finite, the theory developed in the previous section applies and we have at our disposal good notions of positivity and Markovianity, for quadratic forms and semigroups, as well as a one to one correspondence between them. In the finite trace setting, the theory simplifies due to the fact that the modular operator reduces to the identity so that, essentially, positivity has the same meaning in the algebra as in the standard Hilbert space.

We now briefly indicate the changes needed to cover the case of C*-algebras with a densely defined, faithful, semi-finite, lower semi-continuous trace $\tau : A_+ \to [0, +\infty]$.

In the C*-algebra A define the subset $\mathcal{L} := \{a \in A : \tau(a^*a) < \infty\}$. It is easy to see that $\mathcal{L}$ is a left ideal in A, $\mathcal{N} := \mathcal{L}^*\mathcal{L}$ is a subalgebra of A and τ extends to a linear functional on $\mathcal{N}$. Let $L^2(A,\tau)$ be the Hilbert space defined completing $\mathcal{L}$ with respect to the pre-Hilbert space structure given by the sesquilinear form associating $\tau(a^*b)$ to $a, b \in \mathcal{L}$. Denoting by $\eta_\tau : \mathcal{L} \to L^2(A,\tau)$ the natural injection with dense range, the Gelfand-Naimark-Segal (GNS) representation is defined by

$$\pi_\tau : A \to \mathcal{B}(L^2(A,\tau)) \qquad (\eta_\tau(b)|\pi_\tau(a)\eta_\tau(c)) := \tau(b^*ac)$$

for $a \in A$ and $b, c \in \mathcal{L}$. We denote by $\mathfrak{M}$ or $L^\infty(A,\tau)$ the von Neumann algebra $\pi_\tau(A)''$ generated by A in this representation and by the same symbol τ the normal extension to $\mathfrak{M}$ of the trace on A. Moreover, we shall denote by the same symbols $\mathcal{L}, \mathcal{N}$ we used before for the trace τ on A, the corrisponding spaces associated to its normal extension on $\mathfrak{M}$.

From now on we shall not distinguish between a finite trace element of $\mathfrak{M}$ *and its image in the* $L^2(A,\tau)$.

Sometimes, we will denote by $L^\infty_+(A,\tau)$ the positive cone $\mathfrak{M}_+$.
In the trace case the involution $a \mapsto a^*$ of $\mathfrak{M}$ extends to an anti-unitary map on the GNS space $L^2(A,\tau)$. A self-dual closed, convex cone in the Hilbert space $L^2(A,\tau)$ is then realized as the closure of the subset

$$L^2_+(A,\tau) := \overline{\mathcal{L}_+}$$

and $(\mathfrak{M}, L^2(A,\tau)), L^2_+(A,\tau), J)$ is a standard form of $\mathfrak{M}$.

In particular, the positive part (resp. the modulus) of a self-adjoint element $a \in \mathfrak{M} \cap L^2(A,\tau)$, *w.r.t. the cone* $L^2_+(A,\tau)$, *coincides with the positive part* a_+ *(resp. the modulus* $|a| = a_+ + a_-$*) of* a *in the algebra* $\mathfrak{M}$.

In the framework of this standard form we can apply directly the part of the theory developed in section 2.6 concerning positive semigroups and their characterization in terms of quadratic forms. In particular Theorem 2.53 remains valid in this context.

To extend the notion of Markovianity for semigroup and forms to the present semi-finite setting, we have only to face the fact that sets like

$$\{\xi \in L^2(A,\tau) : \xi \le \xi_\tau\}, \qquad \{\xi \in L^2_+(A,\tau) : \xi \le \xi_\tau\}$$

(on which we based the definitions of Markovian forms and Markovian semigroups w.r.t. states) have to be modified due to the possible lack of a cyclic vector $\xi_\tau \in L^2(A,\tau)$ representing the semi-finite trace τ. Defining the closed convex set $C \subset L^2(A,\tau)$

$$C := \overline{\{a \in \mathcal{L} : a = a^* \leq 1_{\mathfrak{M}}\}}\,, \tag{4.1}$$

we shall denote by $a \wedge 1$ the Hilbertian projection of a onto the closed, convex set C. In case $a = a^* \in A \cap L^2(A,\tau)$ the projection $a \wedge 1$ is an element of the algebra A and coincides with the one obtained, by the continuous functional calculus of A, composing the continuous function $\mathbb{R} \ni t \mapsto f(t) = t \wedge 1$ with a.

Definition 4.1. (Dirichlet form with respect to a faithful, semifinite, lower-semicontinuous trace)
A quadratic functional $\mathcal{E} : L^2(A,\tau) \to (-\infty,+\infty]$ is said to be

- i) *J-real* if $\mathcal{E}[J\xi] = \mathcal{E}[\xi]$ for all $\xi \in L^2(A,\tau)$;
- ii) *Markovian* if

$$\mathcal{E}[\xi \wedge 1] \leq \mathcal{E}[\xi] \qquad \xi = J\xi \in L^2(A,\tau)\,,$$

  where $\xi \wedge 1$ denotes the projection of ξ onto the closed, convex set C;
- iii) *Dirichlet form* if it is a lower semi-continuous, Markovian functional;
- iv) *completely Dirichlet form* if all of its canonical extensions $\mathcal{E}_n$ to $L^2(M_n(A),\tau_n)$

$$\mathcal{E}_n[[a_ij]_{i,j=1}^n] := \sum_{i,j=1}^n \mathcal{E}[a_ij] \qquad [a_{ij}]_{i,j=1}^n \in L^2(M_n(A),\tau_n)$$

  are Dirichlet form for all $n \geq 1$; here τ_n denotes the trace $\tau_n := \tau \otimes \mathrm{tr_n}$ on the C*-algebra $M_n(A) := A \otimes M_n(\mathbb{C})$;
- v) *regular* if the subspace $\mathcal{B} := A \cap \mathcal{F}$ is norm dense in the C*-algebra A and a form core for $(\mathcal{E},\mathcal{F})$; here the subspace

$$\mathcal{F} := \{\xi \in \mathcal{L}^2(A,\tau) : \mathcal{E}[\xi] < +\infty\}$$

  denotes the domain of the quadratic form or functional;
- vi) a C*-Dirichlet form if it is a regular, completely Dirichlet form;
- vii) a J-real, symmetric, strongly continuous, semigroup $\{T_t : t \geq 0\}$ on $L^2(A,\tau)$ will be called Markovian if it leaves globally invariant the subset

$$C \cap L^2_+(A,\tau) = \overline{\{a \in \mathcal{L} : 0 \leq a \leq 1_{\mathfrak{M}}\}};$$

- viii) the semigroup is said to be *completely positive (resp. Markovian)* if all of its canonical extensions to $L^2(M_n(A),\tau_n)$ are positive (resp. Markovian).

As announced before, the one to one correspondence between completely Dirichlet forms, completely Markovian semigroups on $L^2(A,\tau)$ and completely Markovian semigroups on the von Neumann algebra $\mathfrak{M}$ still holds true starting from a densely defined, faithful, semi-finite, lower semi-continuous trace τ on a C^*-algebra A or at least from a densely defined, faithful, semi-finite, normal trace τ on a von Neumann algebra $\mathfrak{M}$.

4.2 Modules and Derivations on C*-algebras and Associated Dirichlet Forms

In this section we show how the construction of the model Dirichlet form, i.e. the Dirichlet integral

$$\mathcal{E}[u] = \int_{\mathbb{R}^d} |\nabla u(x)|^2 \, m(dx) \,,$$

can be generalized in terms of derivations on C*-algebras.

Definition 4.2. (Modules and Derivations on C*-algebras) An A–*bimodule* over the C*-algebra A is a Hilbert space $\mathcal{H}$ with a left representation and a right representation of A, which commute. Equivalently, it can be thought as a representation of the C*–algebra $A \otimes_{\max} A^\circ$, maximal tensor product of A and its opposite C*-algebra A°.
The left action of $a \in A$ on $\xi \in \mathcal{H}$ will be denoted by $a\xi \in \mathcal{H}$, while the right action by $\xi a \in \mathcal{H}$. Since the actions commute, we may denote $(a\xi)b = a(\xi b)$ by a unique symbol $a\xi b$ for $a, b \in A$ and $\xi \in \mathcal{H}$.
The bimodule $\mathcal{H}$ is said to be *symmetric* if there exists an isometric, anti-linear involution $\mathcal{J} : \mathcal{H} \to \mathcal{H}$ exchanging the right and left actions of A

$$\mathcal{J}(a\xi b) = b^* \mathcal{J}(\xi) a^* \qquad \forall\, a, b \in A \,, \quad \xi \in \mathcal{H} \,.$$

A *derivation* $\partial : D(\partial) \to \mathcal{H}$ is defined to be a linear map defined on a subalgebra $D(\partial)$ of A, satisfying the following *Leibniz rule*:

$$\partial(ab) = \partial(a)b + a\partial(b) \quad a, b \in D(\partial).$$

The derivation is called *symmetric* if its domain $D(\partial)$ is a self-adjoint subalgebra, the A–bimodule $(\mathcal{H}, \mathcal{J})$ is symmetric and

$$\partial(a^*) = \mathcal{J}(\partial a) \qquad a \in D(\partial) \,.$$

Example 4.3. (Gradient and square integrable vector fields) The standard example of a symmetric derivation is the gradient operator

$$\nabla : C_c^\infty(M) \to L^2(TM)$$

of a Riemannian manifold M, defined on the subalgebra of smooth functions and taking values in the Hilbert space $L^2(TM)$ of square integrable vector fields. Bounded continuous functions on M, acting by pointwise multiplication on vector fields, give rise to a module with respect to which the Leibniz rule holds true.

Example 4.4. (Derivations associated to martingales and stochastic calculus) An important example of derivation appears naturally in the theory of symmetric Hunt processes $\{X_t : t \geq 0\}$ on locally compact spaces X (i.e. the probabilistic counterpart of the theory of classical Dirichlet forms) and in particular, in the decomposition theory of additive functionals (see [FOT]). There, the algebra is the space $C_0(X)$ of continuous functions f on X, the bimodule $\mathcal{H}$ is the space $\mathcal{M}$ of square integrable martingales M of finite energy, and the left and right actions are given by a suitable defined stochastic integral $f \bullet M$. The derivation ∂f is given by the finite energy martingale part of $M^{[f]}$ of the cadlag additive functional

$$A_t^{[f]} = f(X_t) - f(X_0) \qquad t \geq 0\,.$$

We are going to see that derivations naturally gives rise to Dirichlet forms.

Theorem 4.5. *(Construction of Dirichlet forms by derivations) Let $(\partial, D(\partial))$ be a densely defined, symmetric derivation on the C^*-algebra A, taking values in the symmetric Hilbert A–bimodule $(\mathcal{H}, \mathcal{J})$. Suppose that $D(\partial)$ is contained and dense in $L^2(A,\tau)$ and that $(\partial, D(\partial))$ is a closable operator from $L^2(A,\tau)$ to $\mathcal{H}$.*
Then the closure of the quadratic form $(\mathcal{E}, \mathcal{F})$ given by

$$\mathcal{E} : L^2(A,\tau) \to [0,\infty) \qquad \mathcal{E}[a] = \|\partial a\|^2_{\mathcal{H}}\,, \quad a \in \mathcal{F} := D(\partial) \tag{4.2}$$

is a C^*-Dirichlet form. The generator Δ of the completely Markovian semigroup $T_t = e^{-t\Delta}$ associated to $\mathcal{E}$, can be represented as the composition of the "divergence" ∂^* of the "gradient" ∂:

$$\Delta = \partial^* \circ \partial\,.$$

In other words, the derivation ∂ appears as a differential square root of Δ.

To establish the Markovianity of $\mathcal{E}$ we are going to prove a *chain rule formula for derivations* which generalizes the familiar one we have seen in Example 4.3.

For any self-adjoint element a of A, we shall denote by L_a (resp. R_a) the unique representation of $\mathrm{C}(sp(a))$, the C^*-algebra of continuous, complex valued functions on $sp(a)$ (the spectrum of a), such that

$$L_a(f)\xi = \begin{cases} f(a)\xi \text{ if } f(0) = 0 \\ \xi \text{ if } f \equiv 1 \end{cases} \qquad f \in C(sp(a)) \quad \xi \in \mathcal{H}$$

and

$$R_a(f)\xi = \begin{cases} \xi f(a) \text{ if } f(0)=0 \\ \xi \text{ if } f \equiv 1 \end{cases} \qquad f \in C(sp(a)) \quad \xi \in \mathcal{H}\,.$$

$L_a \otimes R_a$ will be the tensor product representation of $C(sp(a)) \otimes C(sp(a)) = C(sp(a) \times sp(a))$. When $I \subseteq \mathbb{R}$ is a closed interval and $f \in \mathrm{C}^1(I)$, we will denote by $\tilde{f} \in \mathrm{C}(I \times I)$ the *difference quotient* on $I \times I$, sometimes called the *quantum derivative* of f, defined by

$$\tilde{f}(s,t) = \begin{cases} \frac{f(s)-f(t)}{s-t} & \text{if } \; s \neq t \\ f'(s) & \text{if } \; s = t. \end{cases} \tag{4.3}$$

Next lemma shows that the domain of a closed derivation with values in a Hilbertian bimodule is closed under C^1-functional calculus. The case of the standard bimodule $L^2(A,\tau)$ was considered in [GIS], while the case of a C^*-bimodule was analyzed in [S3].

Lemma 4.6. *(Functional calculus in the domain of a derivation) Let $(\mathcal{H}\,,\mathcal{J})$ be a symmetric Hilbert A–bimodule, $(\partial, D(\partial))$ be a symmetric derivation defined on an involutive subalgebra of A into $\mathcal{H}$, and let $a = a^* \in A$. Then*

i) for any polynomial f on $\mathbb{R}$, $f(a)$ belongs to $D(\partial)$, the following chain-rule holds true

$$\partial(f(a)) = (L_a \otimes R_a)(\tilde{f})\,\partial(a)\,, \tag{4.4}$$

and we have the bound

$$\|\partial(f(a))\| \leq \|f'\|_{C(sp(a))}\|\partial(a)\| \qquad a \in D(\partial)\,; \tag{4.5}$$

ii) if $(\partial, D(\partial))$ is closable as operator from A to $\mathcal{H}$, then its closure is a derivation;

iii) if $(\partial, D(\partial))$ is a closed derivation from A to $\mathcal{H}$, the above chain-rule holds true for all $f \in C^1(sp(a))$ such that $f(0)=0$. In particular the domain of a closed derivation is closed under C^1-functional calculus.

Proof. i) When f is a polynomial it is easy to verify (4.4) by direct inspection and then derive (4.5). Statement ii) follows directly from the Leibniz rule and the continuity of the left and right actions. To prove the statement in iii), we may approximate the derivative f' of a function $f \in \mathrm{C}^1(sp(a))$ vanishing at the origin, by polynomials f'_n, uniformly on $sp(a)$, and then approximate uniformly f by the primitive polynomials f_n vanishing at the origin. Applying (4.5) we have that $\partial f_n(a)$ is a Cauchy-sequence in $\mathcal{H}$ so that, since the derivation has been assumed to be closed, $\partial f(a)$ belongs to that domain and (4.4) holds true for all f in $C^1(sp(a))$.

Proof. of Theorem 4.5. Let us denote by $(\overline{\mathcal{E}}, \overline{\mathcal{F}})$ the closure in $L^2(A,\tau)$ of the form $(\mathcal{E}, \mathcal{F})$ defined in the statement of the theorem. First notice that the form is J-real due to the fact the derivation is symmetric. Following the same reasoning as the one used in the proof of Lemma 4.6 iii), we start by proving the bound

$$\overline{\mathcal{E}}[f(a)] \leq \|f'\|^2_{C(sp(a))}\overline{\mathcal{E}}[a] \qquad a \in \mathcal{F} \tag{4.6}$$

for all $f \in C^1(sp(a))$ such that $f(0) = 0$. Let us fix an element $a \in \mathcal{F}$ and denote I the spectrum $sp(a)$. Consider the same polynomial approximation f_n (vanishing at the origin) of the function f. Since f_n and f'_n are uniformly convergent to f and f', respectively, they are uniformly bounded sequence in $C(I)$. An application of the bound (4.5) and the estimate

$$\|f_n(a)\|_2^2 = \tau(|f_n(a)|^2) \leq \|f_n\|^2_{C(I)}\tau(|a|^2) = \|f_n\|^2_{C(I))}\|a\|_2^2\,,$$

tell us that $(f_n(a), \partial f_n(a))$ is bounded sequence with respect to the graph norm of the operator $(\partial, D(\partial))$. Hence, possibly considering a suitable subsequence, it is weakly convergent to some $(b, \xi) \in \overline{\mathcal{F}} \times \mathcal{H}$. Since $f_n(a)$ is also converging in the norm of A to $f(a)$, we have the identification $b = f(a)$ and

$$\overline{\mathcal{E}}[f(a)] = \lim_{n\to\infty} \mathcal{E}[f_n(a)] \leq \lim_{n\to\infty} \|f'_n\|^2_{C(I)}\mathcal{E}[a] = \|f'\|^2_{C(I))}\mathcal{E}[a]\,.$$

In particular $f(a) \in \overline{\mathcal{F}}$ for all $a \in \mathcal{F} = D(\partial)$ and $f \in C^1(sp(a))$ such that $f(0) = 0$. We will denote $\mathrm{Lip}_0(\mathbb{R})$ the algebra of all real Lipschitz functions f on the real line, vanishing at the origin, normed by the infimum $\|f\|_{\mathrm{Lip}_0(\mathbb{R})}$ of all numbers λ such that $|f(s) - f(t)| \leq \lambda|s - t|$, $s, t \in \mathbb{R}$. Approximating locally uniformly the elements of $\mathrm{Lip}_0(\mathbb{R})$ by functions in $C(\mathbb{R})$ vanishing at the origin, we obtain from (4.6) the estimate

$$\overline{\mathcal{E}}[f(a)] \leq \|f\|^2_{\mathrm{Lip}_0(sp(a))}\overline{\mathcal{E}}[a] \qquad a \in \mathcal{F} \quad f \in \mathrm{Lip}_0(sp(a))\,. \tag{4.7}$$

Since $\mathcal{F}$ is a form core for $(\overline{\mathcal{E}}, \overline{\mathcal{F}})$, the estimate (3.7) holds true for all $a \in \overline{\mathcal{F}}$. We get the Markovianity of $(\overline{\mathcal{E}}, \overline{\mathcal{F}})$ just choosing as Lipschitz function $f(t) = t \wedge 1$. Complete Markovianity follows just applying the result to the extension of the derivation to matrix algebras over A.

4.3 Modules and Derivations Associated to Regular Dirichlet Forms

In this section we are going to show how Dirichlet spaces, commutative or not, give rise to a differentiable structure on a C*-algebra. More precisely, we construct an essentially unique, closable derivation on a C*-algebra, representing the Dirichlet form as in Theorem 4.5.

Keeping in mind the model case of the Dirichlet integral on Euclidean spaces or Riemannian manifolds, what we are going to do is to reconstruct the gradient operator and the Hilbert space of square summable vector fields from the energy functional.

The fundamental hint for the search of a differential calculus associated to a Dirichlet form is the following observation made in [DL1]. The original proof, based on the Kadison-Schwartz inequality, works for quadratic forms associated to $1\frac{1}{2}$-Markovian semigroups. It is more general than the one we offer here, which is directly based on the fundamental properties of the Dirichlet form, but requires 2-Markovianity.

Proposition 4.7. *Let $(\mathcal{E}, D(\mathcal{E}))$ be a completely Dirichlet form on $L^2(A,\tau)$. Then $\mathcal{B} := A \cap D(\mathcal{E})$ is an involutive subalgebra of $\mathfrak{M}$, called the Dirichlet algebra of $(\mathcal{E}, D(\mathcal{E}))$. In case $(\mathcal{E}, D(\mathcal{E}))$ is a* C**–Dirichlet form, $\mathcal{B}$ is a dense, involutive sub–algebra of A and a form core for $(\mathcal{E}, D(\mathcal{E}))$.*

Proof. Let $a = a^* \in \mathcal{B}$ be such that $\|a\| = 1$ so that

$$\frac{a^2}{2} = a - \int_0^1 dt\, a \wedge t\,.$$

By convexity, lower semicontinuity and Markovianity of $\mathcal{E}$, we have

$$\mathcal{E}\Big[\int_0^1 dt\, a \wedge t\Big] \le \int_0^1 dt\, \mathcal{E}[a \wedge t] \le \mathcal{E}[a]$$

so that $a^2 \in \mathcal{B}$. By scaling the conclusion remains true for all self-adjoint $a \in \mathcal{B}$. This implies that, if $b = b^*$ and $c = c^*$ are self-adjoint elements in $\mathcal{B}$,

$$bc + cb = (b+c)^2 - b^2 - c^2 \in \mathcal{B}\,.$$

In turn, since $b + c$ and $b - c$ are self-adjoint, we have

$$b^2 - c^2 = \frac{(b+c)(b-c) + (b-c)(b+c)}{2} \in \mathcal{B}\,,$$

so that

$$(b + ic)^2 = (b^2 - c^2) + i(bc + cb) \in \mathcal{B}\,.$$

Decomposing a generic element $a \in \mathcal{B}$ as

$$a = \frac{a + a^*}{2} + i\frac{a - a^*}{2i}\,,$$

we conclude that $a^2 \in \mathcal{B}$. If a, b are generic elements in $\mathcal{B}$, considering the matrix

$$\begin{bmatrix} 0 & a \\ b & 0 \end{bmatrix} \in M_2(\mathcal{B})\,,$$

and applying the above result to the extension $\mathcal{E}_2$ of $\mathcal{E}$ on $M_2(A)$, we obtain

$$\begin{bmatrix} ab & 0 \\ 0 & ba \end{bmatrix} = \begin{bmatrix} 0 & a \\ b & 0 \end{bmatrix}^2 \in M_2(\mathcal{B})$$

so that $ab \in \mathcal{B}$.

Next step will be the construction of a Hilbert space on which the algebra A will act, naturally associated to the Dirichlet form.

Proposition 4.8. *The sesquilinear form on the algebraic tensor product* $\mathcal{B} \otimes \mathcal{B}$*, linear in the right-hand side and conjugate linear in the left-hand one, which, to* $c \otimes d$ *and* $a \otimes b$*, associates*

$$\frac{1}{2}\big(\mathcal{E}(c, abd^*) + \mathcal{E}(cdb^*, a) - \mathcal{E}(db^*, c^*a)\big)\,, \tag{4.8}$$

is positive definite and defines a pre-Hilbert structure on $\mathcal{B} \otimes \mathcal{B}$*.*

Proof. By the complete Markovianity of the semigroup $T_t = e^{-t\Delta}$ associated to $\mathcal{E}$ the resolvent maps

$$(I + \varepsilon\Delta)^{-1} = \frac{I}{I + \varepsilon\Delta} = \int_0^\infty e^{-t}\, T_{\varepsilon t}\, dt \qquad \varepsilon > 0,$$

are bounded, completely positive, self-adjoint contractions on $L^2(A, \tau)$ and bounded, completely positive, normal contractions on $\mathfrak{M}$; by the Stinespring construction ([Sti]), there exists, for a fixed $\varepsilon > 0$, a Hilbert space K_ε, a normal representation π_ε of $\mathfrak{M}$ into $\mathcal{B}(K_\varepsilon)$ and a linear operator W_ε from $L^2(A, \tau)$ into K_ε, with norm less than one, such that

$$\frac{I}{I + \varepsilon\Delta}(a) = W_\varepsilon^* \pi_\varepsilon(a) W_\varepsilon$$

for any a in $\mathfrak{M}$. It is then easy to check, for $a, b, c, d \in \mathfrak{M}$, the identity

$$\begin{aligned} &d^* \frac{\Delta}{I + \varepsilon\Delta}(c)^* ab + d^* c^* \frac{\Delta}{I + \varepsilon\Delta}(a) b - d^* \frac{\Delta}{I + \varepsilon\Delta}(c^* a) b = \\ &\frac{1}{\varepsilon}\, d^* \big(W_\varepsilon c - \pi_\varepsilon(c) W_\varepsilon\big)^* \big(W_\varepsilon a - \pi_\varepsilon(a) W_\varepsilon\big) b + \frac{1}{\varepsilon}\, d^* c^* (I - W_\varepsilon^* W_\varepsilon) ab\,. \end{aligned} \tag{4.9}$$

This implies the positivity of the matrix

$$\Big[\frac{\Delta}{I + \varepsilon\Delta}(a_j)^* a_i + a_j^* \frac{\Delta}{I + \varepsilon\Delta}(a_i) - \frac{\Delta}{I + \varepsilon\Delta}(a_j^* a_i)\Big]_{i,j=1\ldots n} \tag{4.10}$$

in $M_n(A)$, for any n in $\mathbb{N}^*$, $a_1, \ldots, a_n$ in $\mathcal{B}$ and, since the expression in (4.8) is the limit of the one in (4.9), the positivity of the sesquilinear form.

Definition 4.9. (Hilbert space structure) The symbol $\mathcal{H}_0$ will denote the Hilbert space obtained from $\mathcal{B} \otimes \mathcal{B}$ after separation and completion with respect to the seminorm provided by the positive sesquilinear form of Proposition 4.9. The scalar product in $\mathcal{H}_0$ will be denoted by $(\cdot|\cdot)_{\mathcal{H}_0}$ (or $(\cdot|\cdot)$ if no confusion can arise). We will denote by $a \otimes_{\mathcal{E}} b$ the canonical image in $\mathcal{H}_0$ of the elementary tensor $a \otimes b$ of $\mathcal{B} \otimes \mathcal{B}$. The Hilbert space structure is then uniquely identified by the following expression

$$\big(c\otimes_{\mathcal{E}} d\,|\,a\otimes_{\mathcal{E}} b\big)_{\mathcal{H}_0}=\frac{1}{2}\big(\mathcal{E}(c,abd^*)+\mathcal{E}(cdb^*,a)-\mathcal{E}(db^*,c^*a)\big) \qquad (4.11)$$

on any pair of elementary vectors $a\otimes_{\mathcal{E}} b, c\otimes_{\mathcal{E}} d\in\mathcal{H}_0$. In particular, we have

$$||a\otimes_{\mathcal{E}} b||^2_{\mathcal{H}_0}=\frac{1}{2}\big(\mathcal{E}(a,abb^*)+\mathcal{E}(abb^*,a)-\mathcal{E}(bb^*,a^*a)\big) \quad a,b\in\mathcal{B}. \qquad (4.12)$$

The following result guarantees that there exists on $\mathcal{H}_0$, a natural structure of right module over A.

Proposition 4.10. *(Right A-module structure) There exists a structure of right A-module on $\mathcal{H}_0$, i.e. a representation of the opposite* C**–algebra of A into $\mathcal{B}(\mathcal{H}_0)$, characterized by*

$$\Big(\sum_{i=1}^n a_i\otimes_{\mathcal{E}} b_i\Big)b=\sum_{i=1}^n a_i\otimes_{\mathcal{E}} b_ib \quad, \forall n\in\mathbb{N}^*,\ a_1,\dots,a_n,b_1,\dots,b_n\in\mathcal{B},\ b\in\mathcal{B}\,. \qquad (4.13)$$

Proof. The positivity of the matrix in (4.10) provides the positivity of the operator

$$\sum_{i,j=1}^n b_j^*\Big(\frac{\Delta}{I+\varepsilon\Delta}(a_j)^*a_i+a_j^*\frac{\Delta}{I+\varepsilon\Delta}(a_i)-\frac{\Delta}{I+\varepsilon\Delta}(a_j^*a_i)\Big)b_i$$

from which we get the inequality

$$\begin{aligned}
&\|\sum_{i=1}^n a_i\otimes_{\mathcal{E}} b_ib\|^2_{\mathcal{H}_0}\\
&=\frac{1}{2}\lim_{\varepsilon\downarrow 0}\tau\Big(b^*\Big(\sum_{i,j=1}^n b_j^*(\frac{\Delta}{I+\varepsilon\Delta}(a_j)^*a_i+a_j^*\frac{\Delta}{I+\varepsilon\Delta}(a_i)-\frac{\Delta}{I+\varepsilon\Delta}(a_j^*a_i))b_i\Big)b\Big)\\
&\le\frac{1}{2}\|b\|^2\lim_{\varepsilon\downarrow 0}\tau\Big(\sum_{i,j=1}^n b_j^*\Big(\frac{\Delta}{I+\varepsilon\Delta}(a_j)^*a_i+a_j^*\frac{\Delta}{I+\varepsilon\Delta}(a_i)-\frac{\Delta}{I+\varepsilon\Delta}(a_j^*a_i)\Big)b_i\Big)\\
&=\|b\|^2\|\sum_{i=1}^n a_i\otimes_{\mathcal{E}} b_i\|^2_{\mathcal{H}_0}\,.
\end{aligned}$$

By continuity we can then extend the right multiplication by any $b\in A$ to the whole $\mathcal{H}_0$. One easily checks, on the linear span of the elementary vectors, that this operation intertwines the algebraic structures of A and $B(\mathcal{H}_0)$ and their involutions:

$$(c\otimes_{\mathcal{E}} d|\ a\otimes_{\mathcal{E}} be)_{\mathcal{H}_0}=(c\otimes_{\mathcal{E}} de^*|\ a\otimes_{\mathcal{E}} b)_{\mathcal{H}_0} \quad a,b,c,d,e\in\mathcal{B}.$$

A natural left A–module structure of $\mathcal{H}_0$, i.e. a representation of A into $B(\mathcal{H}_0)$, is constructed with the help of the following lemma.

Lemma 4.11. *For any n in $\mathbb{N}^*$, any $a, a_1, \ldots, a_n, b_1, \ldots, b_n$ in $\mathcal{B}$, one has*

$$\|\sum_{i=1}^n aa_i \otimes_{\mathcal{E}} b_i - a \otimes_{\mathcal{E}} \sum_{i=1}^n a_i b_i\|_{\mathcal{H}_0} \leq \|a\| \cdot \|\sum_{i=1}^n a_i \otimes_{\mathcal{E}} b_i\|_{\mathcal{H}_0} . \tag{4.14}$$

Proof. For a fixed $\varepsilon > 0$ let $(\pi_\varepsilon, K_\varepsilon)$ and W_ε be the representation of $\mathfrak{M}$ and the operator from $L^2(A, \tau)$ to K_ε, respectively, considered in the proof of Proposition 4.8. Recall in particular that $\frac{I}{I+\varepsilon\Delta}(a) = W_\varepsilon^* \pi_\varepsilon(a) W_\varepsilon$ for any a in $\mathfrak{M}$. Using these operators one easily checks that

$$\begin{aligned}
&\sum_{i,j=1}^n b_j^* \Big(\frac{\Delta}{I+\varepsilon\Delta}(aa_j)^* aa_i + (aa_j)^* \frac{\Delta}{I+\varepsilon\Delta}(aa_i) - \frac{\Delta}{I+\varepsilon\Delta}(a_j^* a^* aa_i)\Big) b_i \\
&\qquad - \sum_{i,j=1}^n b_j^* a_j^* \Big(\frac{\Delta}{I+\varepsilon\Delta}(a)^* a + a^* \frac{\Delta}{I+\varepsilon\Delta}(a) - \frac{\Delta}{I+\varepsilon\Delta}(a^* a)\Big) a_i b_i \\
&\qquad = \sum_{i,j=1}^n b_j^* (W_\varepsilon a_j - \pi_\varepsilon(a_j) W_\varepsilon)^* a^* a (W_\varepsilon a_i - \pi_\varepsilon(a_i) W_\varepsilon) b_i \\
&\qquad \leq \|a\|^2 \sum_{i,j=1}^n b_j^* (W_\varepsilon a_j - \pi_\varepsilon(a_j) W_\varepsilon)^* (W_\varepsilon a_i - \pi_\varepsilon(a_i) W_\varepsilon) b_i \,,
\end{aligned}$$

which implies

$$\begin{aligned}
&\|\sum_{i=1}^n aa_i \otimes_{\mathcal{E}} b_i - a \otimes_{\mathcal{E}} \sum_i a_i b_i\|^2 \\
&= \lim_{\varepsilon \downarrow 0} \frac{1}{2} \tau \Big[\sum_{i,j=1}^n b_j^* (\frac{\Delta}{I+\varepsilon\Delta}(aa_j)^* aa_i + (aa_j)^* \frac{\Delta}{I+\varepsilon\Delta}(aa_i) - \frac{\Delta}{I+\varepsilon\Delta}(a_j^* a^* aa_i)) b_i \\
&\qquad - \sum_{i,j=1}^n b_j^* a_j^* (\frac{\Delta}{I+\varepsilon\Delta}(a)^* a + a^* \frac{\Delta}{I+\varepsilon\Delta}(a) - \frac{\Delta}{I+\varepsilon\Delta}(a^* a)) a_i b_i\Big] \\
&\leq \|a\|^2 \cdot \liminf_{\varepsilon \downarrow 0} \frac{1}{2\varepsilon} \tau \Big[\sum_{i,j=1}^n b_j^* (W_\varepsilon a_j - \pi_\varepsilon(a_j) W_\varepsilon)^* (W_\varepsilon a_i - \pi_\varepsilon(a_i) W_\varepsilon) b_i\Big] \\
&\leq \|a\|^2 \cdot \|\sum_{i=1}^n a_i \otimes_{\mathcal{E}} b_i\|^2
\end{aligned}$$

(the last inequality following from identity (4.9)).

Proposition 4.12. *(Left A-module structure) There exists a structure of left A-module on $\mathcal{H}_0$, i.e. a representation of the* C**–algebra A into $\mathcal{B}(\mathcal{H}_0)$, characterized by*

$$a(b \otimes_{\mathcal{E}} c) = ab \otimes_{\mathcal{E}} c - a \otimes_{\mathcal{E}} bc, \quad a, b, c \in \mathcal{B} . \tag{4.15}$$

Proof. By the previous lemma, any $a \in \mathcal{B}$ defines a bounded operator in $B(\mathcal{H}_0)$ whose action $a(b \otimes_{\mathcal{E}} c)$ on $b \otimes_{\mathcal{E}} c$ is given by $ab \otimes_{\mathcal{E}} c - a \otimes_{\mathcal{E}} bc$, so that (4.15) holds true. Extending, by continuity, these maps to the whole A, it is easy to check that this yields a morphism of algebras from A into $B(\mathcal{H}_0)$. To show that it respects involutions, one has to check that

$$(e(a \otimes_{\mathcal{E}} b) \,|c \otimes_{\mathcal{E}} d)_{\mathcal{H}_0} = (a \otimes_{\mathcal{E}} b \,|e^*(c \otimes_{\mathcal{E}} d))_{\mathcal{H}_0} \tag{4.16}$$

for all a, b, c, d, e in $\mathcal{B}$.

We are now in the position to state the main result of this section. Recall that an A–bimodule is a Hilbert space $\mathcal{H}_0$ with a left representation and a right representation of A which commute (or, equivalently, a representation of the C*–algebra $A \otimes_{\max} A^\circ$).

Theorem 4.13. *(A-bimodule structure) Let $(\mathcal{E}, D(\mathcal{E}))$ be a* C**–Dirichlet form on $L^2(A, \tau)$. There exists a canonical A–bimodule structure on the Hilbert space $\mathcal{H}_0$, characterized by*

$$a(b \otimes_{\mathcal{E}} c) = ab \otimes_{\mathcal{E}} c - a \otimes_{\mathcal{E}} bc \tag{4.17}$$

$$(b \otimes_{\mathcal{E}} c)a = b \otimes_{\mathcal{E}} ca \tag{4.18}$$

for all a, b and c belonging to the Dirichlet algebra $\mathcal{B}$.

Proof. We have only to prove that the right and left actions constructed before commute. By continuity, it is enough to show that they commute on the elementary tensors. In fact we have:

$$\begin{aligned}(a_1(b \otimes_{\mathcal{E}} c))a_2 &= (a_1 b \otimes_{\mathcal{E}} c - a_1 \otimes_{\mathcal{E}} bc)a_2 \\ &= a_1 b \otimes_{\mathcal{E}} ca_2 - a_1 \otimes_{\mathcal{E}} bca_2 \\ &= a_1(b \otimes_{\mathcal{E}} ca_2) \\ &= a_1((b \otimes_{\mathcal{E}} c)a_2)\end{aligned}$$

for all $a_1, a_2, b, c \in \mathcal{B}$.

Once the canonical A–bimodule $\mathcal{H}_0$ associated to the C*–Dirichlet form $(\mathcal{E}, D(\mathcal{E}))$ is available, we lead our efforts to the construction of the derivation on the Dirichlet algebra $\mathcal{B}$.

Lemma 4.14. *For $a \in \mathcal{B}$, the map l_a, defined on the linear span of the set of elementary tensor products of elements of $\mathcal{B}$ by*

$$l_a(b \otimes_{\mathcal{E}} c) := \frac{1}{2}\Big(\mathcal{E}(a, bc) + \mathcal{E}(b^*, ca^*) - \mathcal{E}(b^* a, c)\Big) \quad b, c \in \mathcal{B}, \tag{4.19}$$

extends to a continuous linear form on $\mathcal{H}_0$, with norm not greater than $\mathcal{E}[a]^{\frac{1}{2}}$.

Proof. Fix n in $\mathbb{N}^*$, a, $b_1,\dots,b_n,c_1,\dots,c_n$ in $\mathcal{B}$ and consider the representation $\frac{I}{I+\varepsilon\Delta}(a) = W_\varepsilon^*\pi_\varepsilon(a)W_\varepsilon$ used in the proof of Proposition 4.8. We then have

$$l_a\Big(\sum_{i=1}^n b_i\otimes_{\mathcal{E}} c_i\Big) = \lim_{\varepsilon\downarrow 0}\frac{1}{2\varepsilon}\tau\Big[(W_\varepsilon a - \pi_e(a)W_\varepsilon)^*\Big(\sum_{i=1}^n (W_\varepsilon b_i - \pi_\varepsilon(b_i)W_\varepsilon)c_i\Big) + \\ + a^*(I - W_\varepsilon^* W_\varepsilon)\Big(\sum_{i=1}^n b_i c_i\Big)\Big].$$

Let us apply the Cauchy-Schwarz inequality

$$|\tau(\alpha_\varepsilon^*\beta_\varepsilon + \gamma_\varepsilon^*\delta_\varepsilon)| \le \tau(\alpha_\varepsilon^*\alpha_\varepsilon + \gamma_\varepsilon^*\gamma_\varepsilon)^{1/2}\tau(\beta_\varepsilon^*\beta_\varepsilon + \delta_\varepsilon^*\delta_\varepsilon)^{1/2}$$

to $\alpha_\varepsilon = W_\varepsilon a - \pi_\varepsilon(a)W_\varepsilon$, $\beta_\varepsilon = \sum_i (W_\varepsilon b_i - \pi_\varepsilon(b_i)W_\varepsilon)c_i$, $\gamma_\varepsilon = (I - W_\varepsilon^*W_\varepsilon)^{1/2}a$ and $\delta_\varepsilon = (I - W_\varepsilon^*W_\varepsilon)^{1/2}\sum_i b_i c_i$. We have, as in the proof of Proposition 4.8

$$\overline{\lim}_{\varepsilon\downarrow 0}\frac{1}{2\varepsilon}\tau(\alpha_\varepsilon^*\alpha_\varepsilon + \gamma_\varepsilon^*\gamma_\varepsilon) = \\ \overline{\lim}_{\varepsilon\downarrow 0}\frac{1}{2}\tau\Big(\frac{\Delta}{I+\varepsilon\Delta}(a^*)a + a^*\frac{\Delta}{I+\varepsilon\Delta}(a) - \frac{\Delta}{I+\varepsilon\Delta}(a^*a)\Big) \le \mathcal{E}(a,a)$$

and

$$\lim_{\varepsilon\downarrow 0}\frac{1}{2\varepsilon}\tau(\beta_\varepsilon^*\beta_\varepsilon + \delta_\varepsilon^*\delta_\varepsilon) = ||\sum_{i=1}^n b_i\otimes_{\mathcal{E}} c_i||_{\mathcal{H}_0}\ .$$

Hence we proved that $\Big|l_a\Big(\sum_{i=1}^n b_i\otimes_{\mathcal{E}} c_i\Big)\Big| \le \sqrt{\mathcal{E}[a]}\cdot\|\sum_{i=1}^n b_i\otimes_{\mathcal{E}} c_i\|_{\mathcal{H}_0}$, from which, by continuity, the statement follows.

Notice that, since $\mathcal{B}$ is a form core, l_a can be uniquely defined for any $a\in D(\mathcal{E})$. The above result allows us to consider a map, which will be subsequently verified to be a derivation, providing a first (possibly left-degenerate) representation of Dirichlet forms.

Definition 4.15. We will denote by $\partial_0 : \mathcal{B}\to\mathcal{H}_0$ the following linear map: for any $a\in\mathcal{B}$ let $\partial_0(a)$ be the vector in $\mathcal{H}_0$ associated, by the Riesz representation theorem, to the continuous linear functional l_a provided by the previous lemma. More explicitly, this map is characterized by

$$(\partial_0(a)|b\otimes_{\mathcal{E}} c)_{\mathcal{H}_0} = l_a(b\otimes_{\mathcal{E}} c) \\ = \frac{1}{2}\Big(\mathcal{E}(a,bc) + \mathcal{E}(b^*,ca^*) - \mathcal{E}(b^*a,c)\Big) \quad b,c\in\mathcal{B}. \tag{4.20}$$

Notice that $||\partial_0(a)||^2_{\mathcal{H}_0} \le \mathcal{E}[a]$ for all a in $\mathcal{B}$ and then, since $\mathcal{B}$ is a form core for $\mathcal{E}$, ∂_0 can be extended to the whole form domain $D(\mathcal{E})$.

Proposition 4.16. *(Possibly left-degenerate representation of* C**–Dirichlet forms) Let* $(\mathcal{E}, D(\mathcal{E}))$ *be a* C**–Dirichlet form. Then we have:*

i) $\partial_0 : \mathcal{B} \to \mathcal{H}_0$ *is a* A*–bimodule derivation;*

ii) for any a *in* $\mathcal{B}$ *and* b *in* A *one has*

$$\partial_0(a)b = a \otimes_{\mathcal{E}} b\,; \tag{4.21}$$

iii) the right representation of A *is non degenerate:* $\mathcal{H}_0 A$ *is dense in* $\mathcal{H}_0$*;*

iv) for any a *in* $\mathcal{B}$*, one has*

$$\mathcal{E}(a,a) - \|\partial_0(a)\|^2_{\mathcal{H}_0} = \lim_{\varepsilon \downarrow 0} \frac{1}{2}\tau\Big(\frac{\Delta}{I+\varepsilon\Delta}(a^* a)\Big)\,. \tag{4.22}$$

By the definition of ∂_0 and Theorem 4.13, it is easy to check the identities

$$(\partial_0(a_1 a_2) - a_1\partial_0(a_2) + \partial_0(a_1)a_2 | c \otimes_{\mathcal{E}} d)_{\mathcal{H}_0} = 0$$

and

$$(\partial_0(a)|c \otimes db^*)_{\mathcal{H}_0} = (a \otimes_{\mathcal{E}} b | c \otimes_{\mathcal{E}} d)_{\mathcal{H}_0}\,,$$

for all a_1, a_2, a, b, c, d in $\mathcal{B}$. From these identities the statements i) and ii) follow by continuity. The main point in statement iii) is to prove the existence of the limit. We omit the long proof and refer to [CS1 Proposition 4.4 iii)].

Corollary 4.17. *(Representation of Dirichlet forms generating conservative semigroups) Let* $(\mathcal{E}, D(\mathcal{E}))$ *be a* C*–*Dirichlet form corresponding to a conservative Markovian semigroup:*

$$T_t(1_{\mathfrak{M}}) = 1_{\mathfrak{M}} \qquad t \geq 0\,.$$

Then we have

$$\mathcal{E}[a] = \|\partial_0(a)\|^2_{\mathcal{H}_0} \qquad a \in D(\mathcal{E})\,.$$

To remedy the possible degeneracy of the left A-module structure of $\mathcal{H}_0$, and the asymmetric aspect of the right hand side of (4.22), we have to analyze further the structure of the A-bimodule $\mathcal{H}_0$. The result is that a suitable weight on A will take care of the possible degeneracy of the left action.

Theorem 4.18. *(Non degenerate representation of* C*–*Dirichlet forms) Let* $(\mathcal{E}, D(\mathcal{E}))$ *be a* C*–*Dirichlet form. Then there exists a symmetric derivation* $(\partial_1, \mathcal{H}_1)$ *in a nondegenerate* A*-bimodule and a weight* K *on* A *such that the following representation holds true*

$$\mathcal{E}(\xi,\xi) = \|\partial_1(\xi)\|^2_{\mathcal{H}_1} + \frac{1}{2}K(\xi^*\xi + \xi\xi^*) \qquad \xi \in D(\mathcal{E})\,. \tag{4.23}$$

In the conservative case $K = 0$ *and* $(\partial_0, \mathcal{H}_0) = (\partial_1, \mathcal{H}_1)$

We omit the long proof of the result and refer the interested reader to [CS1 Theorem 8.1]. It is also possible to show [CS1 Theorem 8.2], that even the quadratic form on the right hand side of (4.23), depending on the weight K, may be described in terms of a derivation. The A-bimodule corresponding to K is completely degenerate.

Under the stronger hypothesis that the domain of the generator Δ contains a subalgebra dense in A, the last result has been obtained in [S2,3]. In that case the tangent bimodule supports a richer structure of a *C*-bimodule* (see [Co2] for the definition). The simplest example of such a situation is the one of the Dirichlet integral of a Riemannian manifold M. There one has not only the Hilbert bimodule structure of square integrable vector fields $L^2(TM)$ but also the C*-bimodule $C_0(TM)$ of continuous vector fields vanishing at infinity.

The fact that Dirichlet forms may be represented in terms of modules over C*-algebras, allows to study them along the various decomposition theories of representations of C*-algebras (see [Dix1]). To illustrate this point of view, we re-consider a famous formula due to A. Beurling-J. Deny [BD2] and Y. Le Jan [LJ] concerning the decomposition of Dirichlet forms on locally compact spaces.

Example 4.19. **Dirichlet forms on commutative C*–algebras: Beurling–Deny–Le Jan decomposition revisited I.** Let X be a locally compact, metric space and m a positive Radon measure on X with full topological support. The Beurling–Deny–Le Jan decomposition (see also [FOT]) of a regular Dirichlet form $(\mathcal{E}, D(\mathcal{E}))$ on $L^2(X,m)$, represents $\mathcal{E}$ as a sum

$$\mathcal{E} = \mathcal{E}^{(c)} + \mathcal{E}^{(j)} + \mathcal{E}^{(k)}$$

of Markovian forms, on the Dirichlet algebra $\mathcal{B}$, called the *diffusive*, *jumping* and *killing* parts, respectively.

This decomposition may be obtained in a algebraic way from the representation of a Dirichlet form in terms of bimodules valued derivation, noticing that a bimodule $\mathcal{H}$ on $C_0(X)$ is just a representation of the algebra $C_0(X \times X)$.

- The killing part has the form

$$\mathcal{E}^{(k)}(a,a) = \int_X |a|^2 dk$$

  for a positive Radon measure k on X. It corresponds to the degenerate part of the $C_0(X)$-bimodule associated with $\mathcal{E}$ by our construction.
- The jumping part has the form

$$\mathcal{E}^{(j)}(a,a) = \int_{X\times X - d} |a(x) - a(y)|^2 J(dx,dy)$$

  for some symmetric, positive Radon measure J supported off the diagonal d_X of $X \times X$. It obviously appears as the form $a \mapsto ||\partial_j(a)||^2$, where ∂_j is the universal derivation

$$\partial_j(a) = a \otimes 1 - 1 \otimes a$$

with values in the $C_0(X)$-bimodule $L^2(X \times X \setminus d_X, J)$. Here left action of $a \in C_0(X)$ on $f \in L^2(X \times X \setminus d_X, J)$ is given by

$$(a \cdot f)(x,y) = a(x)f(x,y) \qquad J\text{−a.e.} \qquad (x,y) \in X \times X \setminus d_X\,,$$

while the right action is given by

$$(f \cdot a)(x,y) = f(x,y)a(y) \qquad J\text{−a.e.} \qquad (x,y) \in X \times X \setminus d_X\,.$$

- The diffusive part is characterized by its strong local property:

$$\mathcal{E}^{(c)}[a+b] = \mathcal{E}^{(c)}[a] + \mathcal{E}^{(c)}[b]$$

whenever $a, b \in \mathcal{B}$ and a is constant in a neighborhood of the support of b. By our analysis this part has the form $a \mapsto ||\partial_c(a)||^2_{\mathcal{H}_c}$ for a derivation ∂_c with values in a $C_0(X)$–monomodule $\mathcal{H}_c$ (where left and right actions coincide). This is precisely the part of the $C_0(X)$-bimodule associated with $\mathcal{E}$ by our construction, supported on the diagonal d_X of $X \times X$. As the representation theory of $C_0(X)$ is nothing but measure theory on X, this means that the derivation ∂_c may be decomposed accordingly. The Hilbert module $\mathcal{H}_c$ may be represented as a *Hilbert integral* $\mathcal{H}_c = \int_X^{\oplus} H_x \mu(dx)$ of Hilbert modules $\{H_x : x \in X\}$, μ being a suitable Borel measure on X, where the $C_0(X)$-module structure of $\mathcal{H}_x$, for each fixed $x \in X$, is given by

$$(a \cdot \xi) = a(x)\xi \qquad a \in C_0(X)\,, \quad \xi \in \mathcal{H}_x\,.$$

The derivation ∂_c then decomposes as a direct integral $\partial_c = \int_X^{\oplus} \partial_c^x \mu(dx)$ of derivations $\{\partial_c^x : x \in X\}$ and the corresponding Leibniz rule appears as follows

$$\partial_c^x(ab)(x) = a(x)\partial_c^x(b)(x) + b(x)\partial_c^x(a)(x) \quad \mu\text{−a.s.} \quad x \in X\,.$$

It may be proved that the class of the $C_0(X)$-module $\mathcal{H}_c$ corresponds to the class of the measure μ and both are identified by the $\mathcal{E}$-polar subsets of X.

This illustrates how in the commutative situation the analysis we developed so far, not only gives back the classical Beurling–Deny–Le Jan decomposition, but also provides an algebraic interpretation of each of the three parts plus a description of the diffusion piece in terms of a local derivation.

Example 4.20. **Dirichlet forms on group $\mathbf{C}^*$–algebras associated to functions of negative type.** Let Γ be a countable discrete group, with unit $e \in \Gamma$, and denote its elements by $s, t, \ldots$. On the Hilbert space $l^2(\Gamma)$, endowed with its natural basis $\{\epsilon_t : t \in \Gamma\}$, consider the left and right regular representations defined as follows:

$$\lambda : \Gamma \to B(l^2(\Gamma)) \qquad \lambda(s)\epsilon_t := \epsilon_{st} \qquad s,t \in \Gamma$$
$$\rho : \Gamma \to B(l^2(\Gamma)) \qquad \rho(s)\epsilon_t := \epsilon_{ts} \qquad s,t \in \Gamma\,.$$

The same symbols, λ and ρ, will denote also the associated representations of the convolution algebra $l^1(\Gamma)$. The *reduced* C^**-algebra* of Γ is defined as the norm closure,

$$C^*_{red}(\Gamma) = \overline{\lambda(l^1(\Gamma))} \subseteq B(l^2(\Gamma))\,,$$

of the family of convolution operators associated to λ. The unique trace-state is defined by

$$\tau : C^*_{red}(\Gamma) \to \mathbb{C} \qquad \tau(\lambda(s)) := \delta_{s,e} \qquad s \in \Gamma\,.$$

Since $\tau(\lambda(s)^*\lambda(t)) = \delta_{s,t}$, the von Neumann algebra associated to the GNS representation of τ is isomorphic to the von Neumann algebra generated by the left regular representation λ, i.e. the weak closure $\lambda(l^1(\Gamma))''$ of $\lambda(l^1(\Gamma))$ in $B(l^2(\Gamma))$. The corresponding standard form, described in Example 2.20 lies in the Hilbert space $l^2(\Gamma)$. The positive cone coincides with the subset of positive definite sequences, while the symmetric embedding of $\lambda(l^1(\Gamma))''$ into $l^2(\Gamma)$, extends the map $\lambda(a) \mapsto a$ from $\lambda(l^1(\Gamma))$ to $l^2(\Gamma)$.

Consider now a positive, continuous function $d : G \to [0, +\infty]$, of *negative type*, in the sense that

$$\sum_{i,j=1}^{n} \overline{c_i} c_j d(s_i^{-1} s_j) \leq 0 \qquad s_1\,, \ldots\,, s_n \in \Gamma$$

whenever $c_1\,, \ldots\,, c_n \in \mathbb{C}$ are such that $\sum_{i=1}^n c_i = 0$. Examples, including word-length functions of finitely generated groups, and in particular on free and Coxeter groups, may be found in [Boz], where it is also shown that the class of these groups is stable under free products. The case of the word-length functions on the free groups is explicitly illustrated in Section 12.2 of the Philippe Biane's Lectures in this volume.
A positive, continuous function of negative type defines a semigroup $\{T_t^d : t \geq 0\}$ of completely positive contractions of $C^*_{red}(\Gamma)$, characterized by

$$T_t^d(\lambda(f)) = \lambda(e^{-td} f) \qquad f \in l^1(\Gamma)\,, \quad t \geq 0\,.$$

The dilation of this completely Markovian semigroup corresponds to a quantum stochastic process on $C^*_{red}(\Gamma)$ which is studied in Section 12 of the Phillippe Biane's Lectures in this volume. The semigroup, which can be seen to be of strong Feller type [S8], is easily seen to be symmetric with respect to the trace-state, and the associated completely Dirichlet form is given by

$$\mathcal{E}_d : l^2(\Gamma) \to [0, +\infty) \qquad \mathcal{E}_d[a] = \sum_{s \in \Gamma} d(s)|a(s)|^2\,.$$

The form is regular because, the group algebra $\mathbb{C}\Gamma \subseteq l^1(\Gamma)\cap l^2(\Gamma)$ of finite support functions, on which $\mathcal{E}$ is clearly finite, is both a form core and a norm dense subspace of $\mathrm{C}^*_{red}(\Gamma)$.

To describe the derivation associated to the Dirichlet form $\mathcal{E}_d$, we recall that positive, continuous, functions of negative type d on Γ, may be represented in terms of *1–cocycles of unitary representations* of Γ. There exists in fact a unitary representation $\pi : \Gamma \to B(H)$ and a 1–cocycle $c : \Gamma \to H$, by definition a map satisfying

$$c(st) = c(s) + \pi(s)c(t) \qquad s,t \in \Gamma\,,$$

such that

$$\|c(s)\|^2_H = d(s)$$
$$(c(s)\,|\,c(t))_H = \frac{1}{2}(d(t) + d(s) - d(s^{-1}t))\,.$$

As customary, the same symbol π will denote both the unitary representation of Γ and the induced representation of $C^*_{red}(\Gamma)$. Defining a map $\partial : D(\partial) \to H\otimes l^2(\Gamma)$ by

$$D(\partial) := \lambda(\mathbb{C}\Gamma)\,, \qquad \partial(\lambda(f)) := c\otimes f\,, \qquad f\in\mathbb{C}\Gamma\,,$$

it is easy to check that the following representation holds true

$$\mathcal{E}[a] = \|\partial(a)\|^2_{H\otimes l^2(\Gamma)} \qquad a\in D(\partial)\,.$$

A $C^*_{red}(\Gamma)$–bimodule structure on the Hilbert space $H\otimes l^2(\Gamma)$ is defined by considering the left and right actions given by the representations $\pi_l := \pi\otimes\lambda$ and $\pi_r := id\otimes\rho$, respectively (the symbol id denotes the *identity* representation of Γ on $\mathcal{H}$). This bimodule structure turns out to be symmetric with respect to the anti-linear involution given by

$$\mathcal{J}(\xi\otimes a) := \xi\otimes J(a) \qquad \xi\otimes a\in H\otimes l^2(\Gamma)\,,$$

where $J(a)(s) = \overline{a(s^{-1})}$, $s\in\Gamma$, is just the involution associated to the standard cone. To verify the Leibniz rule it is enough to prove that for all $s,t\in\Gamma$

$$\partial(\lambda(\epsilon_s)\cdot\lambda(\epsilon_t)) = \pi_l(\lambda(\epsilon_s))(\partial(\lambda(\epsilon_t))) + \pi_r(\lambda(\epsilon_t))(\partial(\lambda(\epsilon_s)))\,. \tag{4.24}$$

In fact we have

$$\begin{aligned}
&\pi_l(\lambda(\epsilon_s))(\partial(\lambda(\epsilon_t))) + \pi_r(\lambda(\epsilon_t))(\partial(\lambda(\epsilon_s))) =\\
&\pi_l(\lambda(\epsilon_s))(c(t)\otimes\epsilon_t)) + \pi_r(\lambda(\epsilon_t))(c(s)\otimes\epsilon_s)) =\\
&\pi(\lambda(\epsilon_s))c(t)\otimes\lambda(\epsilon_s)\epsilon_t + c(s)\otimes\rho(\epsilon_t)\epsilon_s =\\
&\pi(s)c(t)\otimes\epsilon_{st} + c(s)\otimes\epsilon_{st} =\\
&(c(s)+\pi(s)c(t))\otimes\epsilon_{st} =
\end{aligned}$$

$$c(st) \otimes \epsilon_{st} =$$
$$\partial(\lambda(\epsilon_{st})) =$$
$$\partial(\lambda(\epsilon_s) \cdot \lambda(\epsilon_t)) .$$

Since d vanishes on $e \in \Gamma$, and the identity of $C^*_{red}(\Gamma)$ is $\lambda(\delta_e)$, it is easy to see that the semigroup is conservative, so that the tangent bimodule $\mathcal{H}_0$ associated with the Dirichlet form as in Corollary 4.17 is a sub–$C^*_{red}(\Gamma)$–bimodule of $H \otimes l^2(\Gamma)$ and the killing weight vanishes identically.

Example 4.21. **Clifford Dirichlet form of free fermion systems.** The following one is historically the first example of noncommutative Dirichlet form. It was studied by L. Gross from the point of view of application to Quantum Field Theory [G1,2]. Let h be an infinite dimensional, separable, real Hilbert space and $Cl(h)$ the complexification of the Clifford algebra over h. See Section 5.2 below for a detailed construction of the Clifford algebra, when h is finite dimensional. It is well known that $Cl(h)$ is a simple C*–algebra with a unique trace state τ. The associated von Neumann algebra being hyperfinite type II_1 factor.
By the Chevalley–Segal isomorphism, here denoted by D, $L^2(A,\tau)$ can be canonically identified with (the complexification of) the antisymmetric Fock space $\Gamma(h)$ over h. L. Gross [G1,2] showed that the Second Quantization $\Gamma(I_h)$ of the identity operator I_h on h is isomorphic to the Number operator $N = D^{-1}\Gamma(I_h)D$, which is the generator of a conservative C*–semigroup over $Cl(h)$. To describe the structure of N, let $\{e_i : i \in \mathbb{N}\}$ be an orthonormal base of h and let $\{A_i : i \in \mathbb{N}\}$ be the corresponding set of *annihilation* operators on $\Gamma(h)$. For each $i \in \mathbb{N}$ the operator $D_i := D^{-1}A_iD$, defined on the domain $D(\sqrt{N})$, is a densely defined, closed operator with values in $L^2(A,\tau)$ and

$$N = \sum_{i\in\mathbb{N}} D_i^* D_i = D^{-1}(\sum_{i\in\mathbb{N}} A_i^* A_i)D .$$

Moreover, $D(\sqrt{N})$ is a sub–algebra of $Cl(h)$ and on it the following *graded* Leibniz rules hold true:

$$D_i(ab) = D_i(a))b + \gamma(a)(D_i(b)) .$$

Here γ is the extension to $L^2(A,\tau)$ of the canonical involution of $Cl(h)$ which is the unique extension of the map $v \mapsto -v$ on h. This shows that, by considering on $L^2(A,\tau)$ the GNS right action of $Cl(h)$ and the new left action given by γ, we obtain a sequence of closed derivations on $Cl(h)$ with values in $L^2(A,\tau)$. The C*–Dirichlet form then is given by the formula

$$\mathcal{E}[a] = ||N^{1/2}(a)||^2_{\mathcal{H}} = \sum_{i\in\mathbb{N}} ||D_i(a)||^2_{L^2(A,\tau)} ,$$

where the tangent bimodule is now a sub-bimodule of $\bigoplus_{i\in\mathbb{N}} L^2(A,\tau)$ and the derivation is $\bigoplus_{i\in\mathbb{N}} D_i$.

Example 4.22. **Heat semigroup on the noncommutative torus.** This is a classical example coming from Noncommutative Geometry [Co2], Let A_θ be the non commutative 2-torus, i.e. the universal C*-algebra generated by two unitaries U and V, satisfying the relation

$$VU = e^{2i\pi\theta}UV\,.$$

Let $\tau : A_\theta \to \mathbb{C}$ be the tracial state given by

$$\tau(U^nV^m) = \delta_{n,0}\delta_{m,0} \qquad n,m \in \mathbb{Z}\,.$$

The *heat semigroup* $\{T_t : t \geq 0\}$ on A_θ is characterized by

$$T_t(U^nV^m) = e^{-t(n^2+m^2)}U^nV^m \qquad n,m \in \mathbb{Z}\,.$$

It is τ-symmetric, and the associated Dirichlet form is given by

$$\mathcal{E}\Big[\sum_{n,m\in\mathbb{Z}} \alpha_{n,m}U^nV^m\Big] = \sum_{n,m\in\mathbb{Z}} (n^2+m^2)|\alpha_{n,m}|^2\,.$$

The derivation associated to $\mathcal{E}$ is the direct sum

$$\partial(a) = \partial_1(a) \oplus \partial_2(a)$$

of the following derivations ∂_1 and ∂_2 defined by

$$\partial_1(U^nV^m) = inU^nV^m\,, \qquad \partial_2(U^nV^m) = imU^nV^m \qquad n,m \in \mathbb{Z}\,.$$

The heat semigroup is clearly conservative, and the A_θ–bimodule $\mathcal{H}_0$ associated with $\mathcal{E}$, as in Corollary 4.17, is a sub–bimodule of the direct sum of two standard bimodules $L^2(A,\tau) \oplus L^2(A,\tau)$.

4.4 Derivations and Dirichlet Forms in Free Probability

Free Probability is a noncommutative probabilistic theory, developed by D. Voiculescu, based on a suitable choice of the notion of independence of random variables, known as *free independence*. The origin of this type of independence may be found in the asymptotic behavior of empirical spectral distributions of *large random matrices* and in properties shared by certain subgroups of *free groups*. Among the various fields of applications, a number of already avaible results suggest that the theory is a useful tool in approaching long standing problems in von Neumann algebra theory. An introduction to the matter may be found in [Voi1].

In the framework of Free Probability an important role is played by the relative Free Entropy χ^* which is a free analogue of the Shannon's entropy. A possible approach to the construction of the Free Entropy is based the free analogue of the Fisher's information Φ^* which in turn depends on the noncommutative generalization of the Hilbert transform. In this section we show how the noncommutative Hilbert transform is related to a suitable derivation and a corresponding Dirichlet form (see [Voi1], [Voi2], [Bi]).
Let $(\mathfrak{M}, \tau)$ be a noncommutative probability space, i.e. a von Neumann algebra $\mathfrak{M}$ with a faithful and normal trace τ on it. Let $1 \in B \subseteq \mathfrak{M}$ be a *-subalgebra and let $X = X^* \in \mathfrak{M}$ be a noncommutative random variable. Denote by $B[X] \subseteq \mathfrak{M}$ the *-subalgebra generated by B and X and consider on $B[X] \otimes_{\mathrm{alg}} B[X]$ the $B[X]$-bimodule structure given by

$$c \cdot (a \otimes b) := ca \otimes b$$
$$(a \otimes b) \cdot c := a \otimes cb\,.$$

If X and B are algebraically free in the sense that no algebraic relation exist between them, there exists a unique derivation $\partial_X : B[X] \to B[X] \otimes_{\mathrm{alg}} B[X]$ such that

$$\partial_X X = 1 \otimes 1$$
$$\partial_X b = 0 \qquad b \in B\,.$$

In other words, if $B[X]$ is regarded as the algebra of noncommutative polynomials in the variable X with coefficients belonging to the algebra B, the operator ∂_X acts as the partial derivation with respect to the noncommutative variable X and the elements of B play the role of *constants*. More explicitly one has

$$\begin{aligned}\partial_X(b_0 X b_1 X \dots X b_n) &= \sum_{k=1}^{n} b_0 X b_1 \dots b_{k-1}(1 \otimes 1) b_k X \dots X b_n \\ &= \sum_{k=1}^{n} b_0 X b_1 \dots b_{k-1} \otimes b_k X \dots X b_n \qquad b_0\,, \dots b_n \in B\,.\end{aligned}$$

Denoting by $W^*(B[X])$ the von Neumann subalgebra of $\mathfrak{M}$ generated by $B[X]$ we may consider on it the restriction of the trace τ and the standard representation in $L^2(W^*(B[X]), \tau)$. The derivation may be considered as a densely defined map from the Hilbert space $L^2(W^*(B[X]), \tau)$ to the Hilbert bimodule $L^2(W^*(B[X]) \otimes W^*(B[X]), \tau \otimes \tau)$.
Under the assumption that $1 \otimes 1 \in D(\partial_X^*)$ it may be proved that

- the derivation is closable
- $B[X] \subset D(\partial_X^* \overline{\partial_X})$ and in particular that $X \in D(\partial_X^* \overline{\partial_X})$.

The element

$$\mathcal{J}(X : B) := \partial_X^*(1 \otimes 1) \in L^2(W^*(B[X]), \tau)$$

is then called the *noncommutative Hilbert transform of X with respect to B* and the square of its norm

$$\Phi^*(X:B) := \|\mathcal{J}(X:B)\|_2^2 = \|\partial_X^* 1 \otimes 1\|_2^2 = \|\partial_X^* \partial_X(X)\|_2^2$$

is by definition the *relative free information* of X with respect to B. In case $B = \mathbb{C}$ and μ_X is the distribution of X given by

$$\int_{\mathbb{R}} f(t)\mu_X(dt) := \tau(f(X)) \qquad f \in C_0(\mathbb{R}),$$

the algebra $W^*(\mathbb{C}[X])$ is identified with $L^\infty(\mathbb{R}, \mu_X)$ and the Hilbert space $L^2(W^*(\mathbb{C}[X]), \tau)$ becomes $L^2(\mathbb{R}, \mu_X)$. The elements $f \in \mathbb{C}[X]$ are just polynomials on $\mathbb{R}$ and $\partial_X f$ coincides with the difference quotient (4.3)

$$\partial_X f(s,t) = \begin{cases} \frac{f(s)-f(t)}{s-t} & \text{if } s \neq t \\ f'(s) & \text{if } s = t. \end{cases}$$

In case the Radon-Nikodym derivative $p := \frac{d\mu_X}{d\lambda}$ with respect to the Lebesgue measure λ exists in $L^3(\mathbb{R}, \lambda)$, it is possible to prove that $\mathcal{J}(X:\mathbb{C})$ is, up to a factor 2π, the Hilbert transform Hp of p:

$$Hp(t) := \text{p.v.}\frac{1}{\pi}\int_{\mathbb{R}} \frac{p(s)}{t-s}\, ds\,.$$

Applying Theorem 4.5 one has that the closure of the quadratic form

$$\mathcal{E}_X[\xi] := \|\partial_X \xi\|^2 \qquad \mathcal{F} := B[X]$$

defined on $L^2(W^*(B[X]), \tau)$ is a completely Dirichlet form generating a completely Markovian, conservative, tracially symmetric C_0^*-semigroup on the von Neumann algebra $W^*(B[X])$. The Dirichlet form $\mathcal{E}_X$ is deeply connected with the relative free Fisher information and with the free entropy. In fact it has been shown by Ph. Biane [Bi] that the Hessian of the free entropy coincides with $\mathcal{E}_X$ on the domain where the relative free Fisher information is finite. Moreover, the Dirichlet form $\mathcal{E}_X$ satisfies the Poincaré inequality if and only if the random variable X is centered, has unital covariance and a semi-circular distribution ([Bi]).

5 Noncommutative Potential Theory and Riemannian Geometry

In this chapter we will explore certain relationships between noncommutative potential theory and classical geometry (see [CS2], [DR1,2]). More precisely we will show the strong interplay among noncommutative Dirichlet integrals and heat semigroups on one hand, and the sign of the curvature of a Riemannian manifold on the other hand.

In any complete Riemannian manifold M without boundary, whose Ricci curvature is bounded from below, the heat semigroup $e^{-t\Delta}$, generated by the Laplace–Beltrami operator Δ, is Markovian, i.e. it is a strongly continuous, positivity preserving, contraction semigroup on the C*-algebra $\mathrm{C}_0(M)$ of complex continuous functions vanishing at infinity.
From an infinitesimal point of view, one has, correspondingly, that the Dirichlet integral $\mathcal{E}[f] := \int_M |\nabla f|^2$ is a Dirichlet form, i.e. a quadratic, lower semicontinuous functional on $\mathrm{C}_0(M)$ satisfying the contraction property $\mathcal{E}[f \wedge 1] \le \mathcal{E}[f]$.

These fundamental properties of classical potential theory are independent of the curvature of the space, even though the Remannian metric is, together with the concept of differential, the main ingredient for the definition of the gradient operator and the energy functional.

Classical potential theory of Riemannian manifolds, suggests however that, if a relationship among curvature and some kind of positivity exists, it should emerge considering energy functionals, heat equations and their solutions, on vector bundles over the manifold.
The first candidates are obviously the exterior bundle $\Lambda^* M$, the Hodge-de Rham Laplacian operator Δ_{HdR} on it and the heat semigroup $e^{-t\Delta_{\mathrm{HdR}}}$ it generates. However, while on scalar functions we have a natural notion of positivity, on exterior forms this is not obvious.

The way to tie together the useful tools of exterior differential calculus with a good notion of positivity is to look at exterior forms, i.e. continuous sections $C_0(\Lambda^* M)$ of the exterior bundle $\Lambda^* M$, from the point of view of its isomorphic Clifford bundle $Cl(M)$. Precisely, we will work with exterior forms as elements of the Clifford algebra $\mathrm{C}^*_0(M)$, i.e. continuous sections of the Clifford bundle, vanishing at infinity:

$$\mathrm{C}^*_0(\Lambda^* M) \cong \mathrm{C}^*_0(M)\,.$$

This is the most natural involutive algebra, indeed a C*-algebra, extending the algebra $\mathrm{C}_0(M)$ of continuous functions, vanishing at infinity on M.

In this framework E.B. Davies and O. Rothaus proved in [DR1] that on any complete Riemannian manifold, the quadratic form associated to the covariant derivation ∇ on $\mathrm{C}^*_0(M)$

$$\mathcal{E}_B[\sigma] := \int_M |\nabla\sigma|^2\, dm$$

is a noncommutative Dirichlet form on $\mathrm{C}^*_0(M)$, with respect to a natural trace, so that the heat semigroup $e^{-t\Delta_{\mathrm{B}}}$ generated by the *Bochner-Laplacian*

$$\Delta_{\mathrm{B}} := \nabla^* \circ \nabla$$

is a Markovian semigroup. In this chapter we provide a proof of the above result verifying that ∇ is a closed derivation in the sense of Chapter 3.

Later we consider the Dirac operator D on $\mathrm{C}_0^*(M)$. It was introduced in the Riemannian setting by M. F. Atiyah and G. B. Singer [AtS] (see also [LM] and reference therein), in their work on the celebrated *Index Theorem* (see [LM]). In the semi-Riemannian setting of relativistic quantum theory it was previously considered by P.A.M. Dirac [Dir].
The Dirac operator is the fundamental elliptic operator of a Riemannian manifold; from the point of view of the exterior algebra it is just the sum of the exterior differential and its adjoint

$$D \cong d + d^* \,.$$

Its square D^2, the so called *Dirac-Laplacian*, is just a version, on the Clifford algebra, of the *Hodge-de Rham-Laplacian* on exterior forms

$$D^2 \cong (d + d^*)^2 = d^*d + dd^* =: \Delta_{\mathrm{HdR}} \,.$$

A first difference between these two Laplacians is that while Δ_{B} reveals the *geometric* aspects of M, the operator D^2 is connected with the *topological* ones. For example, in the kernel of Δ_{B} one finds the *parallel* forms, while the *harmonic* forms are contained in the kernel of D^2.
The second main difference is that, while, by the Davies-Rothaus theorem, the heat semigroup $e^{-t\Delta}$ is always Markovian, the semigroup e^{-tD^2} need not be.

We will show that the heat semigroup e^{-tD^2}, generated by the Dirac-Laplacian D^2, is Markovian if and only if the curvature operator of M is nonnegative. Equivalently, the quadratic form of the operator D^2

$$\mathcal{E}_{\mathrm{D}} : L^2(\mathrm{C}_0^*(M)\,,\tau) \longrightarrow [0,+\infty] \qquad \mathcal{E}_{\mathrm{D}}[\sigma] = \int_M |D\sigma|^2 \,,$$

is a noncommutative Dirichlet form exactly when the curvature operator $\widehat{R}$ of M is nonnegative.

In this way, a geometric property, like the positive sign of the curvature operator, is shown to be equivalent to a potential theoretic property of the Dirac energy functional $\mathcal{E}_D$.

Theorem 5.1. *Let (M,g) be a complete Riemannian manifold without boundary. The following properties are equivalent:*

i) $\{e^{-tD^2} : t \geq 0\}$ is a completely Markovian semigroup, i.e. a strongly continuous, semigroup of completely positive contractions on $\mathrm{C}_0^*(M)$;

ii) $\{e^{-tD^2} : t \geq 0\}$ *is a completely Markovian semigroup on the Hilbert space* $L^2(Cl(M), g)$ *of square integrable sections of the Clifford bundle;*

iii) the Dirac form $\mathcal{E}_{\mathrm{D}}$ *is a* C^**–Dirichlet form on* $L^2(\mathrm{C}^*_0(M), \tau)$*;*

iv) the curvature operator is nonnegative: $\widehat{R} \geq 0$.

The methods we use are based on the Bochner Identity, on the correspondence between noncommutative Dirichlet forms and Markovian semigroups, and on the characterization of Dirichlet forms in terms of derivations which we presented in Chapter 4.

Specializing the above general setting, let us review some applications.

Example 5.2. (Dirichlet forms and topology of Riemann surfaces) Let Σ be a compact, connected, orientable surface. Then there exists a metric g on Σ such that the Dirac form $\mathcal{E}_{\mathrm{D}}$ is a Dirichlet form if and only if Σ is either homeomorphic to the sphere S^2 or to the torus T^2.
In fact in dimension two the curvature operator is just the multiplication operator by the Gauss curvature function k_g; if our surface is homeomorphic to a sphere or a torus, it then carries a metric of nonnegative curvature and the corresponding Dirac form $\mathcal{E}_{\mathrm{D}}$ is a C*-Dirichlet form. On the other hand if g is a metric for which $\mathcal{E}_{\mathrm{D}}$ is a C*-Dirichlet form, then its Gauss curvature is nonnegative so that, by the Gauss–Bonnet formula $\chi(M) = \frac{1}{2\pi}\int_M k_g$, its Euler characteristic is nonnegative.

Example 5.3. (Dirichlet forms on hypersurfaces) Another example in which the Dirac form $\mathcal{E}_D$ is Markovian is the one of a *codimension one convex, hypersurface* $M \subset \mathbb{R}^{n+1}$.

Example 5.4. (Dirichlet forms and topology of Cartan's symmetric spaces) Manifolds which have a nonnegative curvature operator have been intensively studied (and, at the end classified) since the works of E. Cartan on symmetric spaces. Combining these result with the above equivalences we obtain that if M is a compact simply connected Riemannian manifold whose Dirac form $\mathcal{E}_{\mathrm{D}}$ is a complete Dirichlet form then M is homeomorphic to the product of spaces of the following type:

i) Euclidean spaces,
ii) Spheres,
iii) Projective spaces,
iv) Symmetric spaces of compact type.

In the following sections we will explain carefully the ingredients, of geometric and analytic nature needed for the proof of Theorem 5.1. Very good references for all the background we are going to summarize are [LM], [Pet].

5.1 Clifford Algebras

Let (E, g) be a real, Euclidean vector space, with finite dimension $\dim E$. The *Clifford algebra* $Cl(E, g)$ associated to (E, g) can be defined as the unital, associative, complex algebra generated by a unit 1 and the elements of E subject to the relations : $e_1 \cdot e_2 + e_2 \cdot e_1 + 2g(e_1, e_2) \cdot 1 = 0$ for all e_1, e_2 in E. The product of two elements $\sigma_1, \sigma_2 \in Cl(E, g)$ will be denoted by $\sigma_1 \cdot \sigma_2$, and its unit by 1. There is a natural, vector space isomorphism $\phi : \Lambda^*(E) \to Cl(E, g)$ between the complexified exterior algebra $\Lambda^*(E) := \Lambda^*_{\mathbb{R}}(E) \otimes_{\mathbb{R}} \mathbb{C}$ and the Clifford algebra, characterized by

$$\begin{aligned} \phi(1_{\Lambda^*(E)}) &= 1, \\ \phi(v_1 \wedge v_2 \wedge \cdots \wedge v_r) &= v_1 \cdot v_2 \cdots v_r \end{aligned} \tag{5.1}$$

for an orthogonal family $v_1, v_2, \ldots, v_r \in E$ and $r = 1, \ldots, \dim E$. Consequently $\dim_{\mathbb{C}} Cl(E, g) = 2^{\dim E}$ and if $\{e_i : i = 1, \ldots, \dim E\}$ is an orthonormal basis for E, then the unit 1 and the set $\{e_{i_1} \cdot e_{i_2} \cdot \cdots \cdot e_{i_r} : 1 \le i_1 < i_2 < \cdots < i_r \le \dim E \,, r = 1, \ldots, \dim E\}$ form a linear base of the Clifford algebra.

When $\dim E = 2n$ the Clifford algebra is isomorphic to the algebra $M_{2^n}(\mathbb{C})$ of complex matrices with 2^n rows and columns, while when $\dim E = 2n + 1$ it is isomorphic to $M_{2^n}(\mathbb{C}) \bigoplus M_{2^n}(\mathbb{C})$. This suggest that Clifford algebras may be seen as C*-algebras. In fact, the above isomorphism can be used to transfer the canonical Hilbert space structure of $\Lambda^*(E)$ on $Cl(E, g)$ so that the left action of $Cl(E, g)$ on itself gives a representation by which the Clifford algebra became an algebra of operators on a Hilbert space, hence a C*-algebra.

The unit vector 1 determines a faithful trace functional on the Clifford algebra

$$\begin{aligned} &\tau : Cl(E, g) \to \mathbb{C} \\ &\tau(\sigma) := \langle 1, \sigma 1 \rangle \qquad \sigma \in Cl(E, g) \end{aligned} \tag{5.2}$$

such that the G.N.S. Hilbert space $L^2(Cl(E, g), \tau)$ associated with it is canonically isomorphic to $Cl(E, g)$ with its Hilbert space structure.

5.2 Clifford Algebra of a Riemannian Manifold

The very definition of the Clifford algebra of a Euclidean space (E, g) suggests that the group of special orthogonal transformations $SO(E, g)$ acts on $Cl(E, g)$ in a natural way. If a Riemannian manifold (M, g) is given, using this representation, one may consider the vector bundle $Cl(M)$ associated to the tangent bundle TM. The so called Clifford bundle $Cl(M)$ is then a

bundle whose fibers $Cl_x(M)$ at points $x \in M$ are just the Clifford algebras of the Euclidean spaces (T_xM, g_x).
The above algebraic isomorphism between the Clifford algebra and the exterior algebra can be raised to a natural isomorphism of Euclidean bundles $Cl(M) \simeq \Lambda^*(M)$ between the Clifford bundle and the complexified exterior bundle $\Lambda^*(M)$. The great advantage of this is that the exterior algebra of continuous differential forms, vanishing at infinity on M, when considered as the space of sections of the Clifford bundle vanishing at infinity acquires a natural structure of C*-algebra.

Definition 5.5. (Clifford algebra of a Riemannian manifold.) The space $C_0^*(M)$ of sections of the Clifford bundle $Cl(M)$ is called the *Clifford algebra* of the Riemannian manifold (M, g). The multiplication of two sections σ_1, σ_2, or spinors as they are also called, is defined pointwise $(\sigma_1 \cdot \sigma_2)(m) = (\sigma_1)(m) \cdot (\sigma_2)(m)$ by the Clifford product in each Clifford algebra $Cl_m(M)$.

Endowed with the pointwise multiplication and involution in the fibers, it is a C*–algebra with respect to the norm which is the supremum of operator norms on the fibers:

$$\|\sigma\| := \sup_{m \in M} \|\sigma(m)\| . \tag{5.3}$$

Its center contains the algebra $C_0(M)$ of continuous complex functions vanishing at infinity on M.

The Clifford algebra carries a natural faithful, semifinite l.s.c. trace $\tau : \mathrm{C}_0^*(M)_+ \to [0, +\infty]$ obtained by gluing together the traces $\{\tau_m : m \in M\}$ on the fibers by the Riemannian volume measure dm on M:

$$\tau(\sigma) := \int_M \tau_m(\sigma(m))\, \mathrm{d}m \qquad \sigma \in \mathrm{C}_0^*(M)_+ . \tag{5.4}$$

The GNS Hilbert space $L^2(\mathrm{C}_0^*(M), \tau)$ associated to τ coincides with the Hilbert space $L^2(Cl(M))$, with scalar product

$$\begin{aligned}(\sigma_2|\sigma_1) : &= \tau(\sigma_2^* \cdot \sigma_1) = \int_M \tau_m(\sigma_2(m)^* \cdot \sigma_1(m))\mathrm{d}m \\ &= \int_M \langle \sigma_2(m)|\sigma_1(m)\rangle_{Cl(T_mM, g_m)} \cdot \mathrm{d}m .\end{aligned} \tag{5.5}$$

The left and right regular representations of the Clifford algebra onto itself naturally extend, by continuity, to commuting representations in the Hilbert space $L^2(Cl(M)) = L^2(\mathrm{C}_0^*(M), \tau)$. These actions, denoted by $(a, \xi, b) \to a\xi b$, satisfy

$$\|a\xi b\|_2 \le \|a\| \cdot \|\xi\|_2 \cdot \|b\| \qquad a, b \in \mathrm{C}_0^*(M) \quad \xi \in L^2(Cl(M)) \tag{5.6}$$

in such a way that $L^2(Cl(M))$ is naturally endowed with a structure of a $\mathrm{C}_0^*(M)$–*bimodule*.

Extending, again by continuity, the involution of $\mathrm{C}_0^*(M)$ to $L^2(\mathrm{C}_0^*(M),\tau)$, we get an antilinear, isometric involution $J : L^2(\mathrm{C}_0^*(M),\tau) \to L^2(\mathrm{C}_0^*(M),\tau)$ which exchanges the left and right actions of the Clifford algebra,

$$J(a\xi b) = a^* J(\xi) b^* \qquad a, b \in \mathrm{C}_0^*(M) \quad \xi \in L^2(\mathrm{C}_0^*(M),\tau)\,, \tag{5.7}$$

so that $L^2(\mathrm{C}_0^*(M),\tau)$ is in fact a *symmetric* $\mathrm{C}_0^*(M)$–bimodule.

5.3 Covariant Derivative, Bochner and Dirac-Laplacians

We now describe the basic elliptic operators whose potential theoretic properties we want to analyze.
The Levi-Civita connection on the tangent bundle TM induces a hermitian connection in the associated Clifford bundles. We shall denote the associated *covariant derivative*, acting on the spaces of smooth sections of the bundle, by the symbol

$$\nabla : C_c^\infty(Cl(M)) \to C_c^\infty(Cl(M) \otimes T^*M)\,. \tag{5.8}$$

By definition the covariant derivative satisfies the following rules

$$\begin{gathered} \nabla(f\sigma) = \sigma \otimes df + f\nabla\sigma \qquad f \in C_c^\infty(M)\,, \sigma \in C_c^\infty(Cl(M)) \\ X(\sigma_1|\sigma_2) = (\nabla_X\sigma_1|\sigma_2) + (\sigma_1|\nabla_X\sigma_2) \qquad \sigma_1\,, \sigma_2 \in C_c^\infty(Cl(M))\,, X \in C_c^\infty(TM)\,, \end{gathered} \tag{5.9}$$

where ∇_X denotes the composition of ∇ with the contraction associated to the vector field X.

At the Hilbert space level the covariant derivative ∇ can be understood as a closed operator from $L^2(\mathrm{C}_0^*(M),\tau) = L^2(Cl(M))$ to $L^2(Cl(M) \otimes T^*M)$, defined on the Sobolev space $H^1(M)$ of elements of $L^2(Cl(M))$ whose distributional covariant derivative belongs to $L^2(Cl(M) \otimes T^*M)$.
The *Bochner-Lapalcian* is then the nonnegative self-adjoint operator on $L^2(Cl(M))$ defined as

$$\triangle_{\mathrm{B}} := \nabla^*\nabla\,. \tag{5.10}$$

Its associated closed quadratic form coincides with

$$\begin{aligned} \mathcal{E}_{\mathrm{B}} &:= H^1(M) \to [0,\infty) \\ \mathcal{E}_{\mathrm{B}}[\sigma] &:= \|\nabla\sigma\|^2_{L^2(Cl(M)\otimes T^*M)} \qquad \sigma \in H^1(M)\,. \end{aligned} \tag{5.11}$$

Under the natural isomorphism $\mathrm{C}_0^*(M) \simeq \Lambda^*(M)$, the above defined operators ∇, $\triangle_{\mathrm{B}}$ can be naturally identified with the more usual covariant derivative and Bochner-Laplacian acting on the exterior bundle.

The *Dirac operator* $D : C^\infty(\mathrm{C}_0^*(M)) \to C^\infty(\mathrm{C}_0^*(M))$ is defined as

$$D\sigma := \sum_{i=1}^{n} e_i \cdot \nabla_{e_i}\sigma \tag{5.12}$$

at any point $m \in M$, where $\{e_i : i = 1, \dots, n\}$ denotes any orthonormal base of T_mM and "$\cdot$" denotes the product in the Clifford algebra $Cl(T_mM, g_m)$. At the Hilbert space level D is a self-adjoint operator on $L^2(Cl(M))$ with domain $H^1(M)$. The operator D^2 on $L^2(Cl(M))$ is called the *Dirac-Laplacian*. It is a nonnegative self-adjoint operator whose closed quadratic form is given by

$$\begin{aligned} &\mathcal{E}_{\mathrm{D}} : H^1(M) \to [0, \infty) \\ &\mathcal{E}_{\mathrm{D}}[\sigma] := \|D\sigma\|^2_{L^2(Cl(M))} \qquad \sigma \in H^1(Cl(M)) \,. \end{aligned} \tag{5.13}$$

Under the natural isomorphism $Cl(M) \simeq \Lambda^*(M)$, the Dirac operator D and the Dirac-Laplacian D^2 correspond to the operator $d+d^*$ and to the Hodge-de Rham-Laplacian $\Delta_{\mathrm{HdR}} := dd^* + d^*d$, respectively.

5.4 Leibniz Rule for the Covariant Derivative

Here we show that the Bochner-Laplacian generates a completely Markovian semigroup on the Clifford algebra of a Riemannian manifold [DR1 Theorem 13]. The proof is different from the original one and it relies on the Leibniz property of the covariant derivative.
On the Hilbert space $L^2(Cl(M) \otimes T^*M)$ there are continuous and commuting left and right actions of the Clifford algebra $\mathrm{C}_0^*(M)$ which are characterized by the rule

$$\xi \cdot (\zeta \otimes \omega) \cdot \eta = (\xi \cdot \zeta \cdot \eta) \otimes \omega \,, \tag{5.14}$$

for all $\xi, \zeta, \eta \in \mathrm{C}_0^*(M)$ and all sections ω of the cotangent bundle T^*M.
Moreover, since T^*M is the complexification of a real vector bundle, there is on $L^2(T^*M)$ a canonical conjugation whose action we denote by $\omega \to \overline{\omega}$. The map

$$\begin{aligned} \mathcal{J} : L^2(Cl(M) \otimes T^*M) \to L^2(Cl(M) \otimes T^*M) \\ \mathcal{J}(\zeta \otimes \omega) : = \zeta^* \otimes \overline{\omega} \end{aligned} \tag{5.15}$$

is then easily seen to be a natural, antilinear, isometric involution, which intertwines the left and right actions of $\mathrm{C}_0^*(M)$ on $L^2(Cl(M) \otimes T^*M)$:

$$\mathcal{J}(\xi \cdot \zeta \otimes \omega \cdot \eta) := \eta^* \cdot \mathcal{J}(\zeta \otimes \omega) \cdot \xi^* \,. \tag{5.16}$$

Summarizing, we endowed the Hilbert space $L^2(Cl(M) \otimes T^*M)$ with a canonical structure of *symmetric* $\mathrm{C}_0^*(M)$*–bimodule*.

Theorem 5.6. *Let (M, g) be a Riemmanian manifold without boundary and $C_0^*(M)$ its associated Clifford C^*-algebra. Then the covariant derivative defined on the Dirichlet algebra $\mathcal{B}(M) := \mathrm{C}_0^*(M) \cap H^1(M)$*

$$\nabla : \mathcal{B}(M) \to L^2(Cl(M) \otimes T^*M) \tag{5.17}$$

is a symmetric derivation in the sense that $\mathcal{B}(M)$ is a *–algebra, the Leibniz rule

$$\nabla(\sigma_1 \cdot \sigma_2) = (\nabla\sigma_1) \cdot \sigma_2 + \sigma_1 \cdot (\nabla\sigma_1) \qquad \sigma_1\,, \sigma_2 \in \mathcal{B}(M) \tag{5.18}$$

holds true and that ∇ intertwines the involutions J and $\mathcal{J}$

$$\nabla(J\sigma) = \nabla(\sigma^*) = \mathcal{J}(\nabla\sigma) \qquad \sigma \in \mathcal{B}(M)\,. \tag{5.19}$$

As a consequence, the Bochner-Laplacian Δ_B generates a completely Markovian semigroup, both on the Hilbert space $L^2(Cl(M)$ of square integrable sections of the Clifford bundle and on the Clifford C^*-algebra $C_0^*(M)$.

Proof. The symmetry property (5.19) follows directly from the definition of $\mathcal{J}$ in (5.15). The Leibniz property of ∇ is just a consequence of the metric property (5.9) of the Levi-Civita connection. In fact, for any vector field X, from (5.9) and the properties of the Clifford product we have

$$\begin{aligned} X(\sigma|\sigma) &= (\nabla_X\sigma|\sigma) + (\sigma|\nabla_X\sigma) \\ \nabla_X(\sigma \cdot \sigma) &= (\nabla_X\sigma) \cdot \sigma + \sigma \cdot (\nabla_X\sigma) \qquad \sigma \in \mathcal{B}(M)\,. \end{aligned}$$

Since the contraction i_X, with respect to a vector field X, commutes with the left and right actions of the Clifford algebra, and $\nabla_X = i_X \circ \nabla$, we have

$$i_X(\nabla(\sigma \cdot \sigma)) = i_X((\nabla\sigma) \cdot \sigma + \sigma \cdot (\nabla\sigma)) \qquad \sigma \in \mathcal{B}(M)\,.$$

As this is true for any vector field, we have

$$\nabla(\sigma \cdot \sigma) = (\nabla\sigma) \cdot \sigma + \sigma \cdot (\nabla\sigma) \qquad \sigma \in \mathcal{B}(M)\,,$$

from which (5.18) follows by polarization.

5.5 Curvature Operator and Bochner Identity

A large number of results in topology and geometry on Riemannian manifolds, follows from the so called *Bochner method*, based on the splitting of the Dirac Laplacian as the sum of the Bochner-Laplacian and a piece depending the curvature of the manifold. This second part is described in terms of (a bundle of) finite dimensional self-adjoint operators called the *curvature operator*.

The curvature tensor R associated to the Levi–Civita connection of (M, g) can be defined, as a smooth section of $\otimes^4 T^*M$, at the point $m \in M$ by the formula

$$R_m(v_1, v_2, v_3, v_4) = (R_m(v_1, v_2)v_3|v_4)_{T_mM} \qquad v_1, v_2, v_3, v_4 \in T_mM, \quad (5.20)$$

where, for fixed vector fields v_1, v_2 , $R_m(v_1, v_2)$ is the endomorphism of T_mM given by

$$R_m(v_1, v_2)v = -(\nabla_{v_1}\nabla_{v_2}v - \nabla_{v_2}\nabla_{v_1}v - \nabla_{[v_1,v_2]}v)(m) \qquad v \in \mathrm{C}_c^\infty(TM) \quad (5.21)$$

which depends only on values of v_1, v_2 and v at point m.
The symmetries of the curvature tensor (not including the Bianchi's identities) allow to interpret R_m as a self-adjoint operator $\widehat{R}_m$ on the Hilbert space $\Lambda^2_m M$ according to the formula:

$$(\widehat{R}_m(v_1 \wedge v_2)|\, v_3 \wedge v_4)_{\Lambda^2_m M} := R_m(v_1, v_2, v_3, v_4) \qquad v_1, v_2, v_3, v_4 \in T_mM\,. \quad (5.22)$$

Definition 5.7. (Curvature operator of a Riemannian manifold) The field $\widehat{R} := \{\widehat{R}_m : m \in M\}$ is called the *curvature operator* of the Riemannian manifold (M, g). It is said to be *nonnegative* if, at each point m of M, $\widehat{R}_m$ is nonnegative operator in the spectral sense, i.e. if all of its eigenvalues are nonnegative. This property will be denoted by $\widehat{R} \geq 0$.

The curvature operator is related to the *sectional curvature* $K : Gr(2, M) \to \mathbb{R}$ of M, defined on the Grassmannian $Gr(2, M)$ of 2–planes of M by the formula

$$K_m(\pi_m) = (\widehat{R}_m(v_1 \wedge v_2)|v_1 \wedge v_2)_{\Lambda^2_m M} \qquad \pi_m \in Gr_m(2, M) \qquad (5.23)$$

for any orthonormal base $\{v_1, v_2\}$ of the 2–plane π_m at m. The curvature tensor R, the curvature operator $\widehat{R}$ and the sectional curvature K are equivalent algebraic objects in the sense that each of them determines algebraically the others. Attention should be paid to the fact that, while $\widehat{R} \geq 0$ implies $K \geq 0$, the opposite is not always true. The reason for that is that at some point m, $\widehat{R}_m$ may not admit a base of decomposable eigenvectors. Conditions for this are well known and some of them will be used later in the work.

The proof of Theorem 5.1 is based on a repeated use of the *Bochner Identity* (see [LM Theorem 8.2])

$$D^2 = \Delta_{\mathrm{B}} + \Theta_R \qquad (5.24)$$

by which the Dirac-Laplacian D^2 decomposes as a sum of the Bochner-Laplacian Δ_{B} and a symmetric operator Θ_R depending only on the curvature operator $\widehat{R}$. In terms of quadratic forms on $L^2(Cl(M))$, the decomposition reads as follows (see [LM Theorem 8.6])

$$\mathcal{E}_{\mathrm{D}} = \mathcal{E}_{\mathrm{B}} + Q_R \tag{5.25}$$

where Q_R is the quadratic form $Q_R[\sigma] := (\sigma|\Theta_R(\sigma))_{L^2(Cl(M))}$ of the operator Θ_R. The quadratic form Q_R can be explicitly represented as a superposition

$$Q_R[\sigma] = \int_M Q_R(m)[\sigma_m] \cdot \mathrm{d}m \quad \sigma \in L^2(Cl(M)) \tag{5.26}$$

of quadratic forms on the Hilbert spaces $Cl(T_m M, g_m)$ given by

$$Q_R(m)[\sigma] = \frac{1}{4} \sum_{\alpha,\beta=1}^{n(n-1)/2} \left\langle \widehat{R}_m(\xi_\alpha) \,|\, \xi_\beta \right\rangle_{\Lambda^2_m M} \cdot \langle\, [\xi_\alpha, \sigma] \mid [\xi_\beta, \sigma] \,\rangle_{Cl(T_m M, g_m)} \tag{5.27}$$

where $\{\xi_\alpha : \alpha = 1, \ldots, n(n-1)/2\}$ is any orthonormal base of $\Lambda^2_m M$. If we choose a base $\{\eta_\alpha : \alpha = 1, \ldots, n(n-1)/2\}$ of orthonormal eigenvectors of $\widehat{R}_m$ corresponding to the eigenvalues $\{\mu_\alpha : \alpha = 1, \ldots, n(n-1)/2\}$, then (2.38) becomes

$$Q_R(m)[\sigma] = \frac{1}{4} \sum_{\alpha=1}^{n(n-1)/2} \mu_\alpha \| \, [\eta_\alpha, \sigma] \, \|_2^2 \, . \tag{5.28}$$

5.6 Completely Unbounded and Approximately Bounded Parts of a Dirichlet Form

Here we describe a general decomposition of derivations and Dirichlet forms, which will be useful for the proof of the main result of this chapter.

Definition 5.8. Let $\partial : D(\partial) \to \mathcal{H}$ be a derivation, densely defined on a subalgebra of a C*-algebra A (see Definition 4.2) and denote by $\mathcal{L}_{A-A}(\mathcal{H})$, the von Neumann algebra of all bounded operators on $\mathcal{H}$, commuting both with the left and right actions of A.

- An element $B \in \mathcal{L}_{A-A}(\mathcal{H})$ is said to be *∂-bounded* if the map

$$B \circ \partial : D(\partial) \to \mathcal{H}$$

  extends to a bounded map from A to $\mathcal{H}$.
- A projection p in $\mathcal{L}_{A-A}(\mathcal{H})$ is said to be *approximately ∂-bounded* if it is the increasing limit of a net of ∂-bounded projections.
- A projection p in $\mathcal{L}_{A-A}(\mathcal{H})$ is said to be *completely ∂-unbounded* if 0 is the only ∂-bounded projection smaller than p.
- The derivation $(\partial, D(\partial), \mathcal{H})$ is said to be *bounded* (resp. *approximately bounded*, *completely unbounded*) if the identity operator $1_{\mathcal{H}}$ is *bounded* (resp. *approximately bounded*, *completely unbounded*).

Example 5.9. (Structure of bounded completely Dirichlet forms on amenable C*-algebras) By definition (see [Co2]), *amenable C* algebras* are those on which any bounded derivation $\partial : A \to X$, taking values in a dual Banach bimodule X (i.e. a bimodule X such that, as a Banach space it is the dual $X = (X_*)^*$ of some other X_*), are necessarily *inner*: there exists $\xi \in X$ such that

$$\partial(a) = a\xi - \xi a \qquad a \in A\,.$$

Recall that by results due to A. Connes [Co3] and U. Haagerup [H3], A is amenable if and only if is nuclear. Since the derivations representing C*-Dirichlet forms take values in Hilbert bimodule (see Chapter 4), we conclude that if A is amenable, $\tau : A \to \mathbb{C}$ is a finite trace on A, and $\mathcal{E} : L^2(A\,,\tau) \to [0, +\infty)$ is a bounded C*-Dirichlet form, then it can be represented as follows

$$\mathcal{E}[a] = \|a\xi - \xi a\|^2_{\mathcal{H}} \qquad a \in A$$

for some $\xi \in \mathcal{H}$.

Proposition 5.10. *(Decomposition of derivations and Dirichlet forms [CS2 Lemma 4.3]) Let $\partial : D(\partial) \to \mathcal{H}$ be a derivation, densely defined on a subalgebra of a C*-algebra A. Then there exists in $\mathcal{L}_{A-A}(\mathcal{H})$, the greatest approximately ∂-bounded projection P_{ab}. Every ∂-bounded operator B satisfies*

$$B \circ P_{ab} = B\,.$$

As a consequence, the derivation $(\partial\,, D(\partial)\,, \mathcal{H})$ splits, canonically, as direct sum

$$\partial = \partial_{cu} \oplus \partial_{ab}$$

of a smallest completely unbounded derivation

$$\partial_{cu} : D(\partial) \to \mathcal{H}_{cu} \qquad \partial_{cu} := (1_{\mathcal{H}} - P_{cu}) \circ \partial\,, \quad \mathcal{H}_{cu} := (1_{\mathcal{H}} - P_{ab})\mathcal{H}$$

and the greatest approximately bounded derivation

$$\partial_{ab} : D(\partial) \to \mathcal{H}_{ab} \qquad \partial_{ab} := P_{ab} \circ \partial\,, \quad \mathcal{H}_{ab} := P_{ab}\mathcal{H}\,.$$

Applying the decomposition above to the derivation associated to a Dirichlet form $\mathcal{E}$, one gets a decomposition of $\mathcal{E}$ as a sum of two, not necessarily closable, Markovian forms

$$\mathcal{E} = \mathcal{E}_{cu} + \mathcal{E}_{ab}$$

called the completely unbounded part and the approximately bounded one, respectively. To clarify the meaning of the above splitting, let us apply it in the commutative setting.

Example 5.11. (Decomposition of Dirichlet forms on commutative C*-algebras: the Beurling-Deny-Le Jan decomposition revisited II). By the classical

Beurling-Deny-Le Jan decomposition BDLJ (see [FOT]), a regular Dirichlet form $(\mathcal{E}, D(\mathcal{E}))$ on $L^2(X, m)$, splits as a sum

$$\mathcal{E} = \mathcal{E}^{(c)} + \mathcal{E}^{(j)} + \mathcal{E}^{(k)}$$

of three Markovian forms, called the *diffusive*, *jumping* and *killing* parts, respectively. In Example 4.19, we this decomposition was obtained combining, the representation of Dirichlet forms in terms of derivations, with the basic results of representation theory of commutative C*-algebras. Comparing the BDLJ decomposition with the one of Proposition 5.9, it is not difficult to have the following identifications

$$\mathcal{E}_{cu} = \mathcal{E}^{(c)}\,, \qquad \mathcal{E}_{ab} = \mathcal{E}^{(j)} + \mathcal{E}^{k}\,.$$

This result may suggests to interpret the completely unbounded part of Dirichlet form $\mathcal{E}$ on a C*-algebra A, as the strongly local part of $\mathcal{E}$.

5.7 Positive Curvature Operator and Markovianity of the Dirac-Dirichlet Form

In this section we collect the main points in the proof of Theorem 5.1. The equivalence among items ii) and iii) is just the general correspondence between noncommutative Dirichlet form and tracially symmetric Markovian semigroups. Property ii) follows from i) by the results of Section 2.2, 2.3, specialized and simplified to the tracial setting. The reverse implication is a matter of elliptic regularity, i.e. Sobolev estimates, and it is a consequence of the regularization properties of the heat semigroups of Feller type.
To show that iii) is a consequence of iv), let us consider the Bochner Identity in the form (5.25). As the curvature operator is assumed to be nonnegative, by (5.27), quadratic from Q_R is continuous superposition of Dirichlet forms associated to bounded derivations, i.e. the commutators appearing in (5.28). Hence, the quadratic form Q_R itself is a Dirichlet form. Since, by Theorem 5.6, the quadratic form of the Bochner-Laplacian $\mathcal{E}_B$ is a Dirichlet form too, so is their sum $\mathcal{E}_D$.

The proof of the fact that property iv) follows from property iii) is based, essentially, on the decomposition of Dirichlet forms introduced in 5.6.
Suppose that $\mathcal{E}_{\mathrm{D}}$ is a Dirichlet form. Write the curvature operator as the difference of its positive and negative parts: $\widehat{R} = \widehat{R}_+ - \widehat{R}_-$. Correspondingly we have the decomposition $Q_{\widehat{R}} = Q_{\widehat{R}_+} - Q_{\widehat{R}_-}$, where the forms $Q_{\widehat{R}_\pm}$ are defined analogously to $Q_{\widehat{R}}$.
Consider now the following decomposition of the Dirac form:

$$\mathcal{E}_{\mathrm{D}} = \mathcal{E}_+ - \mathcal{E}_-\,, \tag{5.29}$$

where

$$\begin{aligned}\mathcal{E}_+ &:= \mathcal{E}_\mathrm{B} + Q_{\widehat{R}_+} \\ \mathcal{E}_- &:= Q_{\widehat{R}_-} \,.\end{aligned} \tag{5.30}$$

Obviously we then have that $\mathcal{E}_+ = \mathcal{E}_\mathrm{D} + \mathcal{E}_-$ appears as a sum of Dirichlet forms, and we may apply the analysis developed in Section 5.6. Clearly

$$\begin{aligned}(\mathcal{E}_+)_{cu} &= (\mathcal{E}_\mathrm{B} + Q_{\widehat{R}_+})_{cu} = \mathcal{E}_\mathrm{B} \,, \\ (\mathcal{E}_+)_{ab} &= (\mathcal{E}_\mathrm{B} + Q_{\widehat{R}_+})_{ab} = Q_{\widehat{R}_+} \,.\end{aligned} \tag{5.31}$$

On the other hand

$$\begin{aligned}(\mathcal{E}_\mathrm{D} + \mathcal{E}_-)_{cu} &= (\mathcal{E}_\mathrm{D} + Q_{\widehat{R}_-})_{cu} = (\mathcal{E}_\mathrm{D})_{cu} \,, \\ (\mathcal{E}_\mathrm{D} + \mathcal{E}_-)_{ab} &= (\mathcal{E}_\mathrm{D} + Q_{\widehat{R}_-})_{ab} = (\mathcal{E}_\mathrm{D})_{ab} + Q_{\widehat{R}_-}\end{aligned} \tag{5.32}$$

By identification we have

$$Q_{\widehat{R}_+} = (\mathcal{E}_+)_{ab} = (\mathcal{E}_\mathrm{D} + Q_{\widehat{R}_-})_{ab} = (\mathcal{E}_\mathrm{D})_j + Q_{\widehat{R}_-} \tag{5.33}$$

so that the quadratic form associated to the curvature operator can be identified with the jumping part (i.e. approximately bounded part) of the Dirac form:

$$Q_{\widehat{R}} = Q_{\widehat{R}_+} - Q_{\widehat{R}_-} = (\mathcal{E}_\mathrm{D})_{ab} \,. \tag{5.34}$$

This proves, in particular, that $Q_{\widehat{R}}$ is a C*–Dirichlet form. By a purely algebraic result, concerning specific properties of Clifford algebras over finite dimensional Euclidean spaces, one obtains that the coefficients μ_α in (5.28) have to be nonnegative, so that the curvature operator has to be nonnegative too.

We conclude this section with an application of the above main result to the topology of Riemannian spaces with nonnegative curvature operator.

Proposition 5.12. *Let M be a compact Riemannian manifold with nonnegative curvature operator $\widehat{R} \geq 0$. Then the space*

$$\ker D$$

of harmonic spinors is a finite dimensional C^*-algebra hence a finite sum of full matrix algebras

$$\ker D = M_{n_1}(\mathbb{C}) \oplus M_{n_2}(\mathbb{C}) \oplus \cdots \oplus M_{n_k}(\mathbb{C}) \,,$$

where the integer $k \in \mathbb{N}^*$ is the number of maximal ideals of $\ker D$*. Moreover, the evaluation maps*

$$e_x : \ker D \to Cl(T_x M) \quad e_x(\sigma) = \sigma(x) \qquad x \in M$$

are injective morphisms of C^*-algebras. In particular the sum of the Betti numbers $b_i(M)$ of M is a sum of squares

$$\sum_{i=1}^{\dim M} b_i(M) = \sum_{l=1}^{k} n_l^2$$

and if M is irreducible and $\dim M$ *is even this number coincides with Euler's characteristic $\chi(M)$ of M.*

Proof. By elliptic regularity, $\ker D$ is a subspace of the Clifford algebra (in fact its elements are smooth sections of the Clifford bundle). Combining Theorem 5.1 and Theorem 4.18 with the observation that the kernel of a derivation on a C*-algebra is a C*-subalgebra, we get that $\ker D$ is a finite dimensional C*-subalgebra of $C_0^*(M)$. The structure theorem of finite dimensional C*-algebras (see [T2]) allows to conclude that $\ker D$ is finite sum of full matrix algebras. Moreover, since the curvature operator is nonnegative, by the Bochner's identity (5.25), harmonic spinors are parallel (vanishing covariant derivative). Hence for any fixed point $x \in M$, the evaluation map $\ker D \ni \sigma \mapsto \sigma(x) \in Cl(T_x M)$ is an injective morphism of C*-algebras.
The statement concerning the sum of the Betti numbers follows observing that $\ker D$ is isomorphic to the space of harmonic forms of M and in turn, by the de Rham's Theorem (see [LM] for example), to the cohomology of M. The last statement follows because on irreducible manifolds of even dimension having nonnegative curvature operator, the odd Betti numbers vanish (see [Pet page 241]).

Remark 5.13. If a Riemannian manifold whose curvature operator is nonnegative, admits a non constant harmonic form, then the heat semigroup e^{-tD^2} generated by the Dirac Laplacian is nonergodic.

6 Dirichlet Forms and Noncommutative Geometry

In the previous chapter we observed that on Riemannian manifolds there exist noncommutative Dirichlet forms and associated Markovian semigroups reflecting geometrical or topological properties of the space.
In that setting, the powerful tools of differential and integral calculus, as well as tensor algebra, allow to construct topological invariants, as for example the de Rham's currents describing the de Rham homology of X in terms of curvatures. Recall, as a prototype, the case of a Riemann surfaces Σ, whose Euler characteristic may be computed as the integral of the Gauss curvature of a Riemannian metric on Σ (see Example 5.2).

In this chapter we collect some result to corroborate the idea that Dirichlet spaces, commutative or not, exibits a geometry. The idea is to exploit the first order differential calculus, constructed in Chapter 4, to develop tools of differential topology and cyclic cohomology. We limit the presentation to commutative C*-algebras.

6.1 Dirichlet Spaces as Banach Algebras

In this section (X, m) will denote a metrizable, compact, Hausdorff space, endowed with a positive Radon measure of full topological support. We will consider a regular Dirichlet form $(\mathcal{E}, \mathcal{F})$ on $L^2(X, m)$ and denote by $\mathcal{B}$ the associated Dirichlet algebra $C(X) \cap \mathcal{F}$ (see Proposition 4.7). The first hint that a Dirichlet structure on a topological space X may carriy topological information comes from the following result (see [Cip4]).

Proposition 6.1. *(The Dirichlet algebra is semisimple) The Dirichlet algebra $\mathcal{B} := C(X) \cap \mathcal{F}$, normed by*

$$\|a\| := \|a\|_\infty + \sqrt{\mathcal{E}[a]} \qquad a \in \mathcal{B},$$

is an involutive, semisimple Banach algebra. It is unital if and only if $\mathcal{E}[1] = 0$ (i.e. the Dirichlet space is conservative). As a consequence, the Dirichlet algebra $\mathcal{B}$ has a unique Banach algebra topology: any norm, making $\mathcal{B}$ a Banach algebra, is equivalent to the above one.

Proof. By representing $\mathcal{E}$ by a derivation, from the Leibniz rule one obtains for all $a, b \in \mathcal{B}$:

$$\sqrt{\mathcal{E}[ab]} \leq \sqrt{\mathcal{E}[a]} \cdot \|b\|_\infty + \|a\|_\infty \cdot \sqrt{\mathcal{E}[b]} \qquad a, b \in \mathcal{B} \tag{6.1}$$

so that

$$\begin{aligned} \|ab\| = \|ab\|_\infty + \sqrt{\mathcal{E}[ab]} &\leq \|a\|_\infty \|b\|_\infty + \sqrt{\mathcal{E}[a]} \cdot \|b\|_\infty + \|a\|_\infty \cdot \sqrt{\mathcal{E}[b]} \\ &\leq (|a\|_\infty + \sqrt{\mathcal{E}[a]})(|b\|_\infty + \sqrt{\mathcal{E}[b]}) \\ &= \|a\|\|b\| \,. \end{aligned}$$

Clearly $\|1\| = 1$ if and only if $\mathcal{E}[1] = 0$ so that we get that $\mathcal{B}$ is an involutive normed algebra which is complete since the Dirichlet form is closed. Denoting by $\rho(a) = \lim_{n \to \infty} \|a^n\|^{1/n}$ the spectral radius of an element a of $\mathcal{B}$, we get immediately that $\|a\|_\infty \leq \rho(a)$ since $\|a\|_\infty \leq \|a\|$. To prove the converse notice that from (6.1) one has $\sqrt{\mathcal{E}[a^n]} \leq n\|a\|_\infty^{n-1} \cdot \sqrt{\mathcal{E}[a]}$ for all $n \geq 1$. Then we have

$$\|a^n\|_\infty = \|a^n\|_\infty + \sqrt{\mathcal{E}[a^n]} \leq \|a\|_\infty^n + n\|a\|_\infty^{n-1} \cdot \sqrt{\mathcal{E}[a]}$$

which implies

$$\rho(a) \leq \lim_{n \to \infty} (\|a\|_\infty^n + n\|a\|_\infty^{n-1} \cdot \sqrt{\mathcal{E}[a]})^{1/n} = \|a\|_\infty \,.$$

Hence the spectral radius $\rho(a)$ of an element of the Dirichlet algebra $\mathcal{B}$ coincides with its uniform norm $\|a\|_\infty$, which is the spectral radius of the semisimple algebra $C(X)$. This proves that $\mathcal{B}$ is semisimple. The uniqueness of the norm topology of semisimple Banach algebras is a known result (see [Ric]).

The above result still holds true for locally compact spaces X. To carry over the proof one needs to consider the so called the *extended Dirichlet space* of $\mathcal{E}$ (see [FOT], [Cip4]).

A first consequence of the uniqueness above is the fact that *strongly local Dirichlet forms are determined by their Dirichlet algebras.* The result may be considered as a generalization, to Dirichlet spaces, of the fact that, on a differerentiable, paracompact manifold, Riemannan metrics giving rise to Dirichlet integrals having the same domain (the first order Sobolev space) are quasi-conformally equivalent.

Theorem 6.2. *(Quasi-conformal equivalence of Dirichlet forms having the same domain) Let $(\mathcal{E}_1, \mathcal{F}_1)$ and $(\mathcal{E}_2, \mathcal{F}_2)$ be two strongly local, regular Dirichlet spaces on $L^2(X, m)$ having common Dirichlet algebra $\mathcal{B} = C(X) \cap \mathcal{F}_1 = C(X) \cap \mathcal{F}_2$.*
Then $\mathcal{F}_1 = \mathcal{F}_2$ and the Dirichlet forms are quasi-equivalent in the sense that there exists $k > 0$ such that

$$\frac{1}{k}\mathcal{E}_1[a] \leq \mathcal{E}_2[a] \leq k\,\mathcal{E}_1[a] \qquad a \in \mathcal{F}_1 = \mathcal{F}_2\,. \tag{6.2}$$

Proof. By Corollary 6.2 we have, for some $k > 0$

$$\frac{1}{k}(\|a\|_\infty + \sqrt{\mathcal{E}_1[a]}) \leq \|a\|_\infty + \mathcal{E}_2[a] \leq k\,(\|a\|_\infty + \sqrt{\mathcal{E}_1[a]}) \qquad a \in \mathcal{F}_1 = \mathcal{F}_2\,. \tag{6.3}$$

Representing the forms by some derivations ∂_1 and ∂_2 and applying the chain rule, one obtains the identity

$$\mathcal{E}_i[\phi_\lambda(a)] + \mathcal{E}_i[\psi_\lambda(a)] = \mathcal{E}_i[a] \qquad a \in \mathcal{B}$$

where $\phi_\lambda(t) := \lambda^{-1}(1 - \sin(\lambda t))$, $\psi_\lambda(t) := \lambda^{-1}(1 - \cos(\lambda t))$ for all $t \in \mathbb{R}$ and $\lambda \neq 0$. Since $\lim_{\lambda\to 0} \|\phi_\lambda(a)\|_\infty = \lim_{\lambda\to 0} \|\psi_\lambda(a)\|_\infty = 0$ we observe that (6.2) follows from (6.3)

The second consequence we draw from the norm uniqueness result concerns the differential topology of a Dirichlet space. The fact that the spectral radius in the Dirichlet algebra coincides with the uniform norm has another important consequence: *an element $a \in \mathcal{B}$ is invertible in $\mathcal{B}$ if and only if it is invertible in $C(X)$*. This implies a generalization to regular Dirichlet spaces of a well known result of H. Whitney in differential topology according to which finite-dimensional, locally trivial, vector bundles over a smooth manifold admit a smooth structure. The interested reader may find the proof in [Cip4].

Theorem 6.3. *(K-Theory and vector bundles over regular Dirichlet spaces) Let $(\mathcal{E}, \mathcal{F})$ be a regular Dirichlet form on $L^2(X, m)$. Then we have*

i) the K-theory $K_*(\mathcal{B})$ of the Dirichlet algebra $\mathcal{B}$ coincides with the K-theory $K_*(C(X))$ of the algebra $C(X)$ and in turn with the topological K-theory $K^*(X)$ of the topological space X;

ii) every finite-dimensional locally trivial vector bundle E over X admits a Dirichlet structure, namely, a compatible vector bundle atlas whose transition matrices have entries in the Dirichlet algebra $\mathcal{B}$.

6.2 Fredholm Module of a Dirichlet Space

In this section we show how to use the differential calculus associated to Dirichlet form, to construct Fredholm modules, in the sense of Atiyah [At], on Dirichlet spaces. Notice that Fredholm modules and their summability properties lie at the core of Noncommutative Geometry of A. Connes [Co2].

The construction of Fredholm modules $(F, \mathcal{H})$ on compact topological spaces X is a generalization of the theory of elliptic differential operators on compact manifolds [At]. In its (*odd*) form, one requires that the elements f of the algebra of continuous functions $C(X)$ are represented as bounded operators $\pi(f)$ on a Hilbert space $\mathcal{H}$ on which there is a distinguished self-adjoint operator F of square one ($F^2 = 1$), the *symmetry*, such that the commutators $[F, \pi(f)]$ are compact operators.

A nice example of an (even) Fredholm module on an even dimensional oriented conformalmanifold$V$hasbeenconstructedbyA.Connes-D.Sullivan- N. Teleman in [CST] (see also [Co2 Chapter IV, 4-α Theorem 2]). The Fredholm module is uniquely determined by the oriented conformal structure, which can be characterized for example by the L^n-norm on 1-forms on V, where $n := \dim V$. In the particular case where V is an oriented Riemann surface, the conformal structure is uniquely determined by the Dirichlet integral

$$\mathcal{E}[a] = \int_V |\nabla a|^2 \, dm$$

on the algebra of continuous functions over V. We are going to see that the above construction can be carried out on general Dirichlet spaces.

Definition 6.4. (Phase operator of a Dirichlet form) Let us consider a regular Dirichlet form $(\mathcal{E}, \mathcal{F})$ on $L^2(X, m)$. Let $\partial : \mathcal{B} \to \mathcal{H}$ be the associated derivation, defined on the Dirichlet algebra $\mathcal{B} = C(X) \cap \mathcal{F}$ with values in the symmetric Hilbert module $\mathcal{H}$.
Let $P \in \mathrm{Proj}\,(\mathcal{H})$ be the projection onto the closure $\overline{\mathrm{Im}\partial}$ of the range of the derivation ∂,

$$P\mathcal{H} = \overline{\mathrm{Im}\partial} \tag{6.4}$$

We will call $F = P - P^{\perp} : \mathcal{H} \to \mathcal{H}$ the *phase operator* associated to the regular Dirichlet space.

Theorem 6.5. *(Fredholm module of a Dirichlet form) Let $(\mathcal{E}, \mathcal{F})$ be a regular Dirichlet form on $L^2(X, m)$, such that*

i) the spectrum $\{0 < \lambda_1 \leq \lambda_2 < \dots\}$ is discrete and bounded away from zero;

ii) the eigenfunctions $\{a_1, a_2, \dots\}$ are continuous;

iii) the Green function is finite (i.e. bounded).

Then $(F, \mathcal{H})$ is a Fredholm module over $C(X)$ in the sense of [At] and a densely 2-summable Fredholm module over $C(X)$ in the sense of [Co2 Chapter IV 1.γ Definition 8].

Proof. Clearly $F^* = F$, $F^2 = I$. Let us start by proving that $[F, a]$ is Hilbert-Schmidt for all real valued $a \in \mathcal{B}$. Since

$$[P, a] = PaP^{\perp} - P^{\perp}aP \tag{6.5}$$

and a is real valued, we have

$$|[P, a]|^2 = |PaP^{\perp}|^2 + |P^{\perp}aP|^2 \tag{6.6}$$

so that

$$\|[F, a]\|^2_{\mathcal{L}^2} = 4\|[P, a]\|^2_{\mathcal{L}^2} = 8\|P^{\perp}aP\|^2_{\mathcal{L}^2} \,. \tag{6.7}$$

Using the Leibniz rule for the derivation ∂, the fact that $P \circ \partial = \partial$ and $P^{\perp} \circ \partial = 0$, we have, for all $b \in \mathcal{B}$,

$$P^{\perp}aP(\partial b) = P^{\perp}(a\partial b) = P^{\perp}(\partial(ab) - (\partial a)b) = -P^{\perp}((\partial a)b) \tag{6.8}$$

so that

$$\|P^{\perp}aP(\partial b)\| = \|P^{\perp}((\partial a)b)\| \leq \|(\partial a)b\| \,. \tag{6.9}$$

Notice that, by assumption ii), the eigenfunctions belong to the Dirichlet algebra $\mathcal{B}$. Then, the vectors $\xi_k := \lambda_k^{-1/2}\partial a_k$, $k \geq 1$, form an orthonormal complete system in $P\mathcal{H}$. By (6.7) and (6.9) we have

$$\begin{aligned} \|[F, a]\|^2_{\mathcal{L}^2} &= 8\|P^{\perp}aP\|^2_{\mathcal{L}^2} = 8\sum_{k=1}^{\infty} \lambda_k^{-1}\|P^{\perp}aP(\partial a_k)\|^2_{\mathcal{H}} \leq 8\sum_{k=1}^{\infty} \lambda_k^{-1}\|a_k\partial a\|^2_{\mathcal{H}} \\ &= 8\sum_{k=1}^{\infty} \lambda_k^{-1} \int_X a_k^2 d\Gamma(a) = 8\int_K (\sum_{k=1}^{\infty} \lambda_k^{-1} a_k^2) d\Gamma(a) \\ &= 8\int_X G(x, x)\Gamma(a)(dx) \,, \end{aligned} \tag{6.10}$$

where $G(x,y) = \sum_{k=1}^{\infty} \lambda_k^{-1} a_k(x) a_k(y)$ is the *Green function or kernel* of the compact operator H_{D}^{-1} on $L^2(X,m)$ determined by $\mathcal{E}$. Since, by assumption, the Green function is bounded, we have

$$\|[F,a]\|^2_{\mathcal{L}^2} \le 8\Big(\sup_{x\in X} G(x,x)\Big)\mathcal{E}[a] < +\infty$$

for all $a \in \mathcal{B} \subset C(X)$. Since the form is regular, $\mathcal{B}$ is uniformly dense in $C(X)$, $[F,a]$ is norm continuous with respect to $a \in C(X)$ and the space of compact operators is norm closed, we have that $[F,a]$ is compact for all $a \in C(X)$.

Even if the boundedness assumption on the Green function restricts the application of the above construction to situations in which the spectral dimension is low, it applies, however, to the class of Dirichlet forms constructed by J. Kigami [Ki] on self-similar fractal spaces, associated to regular harmonic structures (see [CS4]).

Remark 6.6. The above result indicates a direct connection between the summability properties of the Fredholm module and two of the main objects of potential theory, namely, the Dirichlet form $\mathcal{E}$ and the Green function G.

An immediate consequence of the above construction is the following index theorem [At], [Co2 Chapter IV Proposition 2].

Corollary 6.7. *Let $(\mathcal{H}_q, F_q)$ be the Fredholm module over $M_q(C(X)) = C(X) \otimes M_q(\mathbb{C})$ given by*

$$\mathcal{H}_q := \mathcal{H} \otimes \mathbb{C}^q\,, \qquad F_q := F \otimes 1\,, \qquad \pi_q := \pi \otimes \mathrm{id}\,, \qquad q \in \mathbb{N}^*\,.$$

Define, on the Hilbert space $\mathcal{H}_q$, the projection operator

$$E_q := \frac{1 + F_q}{2}\,.$$

Then for every invertible element $u \in \mathrm{GL}_q(A)$ in $M_q(A)$, the operator

$$E_q \pi_q(u) E_q : E_q\mathcal{H}_q \longrightarrow E_q\mathcal{H}_q$$

is a a Fredholm operator. Its index gives rise to an additive map

$$\phi : \mathcal{K}_1(A) \longrightarrow \mathbb{Z} \qquad \phi([u]) := \mathrm{Index}(E_q\pi_q(u)E_q)$$

on the K-theory group $\mathcal{K}_1(C(X)) = K^1(X)$ of $C(X)$.

Notice that, the Fredholm modules $(\mathcal{H}_q, F_q)$ are those associated by Theorem 6.5 to the family of Dirichlet forms on $M_q(C(X))$ determined by $\mathcal{E}$ (see Definition 4.1).

We conclude this section noticing that the Fredholm module $(\mathcal{H}, F)$ may determine topological invariants of X (see [Co2 Chapter IV]).

In fact, as the *Steenrod K-homology* $K_*(X)$ of the compact space X is isomorphic to the *K-homology* of $K^*(C(X))$ of the algebra $C(X)$, a specific element of it is determined by the equivalence class of the Fredholm module $(\mathcal{H}, F)$. Moreover, the *Chern character*, $\mathrm{ch}_*(\mathcal{H}, F)$, of the finitely summable Fredholm module $(\mathcal{H}, F)$ is the *periodic cyclic cohomology* class of the following *cyclic cocycles* for $n \geq 2$,

$$A \otimes \cdots \otimes A \ni (a^0, a^1, \ldots, a^n) \mapsto \lambda_n \mathrm{Tr}'(a^0[F, a^1] \ldots [F, a^n]),$$

where $\lambda_n := \sqrt{2i}(-1)^{\frac{n(n+1)}{2}} \Gamma(\frac{n}{2} + 1)$ and $\mathrm{Tr}'(B) := \frac{1}{2}\mathrm{Tr}(F(FB + BF))$.

7 Appendix

7.1 Topologies on Operator Algebras

In this subsection we briefly recall some basic definitions concerning operator algebras and collect the relationships among their topologies.

A C*-algebra A is an involutive Banach algebra in which the norm and the involution are related by

$$\|a^* a\| = \|a\|^2 \qquad a \in A.$$

The algebra $C_0(X)$ of continuous functions, vanishing at infinity on a locally compact Hausdorff space X, endowed with the uniform norm and the involution given by the pointwise complex conjugation, is a commutative C*-algebra. A celebrated theorem of I. M. Gelfand (see [Dix1]) ensures that all commutative C*-algebras are of this form for a suitable space X (to be identified with the space of all closed maximal ideals of A).
The simplest examples of noncommutative C*-algebras are the full matrix algebras $M_n(\mathbb{C})$, $n \geq 2$. Finite dimensional C*-algebras are direct sums of full matrix algebras. Examples of infinite dimensional, noncommutative C*-algebras are the algebra $k(\mathcal{H})$ of all compact operators on an infinite dimensional Hilbert space $\mathcal{H}$ and the algebra $B(\mathcal{H})$ of all bounded operators. In all these cases the norm is the usual one and the involution is given by the operation of taking the operator adjoint. By another fundamental theorem of I. M. Gelfand (see [Dix1]), any C*-algebra A may be represented as a norm closed C*-subalgebra of $B(\mathcal{H})$. In particular this implies that the norm in a C*-algebra is uniquely determined by the algebraic structure.

Among the C*-algebras, the von Neumann ones $\mathfrak{M}$ may be defined as those which, as Banach spaces, admit preduals in the sense that $\mathfrak{M} = (\mathfrak{M}_*)^*$ for some Banach space $\mathfrak{M}_*$.

The algebra $L^\infty(X, m)$ of essentially bounded measurable functions on a measured space (X, m) is a commutative von Neumann algebra and all commutative von Neumann algebras arise in this way.
The algebra $B(\mathcal{H})$ of all bounded operators on a Hilbert space $\mathcal{H}$ is a von Neumann algebra (the type I_∞ factor) being the dual of the Banach space of all trace class operators on $\mathcal{H}$.
By a fundamental theorem of J. von Neumann (see [Dix2]), for any given selfadjoint subset $S \subset B(\mathcal{H})$ the set

$$S' := \{x \in B(\mathcal{H}) : xy = yx\,, \quad y \in S\}$$

of all bounded operators on $\mathcal{H}$ which commute with all operators of S, is a von Neumann subalgebra of $B(\mathcal{H})$ and moreover any von Neumann algebra $\mathfrak{M} \subseteq B(\mathcal{H})$ coincides with its own *double commutant*

$$\mathfrak{M} = \mathfrak{M}''\,.$$

Von Neumann algebras $\mathfrak{M} \subseteq B(\mathcal{H})$ whose intersection with its own commutant $\mathfrak{M}'$, reduces to the one dimensional algebra of scalar multiples of the identity operator

$$\mathfrak{M} \cap \mathfrak{M}' = \mathbb{C} \cdot 1_{\mathcal{H}}\,,$$

are called *factors* and may be considered in a precise sense as building blocks for general von Neumann algebras.

On a C*-algebra A, one may consider the *norm topology*, also referred as the *uniform topology* and denoted by τ_u, as well as the *weak topology* $\sigma(A\,, A^*)$, induced by its dual space A^*.

As von Neumann algebras $\mathfrak{M}$ are characterized as C*-algebras which as Banach spaces, admit preduals $\mathfrak{M}_*$ (in the sense that $\mathfrak{M} = (\mathfrak{M}_*)^*$) beside the two topologies above, they carry the *weak*-topology* $\sigma(\mathfrak{M}\,, \mathfrak{M}_*)$ too.

Let $\mathfrak{M}$ act on the Hilbert space $\mathcal{H}$ so that $\mathfrak{M} \subseteq B(\mathcal{H})$. Other useful topologies on $\mathfrak{M}$, are then the following:

- the *strong topology* is the locally convex topology defined by the family of seminorms
  $$\mathfrak{M} \ni a \to \|a\xi\|\,,$$
  parametrized by the vectors $\xi \in \mathcal{H}$;
- the *strong* topology* is the locally convex topology defined by the family of seminorms
  $$\mathfrak{M} \ni a \to \|a\xi\| + \|a^*\xi\|\,,$$
  parameterized by the vectors $\xi \in \mathcal{H}$;
- *σ-strong topology* is the locally convex topology defined by the family of seminorms

$$\mathfrak{M} \ni a \to \Big(\sum_n \|a\xi_n\|^2\Big)^{1/2},$$

parametrized by sequences $\{\xi_n\} \subset \mathcal{H}$ such that $\sum_n \|\xi\|^2 < +\infty$;

- *σ-strong* topology* is the locally convex topology defined by the family of seminorms

$$\mathfrak{M} \ni a \to \Big(\sum_n \|a\xi_n\|^2 + \sum_n \|a^*\xi_n\|^2\Big)^{1/2},$$

parametrized by sequences $\{\xi_n\} \subset \mathcal{H}$ such that $\sum_n \|\xi\|^2 < +\infty$;

- *σ-weak topology* is the locally convex topology defined by the family of seminorms

$$\mathfrak{M} \ni a \to \sum_n |(\xi_n|a\eta_n)|,$$

parametrized by sequences $\{\xi_n\}, \{\eta_n\} \subset \mathcal{H}$ such that $\sum_n \|\xi\|^2 < +\infty$, $\sum_n \|\eta\|^2 < +\infty$.

The σ-weak topology coincides with the weak*-topology $\sigma(\mathfrak{M}, \mathfrak{M}_*)$ (see [BR1 Proposition 2.4.3]), so that bounded sets are relatively compact by the Banach-Alaoglu Theorem. The relation among the various topologies are subsummed as follows:

$$\begin{array}{ccccccc} \text{uniform} < & \sigma\text{-strong}^* & < & \sigma\text{-strong} & < & \sigma\text{-weak} \\ & \wedge & & \wedge & & \wedge \\ & \text{strong}^* & < & \text{strong} & < & \text{weak}^* \end{array}$$

Here "<" means "finer than", and if $\mathcal{H}$ is infinite dimensional, then "<" means "strictly finer then". Moreover, on bounded sets, the σ-strong* topology coincides with the strong* topology (see [T2 Chapter II Lemma 2.5]) and on the set of normal operators, the latter coincides with the strong topology (see [T2 Chapter Proposition 4.1]). Finally, the positive cone $\mathfrak{M}_+$ is σ-weakly closed, being the polar of the positive cone $\mathfrak{M}_{*+}$ of the predual space

$$a \in \mathfrak{M}_+ \qquad \Leftrightarrow \qquad \langle \eta\,|a\rangle \geq 0 \qquad \forall\, \eta \in \mathfrak{M}_{*+}.$$

7.2 One Parameter Continuous Groups and Semigroups

A *one-parameter group* $\mathbf{\Phi} = \{\Phi_t : t \in \mathbb{R}\}$ on a Banach space A, is a family of bounded linear maps $\Phi_t : A \to A$, indexed by a real parameter $t \in \mathbb{R}$, such that

$$\Phi_t \circ \Phi_s = \Phi_{t+s} \qquad \text{and} \qquad \Phi_0 = I_A\,, \qquad s, t \in \mathbb{R}.$$

A *one-parameter semigroup* $\mathbf{\Phi} = \{\Phi_t : t \in \mathbb{R}\}$ on a Banach space A, is a family of linear maps $\Phi_t : A \to A$, indexed by a positive real parameter $t \geq 0$, such that

$$\Phi_t \circ \Phi_s = \Phi_{t+s} \qquad \text{and} \qquad \Phi_0 = I_A\,, \qquad s, t \geq 0\,.$$

In case $\|\Phi_t(a)\| = \|a\|$, for all $a \in A$ and $t \in \mathbb{R}$ or $t \geq 0$, $\mathbf{\Phi}$ ia called a group or semigroup of *isometries*. If, however, $\|\Phi_t(a)\| \leq \|a\|$, for all $a \in A$ and $t \in \mathbb{R}$ or $t \geq 0$, $\mathbf{\Phi}$ is called a *contraction* group or semigroup.

A one-parameter group or semigroup on a C*-algebra A is said to be

- *norm or uniformly continuous* if

$$\lim_{t\to 0} \|\Phi_t - I_A\|_{B(A)} = 0\,;$$

- *strongly continuous* if

$$\lim_{t\to 0} \|\Phi_t(a) - a\|_A = 0 \qquad \forall\, a \in A\,;$$

- *weakly continuous* if

$$\lim_{t\to 0} \langle \eta \,|\, \Phi_t(a) - a\rangle = 0 \qquad \forall a \in A\,, \forall\, \eta \in A^*\,.$$

A one-parameter group or semigroup on a von Neumann algebra $\mathfrak{M}$ is said

- *weakly* continuous* if the maps $\Phi_t : \mathfrak{M} \to \mathfrak{M}$, are weakly* continuous and

$$\lim_{t\to 0} \langle \eta \,|\, \Phi_t(a) - a\rangle = 0 \qquad \forall a \in \mathfrak{M}\,, \forall\, \eta \in \mathfrak{M}_*\,.$$

By a general result, see [BR1 Corollary 3.1.8, Proposition 3.1.3], strong and weak continuity of semigroups are equivalent properties, and both of them imply the bound

$$\|\Phi_t\| \leq M \cdot e^{\beta t} \qquad t \geq 0\,.$$

for suitable constants $M > 0$ and $\beta \in \mathbb{R}$.

Strongly continuous semigroups are also called C_0-semigroups, weakly* continuous semigroups are also called C_0^* or $\sigma(\mathfrak{M}, \mathfrak{M}_*)$-continuous semigroups and weakly continuous semigroups are also called $\sigma(A, A^*)$-continuous semigroups.

The *generator* of a strongly (resp. weakly) continuous semigroup $\{\Phi_t : t \geq 0\}$ on a C*-algebra A, is the operator $(L\,, D(L))$ on A defined as follows: an element $a \in A$ is in the domain $D(L)$ if the limit

$$\lim_{t\to 0} \frac{a - \Phi_t(a)}{t}$$

exists in the strong (resp. weak) topology. The action $L(a)$ of the operator L on the element a of $D(L)$ is defined as the limit above. The *generator* of a weakly* continuous semigroup on a von Neumann algebra $\mathfrak{M}$ is defined similarly, the only difference being that the limit above is understood to exists with respect to the weak* topology.

It can be verified that the generator $(L\,, D(L))$ of a strongly (resp. weakly) continuous semigroup is a norm (resp. weakly) densely defined operator and a norm-norm (resp. $\sigma(A, A^*)$-$\sigma(A, A^*)$) closed operator on a C*-algebra A. Similarly, the generator of a weakly* continuous semigroup, is a weakly* densely defined $\sigma(\mathfrak{M}, \mathfrak{M}_*)$-$\sigma(\mathfrak{M}, \mathfrak{M}_*)$ closed operator on the von Neumann algebra $\mathfrak{M}$. See [BR1 Proposition 3.1.6]. Moreover, the semigroup is uniformly continuous if and only if its generator is a bounded operator. In this case, one has the representation

$$\Phi_t = \sum_{n=0}^{\infty} \frac{t^n}{n!} L^n \qquad t \geq 0\,,$$

where the exponential series converges in the norm of the Banach space of all bounded operators on A.

Theorem 7.1. *(Stinespring Theorem [Sti]). A linear map $\Phi : A \to B(h)$, from a unital C*-algebra A, into the C*-algebra of all bounded operators on a Hilbert space $\mathcal{H}$, is completely positive if and only if it has the form*

$$\Phi(a) = V^* \pi(a) V \qquad a \in A\,, \tag{7.1}$$

for some representation $\pi : A \to B(\mathcal{K})$ and some bounded linear operator $V : \mathcal{H} \to \mathcal{K}$. If A and $\mathcal{H}$ are separable, $\mathcal{K}$ can be taken to be separable. If A is a von Neumann algebra and Φ is normal, then π can be taken to be normal.

7.3 Analytic Elements

Let $\alpha{:=}\{\alpha_t : t \in \mathbb{R}\}$ be a continuous group of isometries of a C*-algebra A. An element $a \in A$ is said to be α-*analytic* if there exists a strip $I_\lambda := \{z \in \mathbb{C} : |\mathrm{Im} z| < \lambda\}$ $(\lambda > 0)$ and an analytic function $f : I_\lambda \to A$ such that

$$f(t) = \alpha_t(a) \qquad t \in \mathbb{R}\,.$$

It may be shown, see [BR1 Chapter 3.1], that an element $a \in A$ is α-analytic if and only if it is analytic for the generator $(L, D(L))$, in the sense that $a \in D(L^n)$ for all $n \geq 1$ and

$$\sum_{n=0}^{\infty} \frac{t^n}{n!} \|L^n(a)\| < +\infty \qquad t \geq 0\,.$$

The set of entire analytic elements A_α is a norm dense, invariant *-subalgebra of A, in the case of a strongly continuous group of isometries of a C*-algebra

A and, a $\sigma(\mathfrak{M}, \mathfrak{M}_*)$-dense, invariant *-subalgebra of $\mathfrak{M}$, in the case of a $\sigma(\mathfrak{M}, \mathfrak{M}_*)$-continuous group of isometries of a von Neumann algebra $\mathfrak{M}$.
In both cases, these extensions form a group of automorphisms of the algebra A_α, denoted by $\{\alpha_z : z \in \mathbb{C}\}$ and indexed by complex numbers.
In particular, if $\{\sigma_t^\omega : t \in \mathbb{R}\}$ is the modular automorphisms group of a von Neumann algebra $\mathfrak{M}$, associated to a normal state ω, and $x \in \mathfrak{M}_\sigma$ is an entire analytic element, one has the identity

$$\sigma_z^\omega(x) = \Delta_\omega^z \, x \Delta_\omega^{-z}\,, \qquad x \in \mathfrak{M}_\alpha \quad z \in \mathbb{C}\,,$$

where Δ_ω denotes the modular operator of ω. Both sides of the above identity are understood as bounded quadratic forms

$$(\xi|\, \sigma_z^\omega(x)\eta) = (\Delta_\omega^{-\overline{z}}\xi|\, x\Delta_\omega^{-z}\eta)\,, \qquad x \in \mathfrak{M}_\alpha \quad z \in \mathbb{C}\,,$$

on the dense subspace of $\mathcal{H}$ of entire analytic elements of the unitary group $\mathbb{R} \ni t \to \Delta_\omega^{it}$ on $\mathcal{H}$. In fact, for fixed $x \in \mathfrak{M}_\alpha$, both sides are entire analytic functions, coinciding for real z. In this way, one may also show that

$$\sigma_{t+is}^\omega(x) = \sigma_t^\omega(\sigma_{is}^\omega(x)) = \sigma_{is}^\omega(\sigma_t^\omega(x)) \qquad t + is \in I_\lambda\,,$$

for all $x \in \mathfrak{M}$ such that the map $\mathbb{R} \ni t \to \sigma_t^\omega(x) \in \mathfrak{M}$ admits an analytic extension to a domain containing the strip I_λ.

8 List of Examples

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Applications of Quantum Stochastic Processes in Quantum Optics

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Abstract These lecture notes provide an introduction to quantum filtering and its applications in quantum optics. We start with a brief introduction to quantum probability, focusing on the spectral theorem. Then we introduce the conditional expectation and quantum stochastic calculus. In the last part of the notes we discuss the filtering problem.

1 Quantum Probability

In quantum theory observables are represented by selfadjoint operators on a Hilbert space. When an observable is being measured, we randomly obtain a measurement result. That is, the result of the measurement is given by a random variable on some classical probability space. In this section we will investigate how we can pass from a selfadjoint operator to a classical random variable. Along the way we will setup a generalised theory of probability, called *noncommutative* or *quantum probability*, that is rich enough to contain quantum mechanics.

1.1 The Spectral Theorem

In these notes we take as a part of its definition that a Hilbert space is separable. The following theorem shows that a self-adjoint operator S on a

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Hilbert space can be identified with a random variable h on a measure space (Ω, Σ, μ). It is the heart of quantum mechanics.

Theorem 1.1. (Spectral Theorem) *Let $\mathcal{H}$ be a Hilbert space and let $S : \mathcal{H} \to \mathcal{H}$ be a bounded selfadjoint operator. Then there exist a measure space (Ω, Σ, μ), a unitary $U : \mathcal{H} \to L^2(\Omega, \Sigma, \mu)$ and a bounded real valued Σ-measurable function h on Ω such that*

$$S = U^* M_h U,$$

where the multiplication operator $M_h : L^2(\Omega, \Sigma, \mu) \to L^2(\Omega, \Sigma, \mu)$ *is given by*

$$(M_h f)(\omega) = h(\omega) f(\omega),$$

for all $\omega \in \Omega$.

Proof. See Reed and Simon volume I [23].

Suppose that the dimension n of $\mathcal{H}$ is finite. Since S is self-adjoint, we can always find an orthonormal basis $(e_1, \ldots, e_n)$ such that S is diagonal, i.e. $S = diag(h_1, \ldots, h_n)$. Note that the real numbers h_i and h_j are not necessarily different numbers, some eigenvalues might be degenerate. Let us define $\Omega = \{1, \ldots, n\}$. Moreover, define $h : \Omega \to \mathbb{R}$ by $h(\omega) = h_\omega$ for all $\omega \in \Omega$. Let $\Sigma = \mathcal{P}(\Omega)$ be the sigma-algebra of all subsets of Ω. We take for μ simply the counting measure. Define $U : \mathcal{H} \to L^2(\Omega, \Sigma, \mu)$ by linear extension of the map

$$U e_\omega = \chi_{\{\omega\}}, \qquad \omega \in \Omega,$$

where $\chi_{\{\omega\}}(\omega')$ is 1 if $\omega' = \omega$ and 0 otherwise. Note that U is unitary and that $S = U^* M_h U$. That means, we have now proved the spectral theorem in finite dimension. We now also see that the main idea of the theorem is to diagonalise an operator. The spectral theorem gives a precize meaning to the notion of diagonalisation also in the infinite dimensional case.

Let $\mathfrak{x} : \mathbb{R} \to \mathbb{R}$ be the map given by $\mathfrak{x}(x) = x$ and let $p = \sum_{m=0}^{l} \alpha_m \mathfrak{x}^m$ be a polynomial. Suppose S is a self-adjoint operator on a Hilbert space $\mathcal{H}$. The spectral theorem provides a measure space (Ω, Σ, μ), a unitary $U : \mathcal{H} \to L^2(\Omega, \Sigma, \mu)$ and a Σ-measurable real valued function h such that $S = U^* M_h U$. It is easy to see that

$$\sum_{m=0}^{l} \alpha_m S^m = U^* M_{p \circ h} U. \tag{1.1}$$

This shows that we can define the polynomial p evaluated at S, denoted $p(S)$, in two equivalent ways, i.e. either by the left hand side or the right hand of Equation (1.1). The *spectrum of an operator* $T : \mathcal{H} \to \mathcal{H}$ is defined as the set

$$\sigma(T) = \big\{ \lambda \in \mathbb{C};\ T - \lambda I \text{ does not have a bounded inverse} \big\}. \tag{1.2}$$

In finite dimensions the spectrum of an operator is just the set of its eigenvalues. The spectrum of a bounded operator T is compact. For the operator S, diagonalised by the spectral theorem as $S = U^* M_h U$, it is not hard to see that $h(\omega) \in \sigma(S)$ for μ-almost all $\omega \in \Omega$ and that $\sigma(S)$ is the smallest compact subset of $\mathbb{C}$ with this property. We denote the range of h by $\mathrm{Ran}(h)$ and are guided by the idea $\mathrm{Ran}(h) = \sigma(S)$.

Definition 1.2. (Functional calculus) Let $S : \mathcal{H} \to \mathcal{H}$ be a bounded, self-adjoint operator and let $j : \sigma(S) \to \mathbb{C}$ be a bounded Borel measurable function. The spectral theorem provides a measure space (Ω, Σ, μ), a unitary $U : \mathcal{H} \to L^2(\Omega, \Sigma, \mu)$ and a Σ-measurable real valued function h such that $S = U^* M_h U$. Define the bounded linear operator $j(S) : \mathcal{H} \to \mathcal{H}$ by

$$j(S) = U^* M_{j \circ h} U.$$

For polynomials p it is clear from Equation (1.1) that this definition does not depend on which 'diagonalisation' of S we choose (the spectral theorem shows existence, not uniqueness of (Ω, Σ, μ), U and h). With polynomials we can uniformly approximate continuous functions arbitrarily well ($\sigma(S)$ is compact) and with continuous functions we can approximate bounded Borel measurable functions arbitrarily well pointwise. In this way it follows that the definition of $j(S)$ does not depend on the diagonalisation for all bounded measurable functions j. See Reed and Simon [23] for further information.

Suppose the bounded self-adjoint operator S represents an observable of some physical system. Suppose the system is in a state given by a vector v of unit length in the Hilbert space $\mathcal{H}$. We now discuss some of the basics of quantum mechanics in this setting. When it is measured, the observable S can only take values in the spectrum $\sigma(S)$. Let B be a Borel subset of $\sigma(S)$. The set B corresponds to the event 'S takes a value in B'. The probability of this event is given by

$$\mathbf{P}\big(S \text{ takes a value in } B\big) = \big\langle v, \chi_B(S) v \big\rangle,$$

where χ_B is the characteristic function of the Borel set B, i.e. $\chi_B(s) = 1$ if $s \in B$ and zero otherwise. The spectral theorem provides a measure space (Ω, Σ, μ), a unitary $U : \mathcal{H} \to L^2(\Omega, \Sigma, \mu)$ and a Σ-measurable real valued function h such that $S = U^* M_h U$. By definition $\chi_B(S) = U^* M_{\chi_B \circ h} U = U^* M_{\chi_{h^{-1}(B)}} U$. Note that since h is measurable, the set $h^{-1}(B)$ is an element of Σ. In fact, we can assign probabilities to all $Q \in \Sigma$ by

$$\mathbf{P}(Q) = \big\langle v, U^* M_{\chi_Q} U v \big\rangle.$$

Summarizing, we can represent S as a random variable h on the probability space $(\Omega, \Sigma, \mathbf{P})$. The spectral theorem transforms quantum mechanics to classical probability theory.

We will now extend the spectral theorem so that we can simultaneously diagonalise a whole class of commuting bounded normal operators. An operator

$S: \mathcal{H} \to \mathcal{H}$ is called *normal* if it commutes with its adjoint, i.e. $SS^* = S^*S$. Before stating the theorem, we need to introduce some mathematical objects. Let $\mathcal{H}$ be a Hilbert space. Denote by $\mathcal{B}(\mathcal{H})$ the algebra of all bounded operators on $\mathcal{H}$ and let $\mathcal{S}$ be a subset of $\mathcal{B}(\mathcal{H})$. We call the set

$$\mathcal{S}' = \big\{R \in \mathcal{B}(\mathcal{H});\ RS = SR\ \forall S \in \mathcal{S}\big\},$$

the *commutant* of $\mathcal{S}$ in $\mathcal{B}(\mathcal{H})$. A *von Neumann algebra* $\mathcal{A}$ on $\mathcal{H}$ is a *-subalgebra of $\mathcal{B}(\mathcal{H})$ that equals its double commutant, i.e. $\mathcal{A}'' = \mathcal{A}$. It is a consequence of von Neumann's double commutant theorem (see e.g. [17]) that a von Neumann algebra is closed in the weak operator topology. It immediately follows from $\mathcal{A}'' = \mathcal{A}$ that the identity $I \in \mathcal{B}(\mathcal{H})$ is an element of the von Neumann algebra $\mathcal{A}$. A *state* is a linear map $\rho: \mathcal{A} \to \mathbb{C}$ such that ρ is *positive* in the sense that $\rho(S^*S) \geq 0$ for all $S \in \mathcal{A}$, and such that ρ is normalised $\rho(I) = 1$. A state is called *normal* if it is weak operator continuous on the unit ball of $\mathcal{A}$.

Theorem 1.3. (Spectral Theorem) *Let $\mathcal{C}$ be a commutative von Neumann algebra and let ρ be a normal state on $\mathcal{C}$. There exist a measure space (Ω, Σ, μ) and a *-isomorphism ι from $\mathcal{C}$ to $L^\infty(\Omega, \Sigma, \mu)$, the space of all bounded measurable functions on Ω. Furthermore, there exists a probability measure $\mathbf{P}$ on Σ such that*

$$\rho(C) = \int_\Omega \iota(C)(\omega)\mathbf{P}(d\omega),$$

for all $C \in \mathcal{C}$.

Theorem 1.3 can be obtained from Theorem 1.1 by using that under mild conditions (which are fulfilled since our von Neumann algebra acts on a separable Hilbert space) a commutative von Neumann algebra $\mathcal{C}$ is generated by a single bounded selfadjoint operator S [27].

Given a probability space $(\Omega, \Sigma, \mathbf{P})$, we can study the commutative von Neumann algebra $\mathcal{C} := L^\infty(\Omega, \Sigma, \mathbf{P})$, acting on the Hilbert space $L^2(\Omega, \Sigma, \mathbf{P})$ by pointwise multiplication equipped with the normal state ρ given by expectation with respect to the measure $\mathbf{P}$. The pair $(\mathcal{C}, \rho)$ faithfully encodes the probability space $(\Omega, \Sigma, \mathbf{P})$ [19]. Indeed, the sigma-algebra Σ can be reconstructed (up to equivalence of sets with $\mathbf{P}$-null symmetric difference, a point on which we will not dwell here) as the set of projections in $\mathcal{C}$, i.e. the set of characteristic functions of sets in Σ, and the probability measure is given by acting with the state ρ on this set of projections. We conclude that studying commutative von Neumann algebras equipped with normal states is the same as studying probability spaces. This motivates the following definition.

Definition 1.4. A *non-commutative* or *quantum* probability space is a pair $(\mathcal{A}, \rho)$ where $\mathcal{A}$ is a von Neumann algebra on some Hilbert space $\mathcal{H}$ and ρ is a normal state.

Note that we do not require the state ρ to be faithful. We use quantum probability spaces to model experiments involving quantum mechanics. The first thing to do is to set a model, say $(\mathcal{A}, \rho)$. It is a feature of quantum mechanics that in one single realization of an experiment only commuting observables can be measured. That is, the experiment is determined by a commutative von Neumann subalgebra $\mathcal{C}$ of $\mathcal{A}$. The pair $(\mathcal{C}, \rho|_{\mathcal{C}})$ is equivalent to a classical probability model $(\Omega, \Sigma, \mathbf{P})$ via the spectral theorem. The operators in $\mathcal{C}$ are mapped to random variables $\iota(C)$ on $(\Omega, \Sigma, \mathbf{P})$ and represent the stochastic measurement results of the experiment. The pair $(\mathcal{A}, \rho)$ describes the collection of all the experiments (i.e. the collection of commutative subalgebras of $\mathcal{A}$) and their statistics in different realizations of the experiment in a concise way.

1.2 Unbounded Operators

Up to now we have only considered bounded operators. In general, however, an observable is given by a selfadjoint, not necessarily bounded, operator on some dense domain of the Hilbert space $\mathcal{H}$. In these notes we will not put emphasis on the problems one encounters when dealing with unbounded operators. When adding or multiplying unbounded operators, it is important to keep track of the domains involved. In this subsection we discuss some techniques for relating an unbounded operator to a von Neumann algebra.

Definition 1.5. Let T be a densely defined linear operator on some Hilbert space $\mathcal{H}$. Denote the domain of T by $\mathrm{Dom}(T)$. The operator T is called *closed* if its graph $\{(x, Tx);\ x \in \mathrm{Dom}(T)\}$ is a closed subset of $\mathcal{H} \times \mathcal{H}$. Define $\mathrm{Dom}(T^*)$ as the set of $x \in \mathcal{H}$ for which there is a $y \in \mathcal{H}$ such that

$$\langle Tz, x\rangle = \langle z, y\rangle, \qquad \forall z \in \mathrm{Dom}(T).$$

For each such $x \in \mathrm{Dom}(T^*)$, we define $T^*x = y$. We call T^* the *adjoint* of T. The operator T is called *symmetric* if $T \subset T^*$, i.e. $\mathrm{Dom}(T) \subset \mathrm{Dom}(T^*)$ and $Tz = T^*z$ for all $z \in \mathrm{Dom}(T)$. Equivalently, T is symmetric if and only if $\langle Tz, y\rangle = \langle z, Ty\rangle$ for all $z, y \in$ Dom(T). The operator T is called *selfadjoint* if $T = T^*$, i.e. if T is symmetric and $\mathrm{Dom}(T) = \mathrm{Dom}(T^*)$.

Theorem 1.6. (basic criterion for selfadjointness) *Let T be a symmetric operator on a Hilbert space $\mathcal{H}$. The following three statements are equivalent*

1. *T is selfadjoint.*
2. *T is closed, $Ker(T^* + iI) = \{0\}$ and $Ker(T^* - iI) = \{0\}$.*
3. *$Ran(T + iI) = \mathcal{H}$ and $Ran(T - iI) = \mathcal{H}$.*

The proof of the above theorem can be found in [23]. Theorem 1.6 shows that $T + iI$ is an injective operator with range $\mathcal{H}$. This means $(T + iI)^{-1}$ is well-defined with domain $\mathcal{H}$. Moreover, since $T + iI$ is closed, $(T + iI)^{-1}$ is also closed. The closed graph theorem (see [23]) then asserts that $(T + iI)^{-1}$

is bounded. A similar argument shows that $T - iI$ is invertible and that $(T - iI)^{-1}$ is bounded. Let λ be in the complement of the spectrum of T (i.e. $T - \lambda I$ has a bounded inverse). Define the *resolvent* of T at λ as $R_\lambda(T) = (T - \lambda I)^{-1}$ (See also Section 3.2 of the lectures by N. Privault). Note that we have the following identity

$$\begin{aligned} R_\lambda(T) - R_\mu(T) &= R_\lambda(T)(T - \mu I)R_\mu(T) - R_\lambda(T)(T - \lambda I)R_\mu(T) \\ &= (\lambda - \mu)R_\lambda(T)R_\mu(T). \end{aligned}$$

Adding this same identity with the roles of μ and λ interchanged shows that $R_\lambda(T)$ and $R_\mu(T)$ commute. Therefore $(T + iI)^{-1}$ and $(T - iI)^{-1}$ commute. The equality

$$\big\langle (T-iI)x,\ (T+iI)^{-1}(T+iI)y\big\rangle = \big\langle (T-iI)^{-1}(T-iI)x,\ (T+iI)y\big\rangle, \quad x, y \in \mathcal{H},$$

and the fact that $\mathrm{Ran}(T \pm iI) = \mathcal{H}$ shows that $(T + iI)^{-1*} = (T - iI)^{-1}$. Therefore $(T + iI)^{-1}$ is normal and therefore the von Neumann algebra generated by $(T + iI)^{-1}$ is commutative.

Definition 1.7. Let $\mathcal{A}$ be a von Neumann algebra on some Hilbert space $\mathcal{H}$. Let T be a selfadjoint operator on a dense domain of $\mathcal{H}$. T is said to be *affiliated* to $\mathcal{A}$ if $(T - iI)^{-1}$ is an element of $\mathcal{A}$. We denote this as $T\eta\mathcal{A}$.

Note that T is affiliated to the commutative von Neumann algebra generated by $(T + iI)^{-1}$. Suppose that $\mathcal{C}$ is a commutative von Neumann algebra on some Hilbert space $\mathcal{H}$ and suppose that T is a selfadjoint operator affiliated to $\mathcal{C}$. Let ρ be a normal state on $\mathcal{C}$. The spectral theorem (Theorem 1.3) provides a measure space (Ω, Σ, μ), a *-isomorphism from $\mathcal{C} \to L^\infty(\Omega, \Sigma, \mu)$ and a probability measure $\mathbf{P}$ on Σ such that $\rho(C) = \mathbb{E}_{\mathbf{P}}(\iota(C))$ for all $C \in \mathcal{C}$. That is, ι allows us to represent the elements in $\mathcal{C}$ as classical random variables on the probability space $(\Omega, \Sigma, \mathbf{P})$. Since $(T + iI)^{-1}$ is an element of $\mathcal{C}$ we can now also represent T on $(\Omega, \Sigma, \mathbb{P})$ by

$$\iota(T)(\omega) = \frac{1}{\iota\big((T + iI)^{-1}\big)(\omega)} - i, \qquad \omega \in \Omega. \tag{1.3}$$

Note that $\iota(T)$ is not bounded. Nevertheless, we have succeeded in representing T as a classical random variable on $(\Omega, \Sigma, \mathbf{P})$.

The following theorem shows there is a one-one correspondence between strongly continuous one-parameter groups of unitaries and selfadjoint operators. The theorem is a classic result and can be found e.g. in [17] or [23].

Theorem 1.8. (Stone's theorem) *Let $\mathcal{A}$ be a von Neumann algebra on some Hilbert space $\mathcal{H}$ and let $\{U_t\}_{t\in\mathbb{R}} \subset \mathcal{A}$ be a group of unitaries that is continuous in the strong operator topology. There exists a unique selfadjoint operator S affiliated to $\mathcal{A}$ such that $U_t = \exp(itS)$ for all $t \in \mathbb{R}$. The operator S is called the* Stone generator *of $\{U_t\}_{t\in\mathbb{R}}$.*

1.3 Wiener and Poisson Processes

We now introduce the quantum probability space with which we will model the quantized electromagnetic field. We will see that the model is rich enough to support an entire family of Wiener and Poisson processes. These different processes do not all commute with each other. In this sense quantum probability is richer than the classical theory.

Definition 1.9. Let $\mathcal{H}$ be a Hilbert space. The *bosonic* or *symmetric Fock space over* $\mathcal{H}$ is the Hilbert space

$$\mathcal{F}(\mathcal{H}) = \mathbb{C} \oplus \bigoplus_{n=1}^{\infty} \mathcal{H}^{\otimes_s n},$$

where $\otimes_s$ denotes the symmetric tensor product.

The Fock space $\mathcal{F}(\mathcal{H})$ describes a field of bosons. The different levels in the Fock space correspond to different numbers of photons present in the field. Note that it is possible to have superpositions between states with different number of particles. For $f \in \mathcal{H}$ we define the exponential vector $e(f)$ by

$$e(f) = 1 \oplus \bigoplus_{n=1}^{\infty} \frac{1}{\sqrt{n!}} f^{\otimes n}.$$

The vector $\Phi = e(0) = 1 \oplus 0 \oplus 0 \oplus \ldots$ is called the *vacuum vector*. The set of all exponential vectors is linearly independent and the linear span of all exponential vectors $\mathcal{D}$ is a dense subset of $\mathcal{F}(\mathcal{H})$ (see e.g. [21]). On the dense domain $\mathcal{D}$ we define for all $f \in \mathcal{H}$ an operator $W(f)$ by

$$W(f)e(g) = e^{-\langle f,g\rangle - \frac{1}{2}\|f\|^2} e(f+g), \qquad g \in \mathcal{H}. \tag{1.4}$$

$W(f)$ is an isometric map $\mathcal{D} \to \mathcal{D}$. Therefore, $W(f)$ extends uniquely to a unitary operator on $\mathcal{F}(\mathcal{H})$. The extension of $W(f)$ to $\mathcal{F}(\mathcal{H})$ is also denoted by $W(f)$. The operators $W(f)$ are called *Weyl operators*. It can be shown (e.g. [21]) that the Weyl operators $W(f),\ f \in \mathcal{H}$ generate the algebra $\mathcal{W} = \mathcal{B}(\mathcal{F}(\mathcal{H}))$ of all bounded operators on $\mathcal{F}(\mathcal{H})$. From the definition in (1.4) it is easy to see that they satisfy the following *Weyl relations*

$$\begin{aligned} &1. \quad W(f)^* = W(-f), \qquad f \in \mathcal{H}, \\ &2. \quad W(f)W(g) = e^{-i\mathrm{Im}\langle f,g\rangle} W(f+g), \qquad f,g \in \mathcal{H}. \end{aligned} \tag{1.5}$$

For a fixed f in $\mathcal{H}$, the family $\{W(sf)\}_{s\in\mathbb{R}}$ forms a one-parameter group of unitaries. This one-parameter group is in fact continuous with respect to the strong operator topology [22]. Denote its Stone generator by $B(f)$, i.e. we have $W(sf) = \exp(isB(f))$. The operators $B(f)$ are called *field operators*. Let $\mathcal{H} = L^2(\mathbb{R}^+)$ and fix $\alpha \in [0, \pi)$. It immediately follows from the Weyl relations Equation (1.5) that all the operators in the set $\mathcal{S} = \{W(sf);\ f = e^{i\alpha}\chi_{[0,t]},\ t \geq 0,\ s \in \mathbb{R}\}$ commute. Here $\chi_{[0,t]}$ is the indicator function of the interval $[0,t]$, i.e. the function that is 1 on $[0,t]$ and 0 elsewhere. Let $\mathcal{C}^\alpha$ be the commutative von Neumann algebra generated by $\mathcal{S}$. Define for all $t \geq 0$ the following selfadjoint operators affiliated to $\mathcal{C}^\alpha$

$$B_t^\alpha := B(e^{i\alpha}\chi_{[0,t]}).$$

Let the *vacuum state* ϕ be given by $\phi = \langle \Phi, \cdot \Phi\rangle$. The spectral theorem (Theorem 1.3) provides a measure space $(\Omega^\alpha, \Sigma^\alpha, \mu^\alpha)$, a *-isomorphism $\iota:\ \mathcal{C}^\alpha \to L^\infty(\Omega^\alpha, \Sigma^\alpha, \mu^\alpha)$, and a probability measure $\mathbf{P}^\alpha$ on Σ^α such that $\phi(C) = \mathbb{E}_{\mathbf{P}^\alpha}(\iota(C))$ for all $C \in \mathcal{C}^\alpha$. Using the definition in Equation (1.3) we can represent the operators B_t^α for $t \geq 0$ as random variables $\iota(B_t^\alpha)$ on $(\Omega^\alpha, \Sigma^\alpha, \mathbf{P}^\alpha)$. Note that in the above discussion the parameter α was fixed. The operators B_t^α and $B_s^{\alpha'}$ for $\alpha \neq \alpha'$ do not commute, i.e. they can not be represented as random variables on the same classical probability space.

We will now study the process $\iota(B_t^\alpha), t \geq 0$ on $(\Omega^\alpha, \Sigma^\alpha, \mathbf{P}^\alpha)$. We calculate the characteristic function of an increment $\iota(B_t^\alpha) - \iota(B_s^\alpha)$ (where $t \geq s$)

$$\begin{aligned}\mathbb{E}_{\mathbf{P}^\alpha}\Big(e^{ik\left(\iota(B_t^\alpha)-\iota(B_s^\alpha)\right)}\Big) &= \mathbb{E}_{\mathbf{P}^\alpha}\Big(\iota\Big(e^{ik\left(B_t^\alpha - B_s^\alpha\right)}\Big)\Big) = \phi\Big(W\big(k\chi_{[s,t]}\big)\Big) \\ &= \Big\langle \Phi, e^{-\frac{1}{2}k^2(t-s)}e\big(k\chi_{[s,t]}\big)\Big\rangle = e^{-\frac{1}{2}k^2(t-s)}, \qquad k \in \mathbb{R}.\end{aligned}$$

This shows that the increment has a mean zero Gaussian distribution with variance $t-s$ (see e.g. [28]). Furthermore, a similar calculation shows that the joint characteristic function of two increments is given by (where $t_1 \geq s_1 \geq t_2 \geq s_2$)

$$\begin{aligned}&\mathbb{E}_{\mathbf{P}^\alpha}\Big(e^{ik_1\left(\iota(B_{t_1}^\alpha)-\iota(B_{s_1}^\alpha)\right)+ik_2\left(\iota(B_{t_2}^\alpha)-\iota(B_{s_2}^\alpha)\right)}\Big) = e^{-\frac{1}{2}(k_1^2(t_1-s_1)+k_2^2(t_2-s_2))} = \\ &\mathbb{E}_{\mathbf{P}^\alpha}\Big(e^{ik_1\left(\iota(B_{t_1}^\alpha)-\iota(B_{s_1}^\alpha)\right)}\Big)\mathbb{E}_{\mathbf{P}^\alpha}\Big(e^{ik_2\left(\iota(B_{t_2}^\alpha)-\iota(B_{s_2}^\alpha)\right)}\Big), \qquad k_1, k_2 \in \mathbb{R}.\end{aligned}$$

Since the joint characteristic function is multiplicative, the increments are independent [28]. That is, the process $\iota(B_t^\alpha)$ has independent mean zero Gaussian increments with variance the length of the increment. This means $\iota(B_t^\alpha)$ is a *Wiener process*. Note that for every $\alpha \in [0,\pi)$ we have now constructed a Wiener process on the Fock space. Note that for different values of α these processes do not commute with each other. The idea to simultaneously diagonalise the fields $\{B_t^\alpha\}_{t\geq 0}$ is implicit in some of the earliest work on quantum field theory. However, Segal [24] in the 1950s was the first to emphasize the connection with probability theory.

We will now construct a Poisson process on the Fock space. The *second quantization* of an element $A \in \mathcal{B}(\mathcal{H})$ such that $\|A\| \leq 1$ (i.e. a contraction) is defined by

$$\Gamma(A) = I \oplus \bigoplus_{n=1}^{\infty} A^{\otimes n}. \tag{1.6}$$

For all contractions $A, B \in \mathcal{B}(\mathcal{H})$ we immediately have $\Gamma(A)\Gamma(B) = \Gamma(AB)$. This means that if A and B commute, then $\Gamma(A)$ and $\Gamma(B)$ also commute. Let S be a selfadjoint element of $\mathcal{B}(\mathcal{H})$. The selfadjoint operator S generates a one-parameter group $U_s = \exp(isS)$ of unitaries in $\mathcal{B}(\mathcal{H})$. After second quantization this leads to a one-parameter group $\Gamma(\exp(isS))$ of unitaries in $\mathcal{W} = \mathcal{B}(\mathcal{F}(\mathcal{H}))$. Denote the Stone generator of $\Gamma(\exp(itS))$ by $\Lambda(S)$, i.e. $\Gamma(\exp(isS)) = \exp(is\Lambda(S))$. Note that $\Lambda(S)$ is affiliated to the commutative von Neumann algebra generated by $\{\Gamma(U_s)\}_{s\in\mathbb{R}}$.

Let $\mathcal{H} = L^2(\mathbb{R}^+)$. For $t \geq 0$, let P_t be the projection given by $P_t = M_{\chi_{[0,t]}}$. P_t is selfadjoint and therefore generates a one-parameter group $U_s^t = \exp(isP_t)$. Let $\mathcal{C}$ be the commutative algebra generated by all U_s^t for $s \in \mathbb{R}, t \geq 0$. Introduce the shorthand Λ_t for the Stone generators $\Lambda(P_t)$. Note that for all $t \geq 0$, Λ_t is affiliated to $\mathcal{C}$. On the nth layer of the symmetric Fock space $\Gamma(\exp(isP_t))$ acts as $\exp(isP_t)^{\otimes n}$. Differentiation with respect to s shows that on the nth layer of the symmetric Fock space $\Lambda_t = P_t \otimes I^{n-1} + I \otimes P_t \otimes I^{n-2} + \ldots + I^{n-1} \otimes P_t$. This shows that Λ_t counts how many particles (i.e. photons) are present in the interval $[0, t]$.

For $f \in L^2(\mathbb{R})$ we define a coherent vector $\psi(f)$ as the exponential vector normalised to unit length, i.e.

$$\psi(f) = e^{-\frac{1}{2}\|f\|^2} e(f) = W(f)e(0) = W(f)\Phi.$$

We can now define a coherent state on $\mathcal{W} = \mathcal{B}(\mathcal{F}(L^2(\mathbb{R}^+)))$ by $\rho(A) = \langle \psi(f), A\psi(f)\rangle$. The spectral theorem (Theorem 1.3) provides a measure space (Ω, Σ, μ), a *-isomorphism $\iota : \mathcal{C} \to L^\infty(\Omega, \Sigma, \mu)$ and a probability measure $\mathbf{P}$ such that $\mathbb{E}_{\mathbf{P}}(\iota(C)) = \rho(C)$ for all $C \in \mathcal{C}$. Since the selfadjoint operators Λ_t are affiliated with $\mathcal{C}$, we can represent them as random variables $\iota(\Lambda_t)$ on $(\Omega, \Sigma, \mathbf{P})$.

For $t_1 \geq s_1 \geq t_2 \geq s_2$ the joint characteristic function of the increments $\iota(\Lambda_{t_1}) - \iota(\Lambda_{s_1})$ and $\iota(\Lambda_{t_2}) - \iota(\Lambda_{s_2})$ is given by

$$\begin{aligned}
&\mathbb{E}_{\mathbf{P}}\Big(e^{ik_1\big(\iota(\Lambda_{t_1})-\iota(\Lambda_{s_1})\big)+ik_2\big(\iota(\Lambda_{t_2})-\iota(\Lambda_{s_2})\big)}\Big) = \\
&\Big\langle \psi(f), \Gamma\Big(e^{ik_1\big(P_{t_1}-P_{s_1}\big)}\Big)\Gamma\Big(e^{ik_2\big(P_{t_2}-P_{s_2}\big)}\Big)\psi(f)\Big\rangle = \\
&e^{-\|f\|^2}\Big\langle e(f), e\Big(e^{ik_1\big(P_{t_1}-P_{s_1}\big)}e^{ik_2\big(P_{t_2}-P_{s_2}\big)}f\Big)\Big\rangle = \\
&e^{\Big\langle f, \Big(e^{ik_1\big(P_{t_1}-P_{s_1}\big)}e^{ik_2\big(P_{t_2}-P_{s_2}\big)}-1\Big)f\Big\rangle} = \\
&e^{\int_{s_1}^{t_1}(e^{ik_1}-1)|f|^2 d\lambda} e^{\int_{s_2}^{t_2}(e^{ik_2}-1)|f|^2 d\lambda}, \qquad k_1, k_2 \in \mathbb{R}.
\end{aligned}$$

This shows that $\{\iota(\Lambda_t)\}_{t\geq 0}$ is a process with independent increments. Moreover, it shows that $\iota(\Lambda_t)_{t\geq 0}$ is a Poisson process with intensity measure $|f|^2 d\lambda$, where λ stands for the Lebesgue measure. Since $\psi(f) = W(f)\Phi$, we can also work with respect to the vacuum by sandwiching Λ_t by $W(f)$. We conclude that in the vacuum the process $W(f)^*\Lambda_t W(f)$ is a Poisson process with intensity measure $|f|^2 d\lambda$.

2 Conditional Expectations

In this section we start with a discussion to illustrate how the classical conditional expectation can be transferred to quantum models using the spectral theorem. In pushing the classical concept as far as possible, we arrive at a definition for the quantum conditional expectation. In Section 4 we state the quantum filtering problem in terms of the newly defined quantum conditional expectation.

2.1 Towards a Definition

Let $\mathcal{B}$ be a von Neumann algebra on a Hilbert space $\mathcal{H}$ and let $\mathbb{P}$ be a normal state on $\mathcal{B}$. Let X and Y be two selfadjoint commuting elements of $\mathcal{B}$. Their expectations are given by $\mathbb{P}(X)$ and $\mathbb{P}(Y)$, respectively. In this subsection we show how to define the conditional expectation $\mathbb{P}(X|Y)$ of X given Y.

Let us first recall the classical definition. Suppose that F and G are random variables on a probability space $(\Omega, \Sigma, \mathbf{P})$. Let us suppose for convenience that Ω is a finite set. Since G is a function on a finite set, its range $\mathrm{Ran}(G)$ is also a finite set. The classical conditional expectation $\mathbb{E}_{\mathbf{P}}(F|G)$ of F given G is the random variable (i.e. a measurable function from Ω to $\mathbb{C}$) given by

$$\mathbb{E}_{\mathbf{P}}(F|G)(\omega) = \sum_{g \in \mathrm{Ran}(G)} \frac{\mathbb{E}_{\mathbf{P}}(F\chi_{[G=g]})}{\mathbf{P}([G=g])}\chi_{[G=g]}(\omega), \qquad \omega \in \Omega, \tag{2.1}$$

where $[G = g]$ is the set $\{\omega \in \Omega;\ G(w) = g\}$ and $\chi_{[G=g]}$ is the indicator function of that set. Note that $\mathbb{E}_{\mathbf{P}}(F|G)$ is not just Σ-measurable, but even $\sigma(G)$-measurable, where $\sigma(G)$ is the σ-algebra generated by G. If Ω is not a finite set, and might even be continuous, this last point is the guiding idea. The conditional expectation is then defined as the orthogonal projection from $L^2(\Omega, \Sigma, \mathbf{P})$ onto $L^2(\Omega, \sigma(G), \mathbf{P})$ (and then extended to L^1), see [28].

Instead of a direct definition as in Equation (2.1), or as an orthogonal projection on an L^2-space, we can provide an abstract characterization of the conditional expectation. Given a σ-subalgebra Σ_0 of Σ, we call a Σ_0-measurable random variable $\mathbb{E}_{\mathbf{P}}(F|\Sigma_0)$ *a version of the conditional expectation of F on Σ_0*, if for all Σ_0-measurable random variables S we have

$$\mathbb{E}_{\mathbf{P}}\big(\mathbb{E}_{\mathbf{P}}(F|\Sigma_0)S\big) = \mathbb{E}_{\mathbf{P}}(FS). \tag{2.2}$$

In geometric terms this is just a characterisation of the projection discussed above. Therefore, there exists an object that satisfies this definition, see [28]. It is easy to see that the direct definition in Equation (2.1) satisfies the abstract characterisation of Equation (2.2) if we take $\Sigma_0 = \sigma(G)$. Furthermore, there is almost surely only one $\mathbb{E}_{\mathbf{P}}(F|\Sigma_0)$ satisfying (2.2) (hence the terminology "... *a* version of *the*..."). The proof of this statement is the same as that for the quantum case, which we will give below. Starting from the definition of the classical conditional expectation $\mathbb{E}_{\mathbf{P}}(F|\Sigma_0)$ in Equation (2.2) we can prove that it has the following properties see e.g. [28]. It is linear in F, it maps positive random variables to positive random variables, it preserves χ_Ω, it has the module property $\mathbb{E}_{\mathbf{P}}(FS|\Sigma_0) = \mathbb{E}_{\mathbf{P}}(F|\Sigma_0)S$ for all Σ_0-measurable functions S, it satisfies the tower property $\mathbb{E}_{\mathbf{P}}(\mathbb{E}_{\mathbf{P}}(F|\Sigma_1)|\Sigma_0) = \mathbb{E}_{\mathbf{P}}(F|\Sigma_0)$ whenever $\Sigma_0 \subset \Sigma_1$, and it is the least mean square estimate of F (see also further below).

Let us return to the commuting selfadjoint operators X and Y in the von Neumann algebra $\mathcal{B}$ equipped with the normal state $\mathbb{P}$. The operators X and Y together generate a commutative von Neumann subalgebra $\mathcal{X}$ of $\mathcal{B}$. The spectral theorem provides a measure space (Ω, Σ, μ), a *-isomorphism ι from $\mathcal{X}$ to $L^\infty(\Omega, \Sigma, \mu)$ and a probability measure $\mathbf{P}$ on Σ such that $\mathbb{P}(C) = \mathbb{E}_{\mathbf{P}}(\iota(C))$ for all $C \in \mathcal{X}$. We know how to condition $\iota(X)$ on $\iota(Y)$, that can be done with the classical conditional expectation $\mathbb{E}_{\mathbf{P}}(\iota(X)|\iota(Y))$. It is natural to define the quantum conditional expectation as

$$\mathbb{P}(X|Y) = \iota^{-1}\Big(\mathbb{E}_{\mathbf{P}}\big(\iota(X)\big|\iota(Y)\big)\Big).$$

We now see that we can only condition those observables $X \in \mathcal{B}$ that commute with Y. That, however, is exactly as it should be. In one realization of an experiment we can only access commuting observables. Two noncommuting observables can never both be assigned a numerical value in a single realization of the experiment, i.e. there is no need for conditioning them on each other. This idea has been called the *nondemolition principle*. Note, however, that two operators X_1 and X_2 that both commute with Y need not necessarily commute with each other.

It is now straightforward to define the conditional expectation of a selfadjoint operator X on a commutative subalgebra $\mathcal{C}$ of $\mathcal{B}$ with which X commutes, i.e. $XC = CX$ for all $C \in \mathcal{C}$. In short, let $\mathcal{X}$ be the commutative algebra generated by the whole of $\mathcal{C}$ and X together. Apply the spectral theorem to $(\mathcal{X}, \mathbb{P})$, that enables the definition of a ι, and then define

$$\mathbb{P}(X|\mathcal{C}) := \iota^{-1}\Bigg(\mathbb{E}_{\mathbf{P}}\Big(\iota(X)\Big|\sigma\big(\iota(C);\ C \in \mathcal{C}\big)\Big)\Bigg). \tag{2.3}$$

In the next subsection we start with the formal definition of the quantum conditional expectation.

2.2 The Quantum Conditional Expectation

Definition 2.1. (Quantum conditional expectation) Let $(\mathcal{B}, \mathbb{P})$ be a quantum probability space. Let $\mathcal{C}$ be a commutative von Neumann subalgebra of $\mathcal{B}$. Denote by $\mathcal{A}$ its *relative commutant*, i.e. $\mathcal{A} = \mathcal{C}' := \{A \in \mathcal{B};\ AC = CA,\ \forall C \in \mathcal{C}\}$. Then $\mathbb{P}(\cdot|\mathcal{C}) :\ \mathcal{A} \to \mathcal{C}$ is (a version of) *the conditional expectation from* $\mathcal{A}$ *onto* $\mathcal{C}$ if

$$\mathbb{P}\big(\mathbb{P}(A|\mathcal{C})C\big) = \mathbb{P}(AC), \qquad \forall A \in \mathcal{A},\ \forall C \in \mathcal{C}. \tag{2.4}$$

Note that the conditional expectation $\mathbb{P}(\,\cdot\,|\mathcal{C})$ is defined only on the commutant $\mathcal{A}$ of $\mathcal{C}$! The definition that we gave here is more restrictive than the one that is usual in quantum probability (see e.g. [26]). There, one also allows for the conditioning on noncommutative subalgebras.

In applications, we start with the quantum probability space $(\mathcal{B} \otimes \mathcal{W}, \mathbb{P})$. Here $\mathcal{B}$ is the algebra with which we model some system of interest (two-level atom, a gas of atoms etc.), $\mathcal{W} = \mathcal{B}(\mathcal{F}(L^2(\mathbb{R})))$ is the algebra with which we model the electromagnetic field and $\mathbb{P} = \rho \otimes \phi$, where ρ some normal state on $\mathcal{B}$ and ϕ is the vacuum state on the field. A commutative subalgebra $\mathcal{C}$ is then generated by the observations we perform (see further below). Next, we choose $\mathcal{A}$ to be the relative commutant of $\mathcal{C}$. The algebra $\mathcal{A}$ consists of the observables that have not been demolished by our observations, i.e. it consists of all operators that are still compatible with $\mathcal{C}$. The following lemma establishes existence and uniqueness for the conditional expectation of Definition 2.1.

Lemma 2.2. *The conditional expectation of Definition 2.1 exists and is unique with probability one, i.e. any two versions* P *and* Q *of* $\mathbb{P}(A|\mathcal{C})$ *satisfy* $\|P - Q\|_{\mathbb{P}} = 0$*, where* $\|X\|^2_{\mathbb{P}} := \mathbb{P}(X^*X)$*.*

Proof. Existence. For a self-adjoint element $A \in \mathcal{A}$ we can define $\mathbb{P}(A|\mathcal{C})$ via Equation (2.3). We now need to check that it satisfies the abstract characterisation Equation (2.4). That, however, follows easily from the classical couterpart Equation (2.2). If $A \in \mathcal{A}$ is not self-adjoint, then we write it as the sum of two self-adjoint elements

$$A = \frac{(A + A^*) - i\big(i(A - A^*)\big)}{2},$$

and simply extend $\mathbb{P}(\,\cdot\,|\mathcal{C})$ linearly. It is easy to see that that obeys Equation (2.4).

Uniqueness w.p. one. Define the pre-inner product $\langle X, Y\rangle := \mathbb{P}(X^*Y)$ on $\mathcal{A}$ (it might have nontrivial kernel if $\mathbb{P}$ is not faithful.) Then $\langle C, A - \mathbb{P}(A|\mathcal{C})\rangle = \mathbb{P}(C^*A) - \mathbb{P}(C^*\mathbb{P}(A|\mathcal{C})) = 0$ for all $C \in \mathcal{C}$ and $A \in \mathcal{A}$, i.e. $A - \mathbb{P}(A|\mathcal{C})$ is orthogonal to $\mathcal{C}$. Now let P and Q be two versions of $\mathbb{P}(A|\mathcal{C})$. It follows that $\langle C, P - Q\rangle = 0$ for all $C \in \mathcal{C}$. But $P - Q \in \mathcal{C}$, so $\langle P - Q, P - Q\rangle = \|P - Q\|^2_{\mathbb{P}} = 0$.

The next lemma asserts that, as in the classical case, the conditional expectation is the least mean square estimate.

Lemma 2.3. $\mathbb{P}(A|\mathcal{C})$ *is the least mean square estimate of* A *given* $\mathcal{C}$*, i.e.*

$$\|A - \mathbb{P}(A|\mathcal{C})\|_{\mathbb{P}} \leq \|A - K\|_{\mathbb{P}}, \qquad \forall\, K \in \mathcal{C}.$$

Proof. For all $K \in \mathcal{C}$ we have

$$\begin{aligned}\|A - K\|_{\mathbb{P}}^2 &= \big\|A - \mathbb{P}(A|\mathcal{C}) + \mathbb{P}(A|\mathcal{C}) - K\big\|_{\mathbb{P}}^2 \\ &= \big\|A - \mathbb{P}(A|\mathcal{C})\big\|_{\mathbb{P}}^2 + \big\|\mathbb{P}(A|\mathcal{C}) - K\big\|_{\mathbb{P}}^2 \geq \big\|A - \mathbb{P}(A|\mathcal{C})\big\|_{\mathbb{P}}^2,\end{aligned}$$

where, in the next to last step, we used that $A - \mathbb{P}(A|\mathcal{C})$ is orthogonal to $\mathbb{P}(A|\mathcal{C}) - K \in \mathcal{C}$.

Remark. We have now highlighted the existence, uniqueness with probability one, and the mean least squares property of the quantum conditional expectation. The other elementary properties of classical conditional expectations and their proofs [28] carry over directly to the noncommutative setting. In particular, we have linearity, positivity, preservation of the identity, the tower property $\mathbb{P}(\mathbb{P}(A|\mathcal{B})|\mathcal{C}) = \mathbb{P}(A|\mathcal{C})$ if $\mathcal{C} \subset \mathcal{B}$, the module property $\mathbb{P}(AB|\mathcal{C}) = \mathbb{P}(A|\mathcal{C})B$ for $B \in \mathcal{C}$, etc. As an example, let us prove linearity. It suffices to show that $Z = \alpha\mathbb{P}(A|\mathcal{C}) + \beta\mathbb{P}(B|\mathcal{C})$ satisfies the definition of $\mathbb{P}(\alpha A + \beta B|\mathcal{C})$, i.e. $\mathbb{P}(ZC) = \mathbb{P}((\alpha A + \beta B)C)$ for all $C \in \mathcal{C}$. But this is immediate from the linearity of $\mathbb{P}$ and Definition 2.1.

In Section 4 we will need to relate conditional expectations with respect to different states to each other. This is done by the following Bayes-type formula.

Lemma 2.4. (Bayes formula [8] [7]) *Let* $(\mathcal{B}, \mathbb{P})$ *be a noncommutative probability space. Let* $\mathcal{C}$ *be a commutative von Neumann subalgebra of* $\mathcal{B}$ *and let* $\mathcal{A}$ *be its relative commutant, i.e.* $\mathcal{A} = \mathcal{C}' := \{A \in \mathcal{B};\ AC = CA,\ \forall C \in \mathcal{C}\}$. *Furthermore, let* Q *be an element in* $\mathcal{A}$ *such that* Q^*Q *is invertible and* $\mathbb{P}(Q^*Q) = 1$. *We can define a state on* $\mathcal{A}$ *by* $\mathbb{Q}(A) := \mathbb{P}(Q^*AQ)$ *and we have*

$$\mathbb{Q}\big(X\big|\mathcal{C}\big) = \frac{\mathbb{P}\big(Q^*XQ\big|\mathcal{C}\big)}{\mathbb{P}\big(Q^*Q\big|\mathcal{C}\big)}, \qquad X \in \mathcal{A}.$$

Proof. Let K be an element of $\mathcal{C}$. For all $X \in \mathcal{A}$, we can write

$$\begin{aligned}&\mathbb{P}\Big(\mathbb{P}\big(Q^*XQ|\mathcal{C}\big)K\Big) = \mathbb{P}\big(Q^*XKQ\big) = \mathbb{Q}\big(XK\big) = \mathbb{Q}\Big(\mathbb{Q}\big(X|\mathcal{C}\big)K\Big) = \\ &\mathbb{P}\Big(Q^*Q\mathbb{Q}\big(X|\mathcal{C}\big)K\Big) = \mathbb{P}\Big(\mathbb{P}\Big(Q^*Q\mathbb{Q}\big(X|\mathcal{C}\big)K\Big|\mathcal{C}\Big)\Big) = \\ &\mathbb{P}\Big(\mathbb{P}\big(Q^*Q\big|\mathcal{C}\big)\mathbb{Q}\big(X|\mathcal{C}\big)K\Big).\end{aligned}$$

Note that the invertibility of $\mathbb{P}\big(Q^*Q\big|\mathcal{C}\big)$ follows immediately from the invertibility of Q^*Q.

3 Quantum Stochastic Calculus

We have seen in Section 1.3 that the quantum probability space $(\mathcal{W}, \phi)$ contains a rich variety of Wiener and Poisson processes. We will now introduce stochastic integrals with respect to these processes and study their stochastic calculus. Quantum stochastic calculus has been introduced by Hudson and Parthasarathy [16]. Quantum stochastic differential equations describe the interaction between atoms and the electromagnetic field in the weak coupling limit.

3.1 The Stochastic Integral

Lemma 3.1. *Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces. There exists a unique unitary isomorphism $U:\ \mathcal{F}(\mathcal{H}_1 \oplus \mathcal{H}_2) \to \mathcal{F}(\mathcal{H}_1) \otimes \mathcal{F}(\mathcal{H}_2)$ such that*

$$Ue(x \oplus y) = e(x) \otimes e(y), \qquad x \in \mathcal{H}_1,\ y \in \mathcal{H}_2. \tag{3.1}$$

Proof. By linear extension of the relation in Equation (3.1) we get a surjective map from $\mathcal{D} = \text{span}\{e(x);\ x \in \mathcal{H}_1 \oplus \mathcal{H}_2\}$ to $\mathcal{D}_1 \otimes \mathcal{D}_2$ where $\mathcal{D}_i = \text{span}\{e(x);\ x \in \mathcal{H}_i\}$. Note that $\mathcal{D}$ is dense in $\mathcal{F}(\mathcal{H}_1 \oplus \mathcal{H}_2)$ and $\mathcal{D}_1 \otimes \mathcal{D}_2$ is dense in $\mathcal{F}(\mathcal{H}_1) \otimes \mathcal{F}(\mathcal{H}_2)$. Moreover, for all $x_1, y_1 \in \mathcal{H}_1$ and $x_2, y_2 \in \mathcal{H}_2$ we have

$$\begin{aligned}\big\langle e(x_1 \oplus x_2), e(y_1 \oplus y_2)\big\rangle &= e^{\langle x_1 + x_2, y_1 + y_2\rangle} = e^{\langle x_1, y_1\rangle} e^{\langle x_2, y_2\rangle} \\ &= \big\langle e(x_1), e(y_1)\big\rangle \big\langle e(x_2), e(y_2)\big\rangle,\end{aligned}$$

i.e. $U:\ \mathcal{D} \to \mathcal{D}_1 \otimes \mathcal{D}_2$ is isometric and therefore extends uniquely to a unitary.

We will often identify $\mathcal{F}(\mathcal{H}_1 \oplus \mathcal{H}_2)$ and $\mathcal{F}(\mathcal{H}_1) \otimes \mathcal{F}(\mathcal{H}_2)$ using the unitary of Lemma 3.1. For all $t \geq s \geq 0$ we define $\mathcal{F} = \mathcal{F}(L^2(\mathbb{R}^+))$, $\mathcal{F}_{t]} = \mathcal{F}(L^2([0,t]))$, $\mathcal{F}_{[s,t]} = \mathcal{F}(L^2([s,t]))$ and $\mathcal{F}_{[t} = \mathcal{F}(L^2([t,\infty)))$. For $t_n > ... > t_1 > 0$ we have $L^2(\mathbb{R}^+) = L^2([0,t_1]) \oplus L^2([t_1,t_2]) \oplus \ldots \oplus L^2([t_n,\infty))$. Therefore, in the sense of Lemma 3.1, we get

$$\mathcal{F} = \mathcal{F}_{t_1]} \otimes \mathcal{F}_{[t_1,t_2]} \otimes \ldots \otimes \mathcal{F}_{[t_{n-1},t_n]} \otimes \mathcal{F}_{[t_n}.$$

Every partition leads to a tensor product splitting of the symmetric Fock space. In this sense the symmetric Fock space is a *continuous tensor product.* Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces. Denote $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$. It easily follows from the definition Equation (1.4) that

$$W(x_1 \oplus x_2) = W(x_1) \otimes W(x_2), \qquad x_1 \in \mathcal{H}_1,\ x_2 \in \mathcal{H}_2. \tag{3.2}$$

This means that the algebra generated by the Weyl operators also splits as a continuous tensor product, i.e. for $t_n > ... > t_1 > 0$ we have

$$\mathcal{W} = \mathcal{W}_{t_1]} \otimes \mathcal{W}_{[t_1,t_2]} \otimes \ldots \otimes \mathcal{W}_{[t_{n-1},t_n]} \otimes \mathcal{W}_{[t},$$

where $\mathcal{W} = \mathcal{B}(L^2([0,\infty)))$, $\mathcal{W}_{t]} = \mathcal{B}(L^2([0,t]))$, $\mathcal{W}_{[s,t]} = \mathcal{B}(L^2([s,t]))$ and $\mathcal{W}_{[t} = \mathcal{B}(L^2([t,\infty)))$. Furthermore, from the definition in Equation (1.6) it follows that

$$\Gamma(S_1 \oplus S_2) = \Gamma(S_1) \otimes \Gamma(S_2) \tag{3.3}$$

for all contractions $S_1 \in \mathcal{B}(\mathcal{H}_1)$ and $S_2 \in \mathcal{B}(\mathcal{H}_2)$.

Definition 3.2. On the dense domain $\mathcal{D} = \text{span}\{e(f);\ f \in L^2(\mathbb{R}^+)\}$ we introduce *annihilation* A_t and *creation* A_t operators by

$$A_t = \frac{1}{2}\Big(B(i\chi_{[0,t]}) - iB(\chi_{[0,t]})\Big), \qquad A_t^* = \frac{1}{2}\Big(B(i\chi_{[0,t]}) + iB(\chi_{[0,t]})\Big),$$

where $B(f)$ denotes the Stone generator of $W(tf)$. The restriction of Λ_t to $\mathcal{D}$ is also denoted by Λ_t and is called the *gauge process*. The operators A_t, A_t^* and Λ_t are called the *fundamental noises*.

It can be shown e.g. [21] that the domain of the Stone generators $B(f)$, $f \in L^2(\mathbb{R}^+)$ contains $\mathcal{D}$, that $A_t e(f) = \langle \chi_{[0,t]}, f\rangle e(f)$ and that A_t^* is the adjoint of A_t restricted to $\mathcal{D}$. Moreover, from its definition it follows that $\langle e(f), \Lambda_t e(f)\rangle = \langle g, \chi_{[0,t]} f\rangle\langle e(g), e(f)\rangle$. In particular this means that $A_t\Phi = A_t e(0) = 0$ and $\Lambda_t \Phi = 0$, properties that we will exploit later on. Let M_t be one of the fundamental noises. It is a consequence of Equations (3.2) and (3.3) and the definition of the fundamental noises as (linear combinations of) generators of one-parameter groups that

$$(M_t - M_s)e(f) = e(f_{s]}) \otimes \Big((M_t - M_s)e(f_{[s,t]})\Big) \otimes e(f_{[t}), \tag{3.4}$$

where $f \in L^2(\mathbb{R}^+)$, $f_{s]} = \chi_{[0,s]}f$, $f_{[s,t]} = \chi_{[0,t]}f$, $f_{[t} = \chi_{[t,\infty)}f$ and $(M_t - M_s)e(f_{[s,t]}) \in \mathcal{F}_{[s,t]}$. In the following we will for notational convenience often omit the tensor product signs between exponential vectors. Let $\mathcal{H}$ be a Hilbert space, called the *initial space*. We tensor the initial space to $\mathcal{F}$ and extend the operators A_t, A_t^* and Λ_t to $\mathcal{H} \otimes \mathcal{F}$ by ampliation, i.e. by tensoring the identity to them on $\mathcal{H}$ (however, to keep notation light we will not denote it). We denote the algebra of all bounded operators on $\mathcal{H}$ by $\mathcal{B}$.

Definition 3.3. (Simple quantum stochastic integral) Let $\{L_s\}_{0\le s\le t}$ be an adapted (i.e. $L_s \in \mathcal{B} \otimes \mathcal{W}_{s]}$ for all $0 \le s \le t$) simple process with respect to the partition $\{s_0 = 0, s_1, \ldots, s_p = t\}$ in the sense that $L_s = L_{s_j}$ whenever $s_j \le s < s_{j+1}$. The stochastic integral of L with respect to a fundamental noise M on $\mathcal{H} \otimes \mathcal{D}$ is then defined as [16, 21]

$$\int_0^t L_s dM_s\ xe(f) := \sum_{j=0}^{p-1} \Big(L_{s_j} xe(f_{s_j]})\Big)\Big((M_{s_{j+1}} - M_{s_j})e(f_{[s_j,s_{j+1}]})\Big)e(f_{[s_{j+1}}),$$

for all $x \in \mathcal{H}$ and $f \in L^2(\mathbb{R}^+)$.

Let $\{L_s\}_{0\leq s\leq t}$ be an adapted process, i.e. $L_s \in \mathcal{B} \otimes \mathcal{W}_{s]}$ for all $0 \leq s \leq t$. We would like to define the integral

$$I_t = \int_0^t L_s dM_s,$$

as a limit of simple integrals $I_t^n = \int_0^t L_s^n dM_s$ where L^n is an approximation of L by simple adapted processes. In the classical case we use the Itô isometry to define the stochastic integral as a mean square limit of simple processes. Moreover, one can show that each mean square integrable process can be approximated by simple processes. Let us see how far we would get using this procedure in the quantum case. For simplicity suppose that the initial space is trivial $\mathcal{H} = \mathbb{C}$. Suppose that we are working with respect to the vacuum state ϕ on $\mathcal{W}$. Following the classical reasoning, we are looking for an operator I_t such that $\langle (I_t - I_t^n)\Phi, (I_t - I_t^n)\Phi\rangle \to 0$ as $n \to \infty$ where I_t^n are simple integrals corresponding to simple approximations of L. This however, would only fix the action of I_t on the vacuum vector Φ. It remains unclear what the domain of I_t is and what the action of I_t is on the vectors in that domain that are not the vacuum.

The solution to this problem was given by Hudson and Parthasarathy [16]. They simply fix the domain for a stochastic integral I_t to $\mathcal{H} \otimes \mathcal{D}$ (one could choose a dense domain in $\mathcal{H}$, for simplicity we have chosen $\mathcal{H}$). Moreover, they consider I_t^n to be an approximation of I_t if $\langle (I_t - I_t^n)x\otimes\psi, (I_t - I_t^n)x\otimes\psi\rangle \to 0$ as $n \to \infty$ for all $x \in \mathcal{H}$ and $\psi \in \mathcal{D}$. This limit exists if $\int_0^t \|L_s - L_s^n\| ds \to 0$ as $n \to \infty$ for all $x \in \mathcal{H}$, $\psi \in \mathcal{D}$ and the limit is independent of the approximation [16]. Moreover, every adapted square integrable process L, i.e. $\int_0^t \|L_s x \otimes \psi\|^2 ds < \infty$ for all $x \in \mathcal{H}$, $\psi \in \mathcal{D}$ admits a simple approximation [16]. This means that for every adapted square integrable L_s we now have an unambiguous definition of the stochastic integral $\int_0^t L_s dM_s$, where M_s can be any of the three fundamental noises. Adapted square integrable processes are said to be *stochastically integrable*. We use the following shorthand for stochastic integrals $dX_t = L_t dM_t$ means $X_t = X_0 + \int_0^t L_s dM_s$.

Since $A_t\Phi = \Lambda_t\Phi = 0$ it is immediate from the definition that quantum stochastic integrals with respect to A_t and Λ_t acting on Φ are zero, or infinitesimally $d\Lambda_t\Phi_{[t} = dA_t\Phi_{[t} = 0$. From this we can immediately conclude that vacuum expectations of stochastic integrals with respect to A_t and Λ_t vanish. Furthermore, we have $\left\langle \Phi, \int_0^t L_s dA_s^*\Phi\right\rangle = \left\langle \int_0^t L_s^* dA_s\Phi, \Phi\right\rangle = 0$, i.e. vacuum expectation of stochastic integrals with respect to A_t^* are zero as well. Note, however, that $dA_t^*\Phi_{[t} \neq 0$.

To get some more feeling for the definition of the quantum stochastic integral we will now investigate which quantum stochastic differential equation is satisfied by the Weyl operators $W(f_{t]})$ ($f \in L^2(\mathbb{R}^+)$). Note that the stochastic integrals are defined on the domain $\mathcal{D}$. Therefore we calculate for g and h in $L^2(\mathbb{R}^+)$

$$\begin{aligned}\phi(t) &:= \big\langle e(g), W(f_{t]})e(h)\big\rangle = e^{-\langle f_{t]},h\rangle - \frac{1}{2}\|f_{t]}\|^2}\big\langle e(g), e(h+f_{t]})\big\rangle \\ &= e^{\langle g,f_{t]}\rangle - \langle f_{t]},h\rangle - \frac{1}{2}\|f_{t]}\|^2}e^{\langle g,h\rangle},\end{aligned}$$

which means that

$$\phi(t) - \phi(0) = \int_0^t \Big\langle e(g), \frac{d}{ds}\Big(\langle g, f_{s]}\rangle - \langle f_{s]}, h\rangle - \frac{1}{2}\|f_{s]}\|^2\Big)\phi(s)e(h)\Big\rangle ds.$$

Let us turn to the definition of the stochastic integral, Definition 3.3. Let $\{0 = s_0, s_1, \ldots, s_p = t\}$ be a partition of $[0,t]$ and choose $L_s = \overline{f}(s_j)W(f_{s_j]})$ for $s_j \le s < s_{j+1}$. Let further M_t be A_t, then the definition of the stochastic integral gives (heuristically in the last step)

$$\begin{aligned}&\sum_{j=0}^{p-1}\Big(\overline{f}(s_j)W(f_{s_j]})e(h_{s_j]})\Big)\Big((A_{s_{j+1}} - A_{s_j})e(h_{[s_j,s_{j+1}]})\Big)e(h_{[s_{j+1}}) = \\ &\sum_{j=0}^{p-1}\Big\langle f(s_j)\chi_{[s_j,s_{j+1}]}, h\Big\rangle W(f_{s_j]})e(h) = \\ &\sum_{j=0}^{p-1}\Big(\big\langle f(s_j)\chi_{s_{j+1}]}, h\big\rangle - \big\langle f(s_j)\chi_{s_j]}, h\big\rangle\Big)W(f_{s_j]})e(h) \\ &\longrightarrow \int_0^t d\big\langle f_{s]}, h\big\rangle\, W(f_{s]})\, e(h).\end{aligned}$$

Together with a similar calculation for $M_t = A_t^*$, this yields the following quantum stochastic differential equation for the Weyl operator $W(f_{t]})$

$$dW(f_{t]}) = \Big\{f(t)dA_t^* - \overline{f}(t)dA_t - \frac{1}{2}\big|f(t)\big|^2 dt\Big\}W(f_{t]}). \tag{3.5}$$

3.2 The Calculus

We now turn to the calculus satisfied by the quantum stochastic integrals we defined in the previous subsection. It is the calculus that makes the theory useful, it allows us to forget the tedious definition of the integral in computations and instead to perform algebraic manipulations with increments.

Definition 3.4. A pair $(L, L^\dagger)$ of adapted processes defined on $\mathcal{H} \otimes \mathcal{D}$ is called an *adjoint pair* if

$$\langle x\otimes e(f), L_t y\otimes e(f)\rangle = \langle L_t^\dagger x\otimes e(f), y\otimes e(f)\rangle, \quad x, y \in \mathcal{H},\ f, g \in L^2(\mathbb{R}^+),\ t \geq 0.$$

The dagger replaces the adjoint on the domain $\mathcal{H} \otimes \mathcal{D}$. It is easy to see that (A, A^*) and (Λ, Λ) are adjoint pairs. Moreover, if $(L, L^\dagger)$ is an adjoint pair, then $(X, X^\dagger)$ is an adjoint pair, where $dX_t = LdM_t$ and $dX_t^\dagger = L^\dagger dM_t^\dagger$.

Theorem 3.5. ***(Quantum Itô rule [16])*** *Let $(B, B^\dagger)$, $(C, C^\dagger)$, $(D, D^\dagger)$, $(E, E^\dagger)$ be adjoint pairs of stochastically integrable processes. Let F_t, G_t, H_t and I_t be stochastically integrable processes. Let X_t and Y_t be stochastic integrals of the form*

$$dX_t = B_t d\Lambda_t + C_t dA_t + D_t dA_t^* + E_t dt,$$
$$dY_t = F_t d\Lambda_t + G_t dA_t + H_t dA_t^* + I_t dt,$$

Suppose X_tY_t is an adapted process defined on $\mathcal{H} \otimes \mathcal{D}$ and XF, XG, XH, XI, BY, CY, DY, EY, BF, CF, BH and CH are stochastically integrable, then

$$d(X_tY_t) = X_t\, dY_t + (dX_t)\, Y_t + dX_t\, dY_t,$$

where dX_tdY_t should be evaluated according to the quantum Itô table

	dA_t	$d\Lambda_t$	dA_t^*	dt
dA_t	0	dA_t	dt	0
$d\Lambda_t$	0	$d\Lambda_t$	dA_t^*	0
dA_t^*	0	0	0	0
dt	0	0	0	0

i.e. $dX_tdY_t = B_tF_td\Lambda_t + C_tF_tdA_t + B_tH_tdA_t^* + C_tH_tdt.$

Suppose that the product X_tY_t is an adapted process defined on $\mathcal{H} \otimes \mathcal{D}$. Then we can read off an expression for X_tY_t from the matrix elements $\langle X_t^\dagger x\otimes e(f), Y_t y\otimes e(g)\rangle$, which explains the need for the concept of an adjoint pair. Writing out these matrix elements using the definition of the stochastic integral is the basic ingredient of the proof of the quantum Itô rule, see [16] and [21]. To get some more feeling for the proof of the quantum Itô rule we compute for $x, y \in \mathcal{H}$ and $f, g \in L^2(\mathbb{R}^+)$

$$\langle xe(f), A_tA_t^* ye(g)\rangle = \langle xe(f), \big(A_t^*A_t + [A_t, A_t^*]\big) ye(g)\rangle =$$
$$\langle A_t xe(f), A_t ye(g)\rangle + t\langle xe(f), ye(g)\rangle = \Big(\langle f, \chi_{[0,t]}\rangle\langle \chi_{[0,t]}, g\rangle + t\Big)\langle xe(f), ye(g)\rangle.$$

Infinitesimally that reads $d(A_tA_t^*) = A_tdA_t^* + A_t^*dA_t + dt$. Note that the Itô correction term finds its origins in the commutator between A_t and A_t^*.

Note that we need to check many conditions before we are allowed to apply the quantum Itô rule. In practice though we mostly work with ‘noisy

Schrödinger equations', which have unitary and therefore bounded solutions. If the integrals and coefficients are bounded, then all the requirements of the theorem are satisfied. In the remainder of these notes we will not worry much about these issues and just assume that we can apply the quantum Itô rule.

In Section 1 we encountered the classical Wiener processes $B_t^\alpha = ie^{-i\alpha}A_t - ie^{i\alpha}A_t^*$ for $\alpha \in [0, \pi)$. Since $dB_t^\alpha = ie^{-i\alpha}dA_t - ie^{i\alpha}dA_t^*$, we recover the classical Itô rule for these Wiener processes, i.e. $(dB_t^\alpha)^2 = dt$, from the quantum Itô rule. For an $f \in L^2(\mathbb{R}^+)$ we can write the Weyl operator $W(f_{t]})$ as $W(f_{t]}) = \exp\big(\int_0^t f(s)d(A_s^* - A_s)\big)$. Therefore it follows from the quantum Itô rule that the Weyl operators $W(f_{t]})$ satisfy equation (3.5), where $-\frac{1}{2}\|f\|^2 W(f_{t]})dt$ is the Itô correction term. The Poisson process of the previous section was given by $\Lambda_t^f := W(f)^*\Lambda_t W(f)$ in the vacuum state, for which the quantum Itô rule gives

$$d\Lambda_t^f = d\Lambda_t + \overline{f}(t)dA_t + f(t)dA_t^* + |f(t)|^2 dt,$$

which leads to the classical Itô rule $(d\Lambda_t^f)^2 = d\Lambda_t^f$ for the Poisson process. Furthermore, integrating the above equation, we see that $\Lambda_t^f = \Lambda_t + B(if_{t]}) + \int_0^t |f(s)|^2 ds$.

3.3 Open Quantum Systems

In quantum optics the basic model consists of some physical system of interest, e.g. a two-level atom, a cloud of atoms, or an atom in a cavity, in interaction with the electromagnetic field. The interaction between the electromagnetic field and the system of interest is described by quantum electrodynamics, see e.g. [10]. The dynamics is given by a Schrödinger equation in which the atomic dipole operator couples to a stationary Gaussian wide band noise. The next step is to approximate the wide band noise by white noise. See [1], [14] and [11] for rigorous limits implementing this Markovian approximation. In this procedure the Schrödinger equation given by quantum electrodynamics transforms to a quantum stochastic differential equation of the form

$$dU_t = \left\{(S - I)d\Lambda_t + LdA_t^* - L^*SdA_t - \frac{1}{2}L^*Ldt - iHdt\right\}U_t, \qquad U_0 = I, \tag{3.6}$$

where S, L and H are operators on the system of interest, H being selfadjoint and S being unitary. See [14] for a description of how gauge terms can arise from QED Hamiltonians in a Markovian approximation. For simplicity we have considered only one channel in the field. In the examples below we will briefly describe systems that interact with two field channels.

A Picard iteration scheme shows that there exists a unique solution to Equation (3.6). Using the quantum Itô rule we can calculate $dU_t^*U_t = dU_tU_t^* = 0$, i.e. the solution to Equation (3.6) is unitary. We define the time evolution of observables of the system of interest by the flow $j_t(X) = U_t^*(X \otimes I)U_t$. Using the quantum Itô rule, we find

$$dj_t(X) = j_t\big(\mathcal{L}(X)\big)dt + j_t\big(S^*XS - X\big)d\Lambda_t + j_t\big([L^*, XS]\big)dA_t + j_t\big([S^*X, L]\big)dA_t^*,$$

where the Lindblad generator [18] is given by

$$\mathcal{L}(X) = i[H, X] + L^*XL - \frac{1}{2}(L^*LX - XL^*L).$$

Instead of going through a rigorous Markov limit, we will always take the quantum stochastic differential equation (3.6) as our starting point.

Example 3.6. Suppose we are studying a two-level atom in interaction with the electromagnetic field. The two-level atom is described by the quantum probability space $(M_2(\mathbb{C}), \rho)$ and the field is described by $(\mathcal{W}, \phi)$. The operators S, L and H are given by

$$S = I, \qquad L = \gamma\sigma_- = \begin{pmatrix} 0 & 0 \\ \gamma & 0 \end{pmatrix}, \qquad H = \frac{\hbar\omega_0}{2}\sigma_z = \begin{pmatrix} \frac{\hbar\omega_0}{2} & 0 \\ 0 & -\frac{\hbar\omega_0}{2} \end{pmatrix},$$

where $\hbar$ is Planck's constant, $\gamma \geq 0$ is a decay parameter, and $\omega_0 \in \mathbb{R}$ is the so-called atomic frequency, determined by the fact that $\hbar\omega_0$ is the energy difference between the two levels. That is, the interaction between the two-level atom and the electromagnetic field is given by the following quantum stochastic differential equation ($\sigma_+ = \sigma_-^*$)

$$dU_t = \left\{\gamma\sigma_- dA_t^* - \gamma\sigma_+ dA_t - \frac{\gamma^2}{2}\sigma_+\sigma_- dt - i\frac{\hbar\omega_0}{2}\sigma_z dt\right\}U_t, \qquad U_0 = I.$$

A laser driving the two-level atom could be modelled by an additional Hamiltonian $\Omega\sigma_x = \Omega(\sigma_- + \sigma_+)$, with $\Omega \in \mathbb{R}$. A more realistic model is obtained by adding an extra field channel in a coherent state (the laser). If we distinguish two field channels, then the two-level atom and the field together are described by the quantum probability space $(M_2(\mathbb{C}) \otimes \mathcal{W}_1 \otimes \mathcal{W}_2,\ \rho \otimes \phi \otimes \sigma)$ where σ is the state given by the inner product with the vector $\psi(f) = W(f)e(0)$, for some $f \in L^2(\mathbb{R}^+)$. Here $|f|$ is the amplitude of the laser and the phase of f represents the phase of the driving laser. The quantum stochastic differential equation is given by

$$\begin{aligned} dU_t = \Big\{&\gamma_1\sigma_- dA_{1t}^* - \gamma_1\sigma_+ dA_{1t} + \gamma_2\sigma_- dA_{2t}^* - \gamma_2\sigma_+ dA_{2t} - \\ &\frac{\gamma_1^2 + \gamma_2^2}{2}\sigma_+\sigma_- dt - i\frac{\hbar\omega_0}{2}\sigma_z dt\Big\}U_t, \qquad U_0 = I, \end{aligned}$$

with $\gamma_1, \gamma_2 \geq 0$. If we are only interested in the evolution of adapted observables, then we have $W(f)^*U_t^*XU_tW(f) = W(f_{t]})^*U_t^*XU_tW(f_{t]})$. Therefore we can describe the system by the quantum probability space

$(M_2(\mathbb{C}) \otimes \mathcal{W}_1 \otimes \mathcal{W}_2,\ \rho \otimes \phi \otimes \phi)$, and interaction given by $\tilde{U}_t = U_t W(f_{t]})$. Using the quantum Itô rule it is easy to see that

$$d\tilde{U}_t = \Big\{\gamma_1 \sigma_- dA_{1t}^* - \gamma_1 \sigma_+ dA_{1t} + L dA_{2t}^* - L^* dA_{2t} - \frac{\gamma_1^2 \sigma_+\sigma_- + L^*L}{2} dt - i\frac{\hbar}{2}\sigma_z - iH dt\Big\}\tilde{U}_t, \qquad \tilde{U}_0 = I,$$

with $L = \gamma_2 \sigma_- + f(t)$ and $H = i(\gamma_2 f(t)\sigma_+ - \gamma_2 \overline{f(t)}\sigma_-)/2$. The Hamiltonian H reduces to the simpler form $\Omega\sigma_x$ if $\Omega = i\gamma_2 f(t)/2$ and $f(t) = -i$.

Example 3.7. We consider a two-level atom inside a cavity. The cavity has one leaky mirror which couples it to the outside field. The cavity is described by the Hilbert space $\ell^2(\mathbb{N})$. Let $n \in \mathbb{N}$. Denote by δ_n the element of $\ell^2(\mathbb{N})$ given by $\delta_n(n) = 1$ and $\delta_n(m) = 0$ for all $m \in \mathbb{N}\backslash\{n\}$. The annihilation operator is given by $b\delta_n = \sqrt{n}\delta_{n-1},\ n \in \mathbb{N}^*$ and $b\delta_0 = 0$ (we will not worry about defining a domain for b). The creation operator b^* is the adjoint of b. The two-level atom in the cavity coupled to the field can be described by the quantum probability space $(M_2(\mathbb{C}) \otimes \mathcal{B}(\ell^2(\mathbb{N})) \otimes \mathcal{W},\ \rho \otimes \sigma \otimes \phi)$, where ρ is some state of the two-level atom, σ is some state on $\mathcal{B}(\ell^2(\mathbb{N}))$ (the cavity) and ϕ is the vacuum state of the field. The quantum stochastic differential equation describing the two-level atom, the cavity, and the field together is

$$dU_t = \Big\{\gamma b dA_t^* - \gamma b^* dA_t - \frac{\gamma^2}{2} b^* b dt + g(\sigma_+ b - \sigma_- b^*)dt - i(\Delta_a \sigma_z + \Delta_c b^* b)dt\Big\}U_t, \qquad U_0 = I.$$

Here γ and g are positive parameters, determined by the cavity. The parameters Δ_a and Δ_c are real. More information about cavity QED can be found in [10]. See [13] for rigorous results on systems including a cavity.

Example 3.8. We consider a gas of atoms in free space in interaction with a linearly polarized laser beam [25]. Suppose the atoms are all two-level atoms, i.e. the Hilbert space of the gas is given by $\mathcal{H} := \mathbb{C}^{2^N}$. Here N represents the number of atoms in the gas. The gas is described by the quantum probability space $(\mathcal{B}(\mathcal{H}), \rho)$, where ρ is a state on the algebra $\mathcal{B}(\mathcal{H})$ of all bounded operators on $\mathcal{H}$. We model the laser beam by the symmetric Fock space over the one photon space $\mathbb{C}^2 \otimes L^2(\mathbb{R}^+)$. Here $\mathbb{C}^2$ describes the polarization and $L^2(\mathbb{R}^+)$ describes the spatial degree of freedom of a photon in the beam. Since the speed of light is constant, we can identify the spatial degree of freedom with time. Let $\{e_x, e_y\}$ be the orthonormal basis in $\mathbb{C}^2$ such that e_x corresponds to an x-polarized photon and e_y to a y-polarized photon. We can identify $\mathbb{C}^2 \otimes L^2(\mathbb{R}^+)$ with $L^2(\mathbb{R}^+) \oplus L^2(\mathbb{R}^+)$ by the linear map that maps $e_x \otimes f$ to $(f, 0)$ and $e_y \otimes g$ to $(0, g)$ for all $f, g \in L^2(\mathbb{R}^+)$. That is, the laser beam consists out of two polarization channels

$$\mathcal{F}(\mathbb{C}^2 \otimes L^2(\mathbb{R}^+)) = \mathcal{F}_x \otimes \mathcal{F}_y.$$

Let $\mathcal{W}_x$ and $\mathcal{W}_y$ be the algebras of all bounded operators on $\mathcal{F}_x$ and $\mathcal{F}_y$, respectively. The gas and the x-polarized laser beam together are modelled by the quantum probability space $\big(\mathcal{B}(\mathcal{H})\otimes\mathcal{W}_x\otimes\mathcal{W}_y, \rho\otimes\sigma\big)$ where σ is given by the inner product with the coherent vector $\psi(e_x\otimes f)$ in $\mathcal{F}(\mathbb{C}^2\otimes L^2(\mathbb{R}^+))$ given by

$$\psi(e_x\otimes f) = \exp\left(-\frac{1}{2}\|f\|^2\right) 1 \oplus \bigoplus_{n=1}^{\infty} \frac{(e_x\otimes f)^{\otimes n}}{\sqrt{n!}}.$$

The modulus and phase of $f(t)$ correspond to the amplitude and phase of the laser at time t.

We can also choose the circularly polarized basis $\{e_+, e_-\}$ in $\mathbb{C}^2$, given by $e_+ = -(e_x + ie_y)/\sqrt{2}$ and $e_- = (e_x - ie_y)/\sqrt{2}$. In an analogous way as for the linear basis $\{e_x, e_y\}$ this leads to an identification

$$\mathcal{F}(\mathbb{C}^2\otimes L^2(\mathbb{R}^+)) = \mathcal{F}_+\otimes\mathcal{F}_-.$$

In a suitable appproximation [25], the interaction between the laser beam and the gas of atoms can be described by the following quantum stochastic differential equation [5]

$$dU_t = \Big\{\big(e^{i\kappa F_z} - I\big)d\Lambda_t^{++} + \big(e^{-i\kappa F_z} - I\big)d\Lambda_t^{--}\Big\}U_t, \qquad U_0 = I. \tag{3.7}$$

Here κ is a real coupling parameter. The processes Λ_t^{++} and Λ_t^{--} are the gauge processes on $\mathcal{F}_+$ and $\mathcal{F}_-$, respectively. The operator $F_z:\ \mathbb{C}^{2^N}\to\mathbb{C}^{2^N}$ is the collective z-component of the spin of the atoms

$$F_z = \sum_{i=1}^{N} I_2^{\otimes i-1}\otimes\sigma_z\otimes I_2^{\otimes N-i}.$$

Equation (3.7) shows that right polarized photons rotate the spin over a positive angle κ along the z-axis and left polarized photons rotate the spin over a negative angle κ along the z-axis.

4 Quantum Filtering

In this section we formulate the filtering problem and solve it by a change of measure technique that is inspired by classical filtering theory [20, 12, 29]. Quantum filtering has been introduced by Belavkin using martingale methods [3, 4], see also [6]. The treatment below follows [8, 9] and is based on the quantum Bayes formula and a trick introduced by Holevo [15].

4.1 The Filtering Problem

Let $(\mathcal{B}, \rho)$ be the quantum probability space with which we model a certain system of interest, e.g. a two-level atom, a dilute gas of atoms, an atom in a cavity, or a harmonic oscillator. The system of interest is coupled to the electromagnetic field $(\mathcal{W}, \phi)$ which we will take to be in the vacuum state. The combined system is then described by the quantum probability space $(\mathcal{B} \otimes \mathcal{W}, \mathbb{P})$ where $\mathbb{P} = \rho \otimes \phi$. Suppose the interaction between the system of interest and the electromagnetic field is given by a QSDE of the following type

$$dU_t = \left\{ L dA_t^* - L^* dA_t - \frac{1}{2} L^* L dt - iH dt \right\} U_t, \qquad U_0 = I, \tag{4.1}$$

where L and H are elements in $\mathcal{B}$, H being selfadjoint. For reasons of convenience we have restricted ourselves to only a single channel in the field and no gauge terms in the QSDE.

We will work in the Heisenberg picture, i.e. the state $\mathbb{P}$ remains fixed and the observables evolve in time according to $j_t(S) = U_t^* S U_t$ where S is an element in $\mathcal{B} \otimes \mathcal{W}$. Let X be a system operator, i.e. $X \in \mathcal{B}$, then it follows from the quantum Itô rule that

$$dj_t(X) = j_t\big(\mathcal{L}(X)\big)dt + j_t\big([L^*, X]\big)dA_t + j_t\big([X, L]\big)dA_t^*. \tag{4.2}$$

We will call Equation (4.2) the *system*.

In the field we are doing a measurement continuously in time. We will allow for two possible measurement setups, direct photon detection, for which the observations are given by $Y_t^\Lambda = U_t^* \Lambda_t U_t$, and homodyne detection, for which the observations are given by $Y_t^W = U_t^*(e^{-i\phi_t} A_t + e^{i\phi_t} A_t^*)U_t$. For convenience we will choose $\phi_t = 0$. We will not go further into the details of the homodyne detection setup here, but instead refer to [2]. Using the quantum Itô rule we obtain

$$\begin{aligned} dY_t^\Lambda &= d\Lambda_t + j_t(L)dA_t^* + j_t(L^*)dA_t + j_t(L^*L)dt, \\ dY_t^W &= j_t(L + L^*)dt + dA_t + dA_t^*. \end{aligned} \tag{4.3}$$

The quantum probability space $(\mathcal{B} \otimes \mathcal{W}, \mathbb{P})$ together with Equations (4.2) and (4.3) define a system-observations model, in analogy to the system-observation models in classical stochastic control theory.

Only if the observations at different times commute with each other, can we observe them in a single realization of an experiment. The requirement that the observations are commutative is called the *self-nondemolition* property. Note that if the observations are self-nondemolition, then they can be mapped onto a classical stochastic process via the spectral theorem. This classical stochastic process can be read off from the measurement apparatus while the measurement is taking place continuously in time. Let us now check that the observation processes Y_t^Λ and Y_t^W are indeed self-nondemolition. Let Z be an operator of the form $I \otimes Z \otimes I_{[s}$ on $\mathcal{H} \otimes \mathcal{F}_{s]} \otimes \mathcal{F}_{[s}$. It follows from the quantum Itô rules that for all $t \geq s$

$$U_t^* Z U_t = U_s^* Z U_s + \int_s^t U_r^* \mathcal{L}(Z) U_r dr + \int_s^t U_r^* [Z, L] U_r dA_r^* + \int_s^t U_r^* [L^*, Z] U_r dA_r.$$

Since Z is a field operator and L and H are system operators, we have that $\mathcal{L}(Z) = [L, Z] = [L^*, Z] = 0$. Therefore we have $U_t^* Z U_t = U_s^* Z U_s$. Using this result with $Z = \Lambda_s$, we find

$$[Y_t^\Lambda, Y_s^\Lambda] = [U_t^* \Lambda_t U_t, U_s^* \Lambda_s U_s] = [U_t^* \Lambda_t U_t, U_t^* \Lambda_s U_t] = U_t^* [\Lambda_t, \Lambda_s] U_t = 0,$$

where we used that $[\Lambda_t, \Lambda_s] = 0$. In a similar way we find $[Y_t^W, Y_s^W] = 0$. That is, both processes Y^Λ and Y^W are self-nondemolition. Note however that $[Y_t^\Lambda, Y_t^W] \neq 0$, we can not observe both processes in a single realization of the experiment.

Define the von Neumann algebra generated by the observations up to time t by $\mathcal{Y}_t = \mathrm{vN}\{Y_s;\ 0 \leq s \leq t\}$, where Y_s is either Y_s^Λ in case of direct photodetection, or Y_s^W in case of homodyne detection. We would like to estimate $j_t(X)$ for all operators $X \in \mathcal{B}$ based on the observations up to time t. That is, we would like to calculate the conditional expectation $\mathbb{P}(j_t(X)|\mathcal{Y}_t)$ which is the mean least squares estimate of $j_t(X)$ given $\mathcal{Y}_t$. However, in order for $\mathbb{P}(j_t(X)|\mathcal{Y}_t)$ to be well-defined, we have to show that $j_t(X)$ is in the commutant of $\mathcal{Y}_t$. This requirement is called the *nondemolition* property. To show that $j_t(X)$ is nondemolished by $\mathcal{Y}_t$ we again use that $U_s^* Z U_s = U_t^* Z U_t$ for all operators of the form $I \otimes Z \otimes I_{[s}$ on $\mathcal{H} \otimes \mathcal{F}_{s]} \otimes \mathcal{F}_{[s}$. If we take $Z = A_s + A_s^*$ when $Y_s = Y_s^W$ and $Z = \Lambda_s$ when $Y_s = Y_s^\Lambda$, then we obtain

$$[j_t(X), Y_s] = [U_t^* X U_t, U_s^* Z U_s] = [U_t^* X U_t, U_t^* Z U_t] = U_t^* [X, Z] U_t = 0,$$

where we used that $[X, Z] = 0$ since X is a system operator and Z is a field operator. This establishes the nondemolition property and therefore also that $\mathbb{P}(j_t(X)|\mathcal{Y}_t)$ is well-defined.

We will now focus on finding the filtering equation, i.e. a recursive equation for updating $\mathbb{P}(j_t(X)|\mathcal{Y}_t)$ in real time. Note that since $\mathbb{P}(j_t(X)|\mathcal{Y}_t)$ depends linearly on X and is positive and normalized, we can define an *information state* π_t on $\mathcal{B}$ by

$$\pi_t(X) = \iota\left(\mathbb{P}\big(j_t(X)\big|\mathcal{Y}_t\big)\right),$$

where ι maps Y_t to a classical process via the spectral theorem. Note that π_t is a stochastic state, it depends on the observations up to time t. The filtering equation propagates the information state π_t in time and is driven by the observations.

4.2 Change of State

Homodyne Detection

Suppose that we are doing a homodyne detection experiment and that the interaction between the system of interest and the field is given by Equation (4.1). Our system-observations pair is then given by the quantum probability space $(\mathcal{B} \otimes \mathcal{W}, \mathbb{P})$ and the equations

$$dj_t(X) = j_t\big(\mathcal{L}(X)\big)dt + j_t\big([L^*, X]\big)dA_t + j_t\big([X, L]\big)dA_t^*,$$
$$dY_t = j_t(L + L^*)dt + dA_t + dA_t^*.$$

Solving the corresponding filtering problem means to find a recursive equation that propagates $\mathbb{P}(j_t(X)|\mathcal{Y}_t)$ in real time. Our strategy will be to change to a different state $\mathbb{R}^t$, the so-called *reference state*. We will choose the reference state $\mathbb{R}^t$ such that the observations have independent increments. That will make it easier to manipulate conditional expectations. Using the Bayes formula we can relate conditional expectations with respect to $\mathbb{R}^t$ back to conditional expectations with respect to $\mathbb{P}$.

Note that the process $A_s + A_s^*,\ 0 \le s \le t$ is a Wiener process under $\mathbb{P}$, i.e. it has independent increments under $\mathbb{P}$. Therefore, if we define a reference state

$$\mathbb{R}^t(S) = \mathbb{P}(U_t S U_t^*), \qquad S \in U_t^* \mathcal{B} \otimes \mathcal{W} U_t,$$

then we see that under this state the observations $Y_s = j_s(A_s + A_s^*) = j_t(A_s + A_s^*)$ form a Wiener process. That is, under $\mathbb{R}^t$, the observation process $Y_s = j_s(A_s + A_s^*),\ 0 \le s \le t$ has independent increments. Moreover, under $\mathbb{R}^t$ the system $j_t(X)$ $(X \in \mathcal{B})$ and the observations $Y_s,\ 0 \le s \le t$ are independent. From the definition it is immediate that

$$\mathbb{P}(S) = \mathbb{R}^t(U_t^* S U_t), \qquad S \in \mathcal{B} \otimes \mathcal{W}.$$

We would now like to use the Bayes formula with $Q = U_t$ to relate conditional expectations with respect to $\mathbb{P}$ to conditional expectations with respect to $\mathbb{R}^t$. However, U_t is not in the commutant of $\mathcal{Y}_t$. The following trick, in the spirit of [15], resolves this problem.

We search for an element Q_t that satisfies the following two requirements

$$\begin{aligned} &1. \quad \mathbb{R}^t(U_t^* S U_t) = \mathbb{R}^t(Q_t^* S Q_t), \qquad S \in \mathcal{B} \otimes \mathcal{W}, \\ &2. \quad Q_t \text{ is affiliated to the commutant of } \mathcal{Y}_t. \end{aligned} \tag{4.4}$$

We could then use the Bayes formula with $Q = Q_t$, to obtain

$$\mathbb{P}\big(j_t(X)\big|\mathcal{Y}_t\big) = \frac{\mathbb{R}^t\big(Q_t^* j_t(X) Q_t \big| \mathcal{Y}_t\big)}{\mathbb{R}^t\big(Q_t^* Q_t \big| \mathcal{Y}_t\big)}. \tag{4.5}$$

The two conditions of Equation (4.4) are satisfied if we can find an element Q_t that satisfies

$$\begin{array}{ll} 1. & Q_t U_t^* v \otimes \Phi = v \otimes \Phi, \quad \forall v \in \mathcal{H}, \\ 2. & Q_t \text{ is affiliated to the commutant of } \mathcal{Y}_t. \end{array} \tag{4.6}$$

Or equivalently, if we can find an element V_t that satisfies

$$\begin{array}{ll} 1. & V_t v \otimes \Phi = U_t v \otimes \Phi, \quad \forall v \in \mathcal{H}, \\ 2. & V_t \text{ is affiliated to the commutant of } \mathcal{C}_t, \end{array} \tag{4.7}$$

where $\mathcal{C}_t = U_t \mathcal{Y}_t U_t^* = \mathrm{vN}\{A_s + A_s^*;\ 0 \leq s \leq t\}$. Indeed, if V_t satisfies the conditions in Equation (4.7), then $Q_t = j_t(V_t)$ satisfies the conditions in Equation (4.6) and subsequently Equation (4.4). Let V_s for $0 \leq s \leq t$ be given by

$$dV_t = \left\{ L\big(dA_t^* + dA_t\big) - \frac{1}{2} L^* L dt - iH dt \right\} V_t, \quad V_0 = I, \tag{4.8}$$

then $V_t v \otimes \Phi = U_t v \otimes \Phi$ for all $v \in \mathcal{H}$. Moreover, the equation is driven by $dA_t + dA_t^*$ and the coefficients L and H are in the commutant of $\mathcal{C}_t$, i.e. V_s is for all $0 \leq s \leq t$ affiliated to the commutant of $\mathcal{C}_t$. We conclude that V_t given by Equation (4.8) satisfies the conditions in Equation (4.7).

On $\mathcal{B}$ we define an unnormalized information state by

$$\sigma_t(X) = \mathbb{R}^t(Q_t^* j_t(X) Q_t | \mathcal{Y}_t) = \mathbb{R}^t(j_t(V_t^* X V_t) | \mathcal{Y}_t).$$

From the Bayes rule Equation (4.5) it is immediate that

$$\pi_t(X) = \frac{\sigma_t(X)}{\sigma_t(I)}. \tag{4.9}$$

This is the quantum analogue of the classical Kallianpur-Striebel formula. We will now focus on finding an equation that propagates $\sigma_t(X)$ in time. From the definition of conditional expectations it easily follows that $\mathbb{R}^t(j_t(V_t^* X V_t)|\mathcal{Y}_t) = U_t^* \mathbb{P}(V_t^* X V_t | \mathcal{C}_t) U_t$. Since V_t is driven by classical noise, we can resort to the classical Itô calculus from here onwards. The Itô rule gives

$$dV_t^* X V_t = V_t^* \mathcal{L}(X) V_t dt + V_t^* (L^* X + XL) V_t (dA_t + dA_t^*).$$

In integral form this reads

$$V_t^* X V_t = X + \int_0^t V_s^* \mathcal{L}(X) V_s ds + \int_0^t V_s^* (L^* X + XL) V_s (dA_s + dA_s^*).$$

Taking the conditional expectation $\mathbb{P}(\,\cdot\,|\mathcal{C}_t)$ of this equation gives

$$\mathbb{P}\big(V_t^* X V_t \big| \mathcal{C}_t\big) = \mathbb{P}\big(X\big|\mathcal{C}_t\big) + \int_0^t \mathbb{P}\big(V_s^* \mathcal{L}(X) V_s \big| \mathcal{C}_t\big) ds + \int_0^t \mathbb{P}\big(V_s^*(L^*X + XL)V_s\big|\mathcal{C}_t\big)(dA_s + dA_s^*),$$

where we have approximated the integrals by simple functions in the usual way and have taken the integrators out using the module property of the conditional expectation. For adapted processes L_s we have that $\mathbb{P}(L_s|\mathcal{C}_t) = \mathbb{P}(L_s|\mathcal{C}_s)$ for all $s \leq t$. This is where our clever choice for the reference state $\mathbb{R}^t$ pays off. We use here that $\mathcal{C}_{[s,t]}$ is independent of $\mathcal{C}_s$ under $\mathbb{P}$, or equivalently, that $\mathcal{Y}_{[s,t]}$ is independent of $\mathcal{Y}_s$ under $\mathbb{R}^t$. Note that that is exactly how we had chosen the reference state $\mathbb{R}^t$. This means we now have

$$\mathbb{P}\big(V_t^* X V_t \big| \mathcal{C}_t\big) = \mathbb{P}(X) + \int_0^t \mathbb{P}\big(V_s^* \mathcal{L}(X) V_s \big| \mathcal{C}_s\big) ds + \int_0^t \mathbb{P}\big(V_s^*(L^*X + XL)V_s\big|\mathcal{C}_s\big)(dA_s + dA_s^*).$$

Sandwiching with U_t leads to the following linear quantum filtering equation

$$d\sigma_t(X) = \sigma_t\big(\mathcal{L}(X)\big)dt + \sigma_t(L^*X + XL)dY_t.$$

This equation is the quantum analogue of the classical Duncan-Mortensen-Zakai equation [20, 12, 29]. Using the Kallianpur-Striebel formula Equation (4.9) and the Itô rule, we obtain the normalized quantum filtering equation

$$d\pi_t(X) = \pi_t\big(\mathcal{L}(X)\big)dt + \Big(\pi_t(L^*X+XL) - \pi_t(L^*+L)\pi_t(X)\Big)\Big(dY_t - \pi_t(L^*+L)dt\Big). \tag{4.10}$$

This equation is a quantum analogue of the classical Kushner-Stratonovich equation. The process $dY_t - \pi_t(L^* + L)dt$ driving the quantum filter is called the *innovations* or the *innovating martingale*. In subsection 4.3 we will prove that the innovations indeed form a martingale.

Direct Photodetection

Now suppose that instead of a homodyne detection experiment we are directly counting photons in the field. Our system-observations pair is then given by the quantum probability space $(\mathcal{B} \otimes \mathcal{W}, \mathbb{P})$ and the equations

$$dj_t(X) = j_t\big(\mathcal{L}(X)\big)dt + j_t\big([L^*, X]\big)dA_t + j_t\big([X, L]\big)dA_t^*,$$
$$dY_t = d\Lambda_t + j_t(L)dA_t^* + j_t(L^*)dA_t + j_t(L^*L)dt.$$

To solve the corresponding filtering problem, we again change to a different state $\mathbb{R}^t$, the so-called *reference state* for the counting experiment. We choose the reference state such that the observation process has independent increments. Moreover, we want the measure induced on the observations $\mathcal{Y}_t$ by the reference measure $\mathbb{R}^t$ to be absolutely continuous with respect to the measure induced by $\mathbb{P}$. This last requirement rules out the reference state we used previously for the homodyne case, since under this measure the counting observations will be identical zero, whereas under $\mathbb{P}$ this is not the case. If we would ignore this problem and would proceed naively with the reference state from the previous section, we would find that we are unable to find a suitable Radon-Nikodym derivative Q_t.

We solve the above difficulty by using a reference state that turns the observations into a Poisson process. Let the Weyl operator W_t be given by

$$dW_t = \left\{ dA_t - dA_t^* - \frac{1}{2}dt \right\} W_t, \qquad W_0 = I.$$

Define $U_t' = W_t U_t$, then U_t' satisfies the following QSDE

$$dU_t' = \left\{ (L - I)dA_t^* - (L^* - I)dA_t - \frac{1}{2}(L^*L + I - 2L + 2iH)dt \right\}, \quad U_0' = I. \tag{4.11}$$

Let the reference state $\mathbb{R}^t$ be given by

$$\mathbb{R}^t(S) = \mathbb{P}(U'_t S U_t'^*), \qquad S \in U_t'^* \mathcal{B} \otimes \mathcal{W} U_t'.$$

Note that under $\mathbb{R}^t$ we have that the process $Y_s,\ 0 \le s \le t$ is a Poisson process, i.e. the observations have independent increments. Moreover, note that under $\mathbb{R}^t$ $j_t(X)$ and $Y_s = j_s(\Lambda_s) = j_t(\Lambda_s)$ are independent for all $X \in \mathcal{B}$. From the definition it is immediate that

$$\mathbb{P}(S) = \mathbb{R}^t(U_t'^* S U_t'), \qquad S \in \mathcal{B} \otimes \mathcal{W}.$$

As before we would now like to apply the Bayes formula. However, Equation (4.11) shows that U_t' is not in the commutant of $\mathcal{Y}_t$. We will use the same trick as before to solve this problem [15].

We search for an element Q_t that satisfies the following two requirements

$$\begin{aligned} &1. \quad \mathbb{R}^t(U_t'^* S U_t') = \mathbb{R}^t(Q_t^* S Q_t), \qquad S \in \mathcal{B} \otimes \mathcal{W}, \\ &2. \quad Q_t \text{ is affiliated to the commutant of } \mathcal{Y}_t. \end{aligned} \tag{4.12}$$

These conditions are satisfied if we can find an element Q_t that satisfies

$$\begin{aligned} &1. \quad Q_t U_t'^* v \otimes \Phi = v \otimes \Phi, \qquad \forall v \in \mathcal{H}, \\ &2. \quad Q_t \text{ is affiliated to the commutant of } \mathcal{Y}_t. \end{aligned} \tag{4.13}$$

Or equivalently, if we can find an element V_t that satisfies

$$\begin{aligned} &1. \quad V_t' v \otimes \Phi = U_t' v \otimes \Phi, \qquad \forall v \in \mathcal{H}, \\ &2. \quad V_t' \text{ is affiliated to the commutant of } \mathcal{C}_t, \end{aligned} \tag{4.14}$$

where $\mathcal{C}_t = U_t' \mathcal{Y}_t U_t'^* = \mathrm{vN}\{W_s \Lambda_s W_s^*;\ 0 \le s \le t\}$. Indeed, if we can find a V_t' satisfying Equation (4.14), then $Q_t = U_t'^* V_t' U_t'$ satisfies Equations (4.13) and

(4.12). Note that $Z_t = W_t \Lambda_t W_t^*$ is given by

$$dZ_t = d\Lambda_t + dA_t + dA_t^* + dt, \qquad Z_0 = 0.$$

Let V_s' for $0 \le s \le t$ be given by

$$dV_t' = \left\{ (L-1)dZ_t - \frac{1}{2}(L^*L + I + 2iH)dt \right\} V_t', \qquad V_0 = I, \tag{4.15}$$

then $V_t' v \otimes \Phi = U_t' v \otimes \Phi$ for all $v \in \mathcal{H}$. Moreover, the equation is driven by dZ_t and the coefficients L and H are in the commutant of $\mathcal{C}_t$, i.e. V_s' is affiliated to the commutant of $\mathcal{C}_t$ for all $0 \le s \le t$. This means that V_t' given by Equation (4.15) satisfies the conditions in Equation (4.14).

We can now apply the Bayes formula with $Q_t = U_t'^* V_t' U_t'$, i.e.

$$\mathbb{P}\big(j_t(X)\big|\mathcal{Y}_t\big) = \frac{\mathbb{R}^t\big(Q_t^* j_t(X) Q_t\big|\mathcal{Y}_t\big)}{\mathbb{R}^t(Q_t^* Q_t|\mathcal{Y}_t)}, \qquad X \in \mathcal{B}.$$

On $\mathcal{B}$ we define an unnormalized information state by

$$\sigma_t(X) = \mathbb{R}^t\big(Q_t^* j_t(X) Q_t\big|\mathcal{Y}_t\big) = \mathbb{R}^t\big(U_t'^* V_t'^* X V_t' U_t'\big|\mathcal{Y}_t\big),$$

where in the second step we used that $X \in \mathcal{B}$ commutes with W_t. From the Bayes formula it is immediate that

$$\pi_t(X) = \frac{\sigma_t(X)}{\sigma_t(I)}, \qquad X \in \mathcal{B}. \tag{4.16}$$

We will now focus on finding an equation that propagates $\sigma_t(X)$ in time. From the definition of the conditional expectation it easily follows that $\mathbb{R}^t\big(U_t'^* V_t'^* X V_t' U_t'\big|\mathcal{Y}_t\big) = U_t'^* \mathbb{P}(V_t'^* X V_t'|\mathcal{C}_t) U_t'$. The Itô rule gives

$$dV_t'^* X V_t' = V_t'^* \mathcal{L}(X) V_t' dt + V_t'(L^* X L - X) V_t'(dZ_t - dt).$$

Using analogous arguments as in the homodyne case, we obtain the linear quantum filter

$$\sigma_t(X) = \sigma_t\big(\mathcal{L}(X)\big)dt + \big(\sigma_t(L^*XL) - \sigma_t(X)\big)\big(dY_t - dt\big).$$

Using Equation (4.16) and the Itô rule, we obtain the normalized quantum filter for photon counting

$$d\pi_t(X) = \pi_t\big(\mathcal{L}(X)\big)dt + \left(\frac{\pi_t(L^*XL)}{\pi_t(L^*L)} - \pi_t(X)\right)\big(dY_t - \pi_t(L^*L)dt\big).$$

The process $dY_t - \pi_t(L^*L)dt$ is called the *innovations* or the *innovating martingale* for the photon counting experiment. In the next subsection we prove that this process indeed forms a martingale.

4.3 Innovations

In martingale based approaches to quantum filtering [4],[6], the following theorem is the starting point. The proof below is an adaptation to the Heisenberg picture of the proof in [6]. It can also be found in [8], [7].

Theorem 4.1. *Let Y_t be given by $Y_t = U_t^* Z_t U_t$, where $dZ_t = a_t d\Lambda_t + \overline{b}_t dA_t + b_t dA_t^*$, $Z_0 = 0$ and $a_t \in \mathbb{R}$ and $b_t \in \mathbb{C}$ for all $t \geq 0$. Denote by $\mathcal{Y}_t$ the von Neumann algebra generated by Y_s for $0 \leq s \leq t$. Define the* innovations *$\tilde{Y}_t$ by*

$$\tilde{Y}_t = Y_t - \int_0^t \mathbb{P}\Big(a_s U_s^* L^* L U_s + \overline{b}_s U_s^* L U_s + b_s U_s^* L^* U_s \big| \mathcal{Y}_s\Big) ds.$$

The innovations are a martingale, i.e. $\mathbb{P}(\tilde{Y}_t|\mathcal{Y}_s) = \tilde{Y}_s$ for all $0 \leq s \leq t$.

Proof. We have to show that $\mathbb{P}(\tilde{Y}_t - \tilde{Y}_s|\mathcal{Y}_s) = 0$ for all $0 \leq s \leq t$. This means we need to prove that $\mathbb{P}\big((\tilde{Y}_t - \tilde{Y}_s)K\big) = 0$ for all $0 \leq s \leq t$ and $K \in \mathcal{Y}_s$. This is equivalent to showing that

$$\mathbb{P}(Y_t K) - \mathbb{P}(Y_s K) = \int_s^t \mathbb{P}\Big(\mathbb{P}(a_r U_r^* L^* L U_r + \overline{b}_r U_r^* L U_r + b_r U_r^* L^* U_r|\mathcal{Y}_r)K\Big) dr,$$

for all $0 \leq s \leq t$ and for all $K \in \mathcal{Y}_s$. For $t = s$ the above equation is obviously true. It therefore remains to show that for all $K \in \mathcal{Y}_s$ and all $s \leq r \leq t$

$$\begin{aligned} d\mathbb{P}(Y_r K) &= \mathbb{P}\Big(\mathbb{P}(a_r U_r^* L^* L U_r + \overline{b}_r U_r^* L U_r + b_r U_r^* L^* U_r|\mathcal{Y}_r)K\Big) dr \\ &= \mathbb{P}\Big(a_r U_r^* L^* L U_r K + \overline{b}_r U_r^* L U_r K + b_r U_r^* L^* U_r K\Big) dr. \end{aligned}$$

This is just a simple exercise in applying the quantum Itô rule and the relation $Y_r = U_r^* Z_r U_r$.

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Quantum Walks

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Summary. Quantum walks can be considered as a generalized version of the classical random walk. There are two classes of quantum walks, that is, the discrete-time (or coined) and the continuous-time quantum walks. This manuscript treats the discrete case in Part I and continuous case in Part II, respectively. Most of the contents are based on our results. Furthermore, papers on quantum walks are listed in References. Studies of discrete-time walks appeared from the late 1980s from Gudder (1988), for example. Meyer (1996) investigated the model as a quantum lattice gas automaton. Nayak and Vishwanath (2000) and Ambainis et al. (2001) studied intensively the behaviour of discrete-time walks, in particular, the Hadamard walk. In contrast with the central limit theorem for the classical random walks, Konno (2002a, 2005a) showed a new type of weak limit theorems for the one-dimensional lattice. Grimmett, Janson, and Scudo (2004) extended the limit theorem to a wider range of the walks. On the other hand, the continuous-time quantum walk was introduced and studied by Childs, Farhi, and Gutmann (2002). Excellent reviews on quantum walks are found in Kempe (2003), Tregenna et al. (2003), Ambainis (2003), Kendon (2007).

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Part I: Discrete-Time Quantum Walks

1 Limit Theorems

1.1 Two-State Case

Introduction

The classical random walk on the line is the motion of a particle that lives on the set of integers. The particle moves at each time step either one unit to the right with probability p or one unit to the left with probability $1-p$. The directions of different steps are independent of each other. This classical random walk is often called the Bernoulli random walk. For general random walks on a countable space, there is a beautiful theory (see Spitzer (1976)). In this section, we consider quantum variations of the Bernoulli random walk and refer to such processes as quantum walks here.

The quantum walk considered here is determined by a 2×2 unitary matrix U that will be introduced below. We will introduce four other matrices P, Q, R and S which will all be determined by U. The matrices P, Q, R and S will allow us to obtain a combinatorial expression for the characteristic function of the walk and will clarify the dependence of the m-th moment and the symmetry of the distribution of the walk on the unitary matrix U and the initial qubit state φ. Furthermore we give a new type of weak limit theorems for the quantum walk by using our results. Our limit theorem shows that the behavior of quantum walk is remarkably different from that of the classical random walk. As a corollary, it reveals whether some simulation results already known are accurate or not. The results on this section are based on Konno (2002a, 2005a).

The time evolution of the one-dimensional quantum walk studied here is given by the following unitary matrix:

$$U = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \in \mathrm{U}(2)$$

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where $a, b, c, d \in \mathbb{C}$. Here $\mathbb{C}$ is the set of complex numbers, and U(2) is the set of 2×2 unitary matrices. So we have

$$|a|^2 + |c|^2 = |b|^2 + |d|^2 = 1, \qquad a\overline{c} + b\overline{d} = 0,$$
$$c = -\triangle\overline{b}, \qquad d = \triangle\overline{a},$$

where $\overline{z}$ is a complex conjugate of $z \in \mathbb{C}$ and $\triangle = \det U = ad - bc$. We should note that the unitarity of U gives $|\triangle| = 1$.

The quantum walk is a quantum generalization of the classical Bernoulli random walk in one dimension with an additional degree of freedom called the chirality. The walk can also be considered as a quantum version of the so-called correlated random walk. There is a strong structural similarity between them (see Konno (2003)). The chirality takes values *left* and *right*, and means the direction of the motion of the particle. The evolution of the quantum walk is given by the following rule. At each time step, if the particle has the left chirality, it moves one unit to the left, and if it has the right chirality, it moves one unit to the right.

More precisely, the unitary matrix U acts on two chirality states $|L\rangle$ and $|R\rangle$:

$$|L\rangle \;\rightarrow\; a|L\rangle + c|R\rangle, \quad |R\rangle \;\rightarrow\; b|L\rangle + d|R\rangle,$$

where L and R refer to the right and left chirality state respectively. In fact, define

$$|L\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \qquad |R\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix},$$

so we have

$$U|L\rangle = a|L\rangle + c|R\rangle, \quad U|R\rangle = b|L\rangle + d|R\rangle.$$

The study of the dependence of some important quantities (e.g., characteristic function, the m-th moment, limit theorem) on initial *qubit* state is one of the essential parts, so we define the set of initial qubit states as follows:

$$\varPhi = \left\{ \varphi = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \in \mathbb{C}^2 : |\alpha|^2 + |\beta|^2 = 1 \right\}.$$

Let X_n be the *quantum walk* at time n starting from initial qubit state $\varphi \in \varPhi$. It should be noted that $P(X_n = 0) = 1$. In contrast with classical random walks, X_n can not be written as $X_n = Y_1 + \cdots + Y_n$, where $Y_1, Y_2, \ldots$ are independent and identically distributed random variables. The precise definition of X_n will appear in the next subsection. Here we explain X_n briefly. To do so, we introduce the following matrices P and Q:

$$P = \begin{bmatrix} a & b \\ 0 & 0 \end{bmatrix}, \quad Q = \begin{bmatrix} 0 & 0 \\ c & d \end{bmatrix}.$$

Remark that

$$U = P + Q.$$

For fixed l and m with $l + m = n$ and $-l + m = x$,

$$\Xi_n(l,m) = \sum_{l_j,m_j} P^{l_1}Q^{m_1}P^{l_2}Q^{m_2}\cdots P^{l_n}Q^{m_n}$$

summed over all $l_j, m_j \geq 0$ satisfying $l_1 + \cdots + l_n = l$, $m_1 + \cdots + m_n = m$ and $l_j + m_j = 1$. Moreover, to define $P(X_n = x)$, it is convenient to introduce

$$R = \begin{bmatrix} c & d \\ 0 & 0 \end{bmatrix}, \quad S = \begin{bmatrix} 0 & 0 \\ a & b \end{bmatrix}.$$

An expression of $\Xi_n(l,m)$ can be given by using P, Q, R and S (see Lemma 1.1). The definition of $\Xi_n(l,m)$ gives

$$P(X_n = x) = (\Xi_n(l,m)\varphi)^*(\Xi_n(l,m)\varphi) = \|\Xi_n(l,m)\varphi\|^2,$$

where $n = l + m$, $x = -l + m$ and $*$ means the adjoint operator. From this expression, we will obtain the characteristic function of X_n (Theorem 1.3) and the m-th moment of it (Corollary 1.4). One of the interesting results is that when m is even, the m-th moment of X_n is independent of the initial qubit state $\varphi \in \Phi$. On the other hand, when m is odd, the m-th moment depends on the initial qubit state. So the standard deviation of X_n is not independent of the initial qubit state $\varphi \in \Phi$.

By using the characteristic function of X_n, we give the following new type of limit theorems in $abcd \neq 0$ case (Theorem 1.6). If $n \to \infty$, then

$$\frac{X_n}{n} \quad \Rightarrow \quad Z,$$

where Z has a density

$$\begin{aligned} f(x) &= f(x; \varphi = {}^T[\alpha,\beta]) \\ &= \frac{\sqrt{1-|a|^2}}{\pi(1-x^2)\sqrt{|a|^2-x^2}} \left\{1 - \left(|\alpha|^2 - |\beta|^2 + \frac{a\alpha\overline{b\beta} + \overline{a\alpha}b\beta}{|a|^2}\right)x\right\}, \end{aligned}$$

for $x \in (-|a|, |a|)$, and $f(x) = 0$ for $|x| \geq |a|$, where $Y_n \Rightarrow Y$ means that Y_n converges weakly to a limit Y and T indicates the transposed operator. We remark that standard deviation of Z is not independent of initial qubit state $\varphi = {}^T[\alpha,\beta]$.

Moreover if $b = 0$, then $c = 0$ and $|a| = |d| = 1$. So this case is trivial. In fact, Theorem 1.3 (ii) implies that $X_n/n \Rightarrow W^{(1)}$, where $W^{(1)}$ is determined by $P(W^{(1)} = -1) = |\alpha|^2$ and $P(W^{(1)} = 1) = |\beta|^2$. If $a = 0$, then $d = 0$ and $|b| = |c| = 1$. So this case is also trivial. Theorem 1.3 (iii) implies that $X_n/n \Rightarrow W^{(2)}$, where $W^{(2)}$ is determined by $\delta_0(x)$, where $\delta_a(x)$ denotes the pointmass at a.

The above weak limit theorem suggests the following result on the symmetry of the distribution for quantum walks (Theorem 1.5). Define

$$\Phi_s = \{\varphi \in \Phi : \ P(X_n = x) = P(X_n = -x) \ \text{for any} \, n \in \mathbb{Z}_+ \ \text{and} \ x \in \mathbb{Z}\},$$
$$\Phi_0 = \{\varphi \in \Phi : \ E(X_n) = 0 \ \text{for any} \, n \in \mathbb{Z}_+\},$$
$$\Phi_\perp = \left\{\varphi = {}^T[\alpha, \beta] \in \Phi : |\alpha| = |\beta|, \ a\alpha\overline{b\beta} + \overline{a\alpha}b\beta = 0\right\},$$

and $\mathbb{Z}$ (resp. $\mathbb{Z}_+$) is the set of (resp. non-negative) integers. For $\varphi \in \Phi_s$, the probability distribution of X_n is symmetric for any $n \in \mathbb{Z}_+$. Using explicit forms of distribution of X_n (Lemma 1.2) and $E(X_n)$ (Corollary 1.4 (i) for $m = 1$ case), we have

$$\Phi_s = \Phi_0 = \Phi_\perp.$$

Nayak and Vishwanath (2000) discussed the symmetry of distribution and showed that ${}^T[1/\sqrt{2}, \ \pm i/\sqrt{2}] \in \Phi_s$ for the Hadamard walk.

In the rest of this subsection, we focus on the Hadamard walk which has been extensively investigated in the study of quantum walks. The unitary matrix U of the Hadamard walk is defined by the following Hadamard gate (see Nielsen and Chuang (2000)):

$$U = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

The dynamics of this walk corresponds to that of the symmetric random walk in the classical case. However the symmetry of the Hadamard walk depends heavily on initial qubit state, see Konno, Namiki, and Soshi (2004).

For example, in the case of the Hadamard walk with initial qubit state $\varphi = {}^T[1/\sqrt{2}, i/\sqrt{2}]$ (symmetric case), direct computation gives

$$P(X_4 = -4) = P(X_4 = 4) = 1/16,$$
$$P(X_4 = -2) = P(X_4 = 2) = 6/16, \quad P(X_4 = 0) = 2/16.$$

In contrast with the above result, as for the classical symmetric random walk Y_n^o starting from the origin, we see that

$$P(Y_4^o = -4) = P(Y_4^o = 4) = 1/16,$$
$$P(Y_4^o = -2) = P(Y_4^o = 2) = 4/16, \quad P(Y_4^o = 0) = 6/16.$$

In fact, quantum walks behave quite differently from classical random walks. For the classical walk, the probability distribution is a binomial distribution. On the other hand, the probability distribution in the quantum walk has a complicated, oscillatory form.

Now we compare our analytical results (Theorem 1.6) with the numerical ones given by Mackay et al. (2002), Travaglione and Milburn (2002) for the the Hadamard walk. In this case, our weak limit theorem (Theorem 1.6) implies that if $-1/\sqrt{2} \le a < b \le 1/\sqrt{2}$, then as $n \to \infty$,

$$P(a \le X_n/n \le b) \to \int_a^b \frac{1-(|\alpha|^2-|\beta|^2+\alpha\overline{\beta}+\overline{\alpha}\beta)x}{\pi(1-x^2)\sqrt{1-2x^2}}dx,$$

for any initial qubit state $\varphi = {}^T[\alpha,\beta]$. For the classical symmetric random walk Y_n^o starting from the origin, the well-known central limit theorem implies that if $-\infty < a < b < \infty$, then as $n \to \infty$,

$$P(a \le Y_n^o/\sqrt{n} \le b) \to \int_a^b \frac{e^{-x^2/2}}{\sqrt{2\pi}}dx.$$

This result is often called the de Moivre-Laplace theorem. When we take $\varphi = {}^T[1/\sqrt{2}, i/\sqrt{2}]$ (symmetric case), then we have the following quantum version of the de Moivre-Laplace theorem: if $-1/\sqrt{2} \le a < b \le 1/\sqrt{2}$, then as $n \to \infty$,

$$P(a \le X_n/n \le b) \to \int_a^b \frac{1}{\pi(1-x^2)\sqrt{1-2x^2}}dx.$$

There is a remarkable difference between the quantum walk X_n and the classical one Y_n^o even in a symmetric case for $\varphi = {}^T[1/\sqrt{2}, i/\sqrt{2}]$. Noting that $E(X_n) = 0$ $(n \ge 0)$ for any $\varphi \in \Phi_s$, we have

$$sd(X_n)/n \to \sqrt{(2-\sqrt{2})/2} = 0.54119\ldots$$

where $sd(X)$ is the standard deviation of X. This rigorous result reveals that the numerical simulation result $3/5 = 0.6$ given by Travaglione and Milburn (2002) is not so accurate.

As in a similar way, when we take $\varphi = {}^T[0, e^{i\theta}]$ where $\theta \in [0, 2\pi)$ (asymmetric case), we see that if $-1/\sqrt{2} \le a < b \le 1/\sqrt{2}$, then as $n \to \infty$,

$$P(a \le X_n^{\varphi}/n \le b) \to \int_a^b \frac{1}{\pi(1-x)\sqrt{1-2x^2}}dx.$$

So we have

$$E(X_n)/n \to (2-\sqrt{2})/2 = 0.29289\ldots,$$
$$sd(X_n)/n \to \sqrt{(\sqrt{2}-1)/2} = 0.45508\ldots$$

When $\varphi = {}^T[0,1]$ $(\theta = 0)$, Nayak and Vishwanath (2000) and Ambainis et al. (2001) gave a similar result, but both papers did not treat weak convergence. The former paper took the Fourier analysis, and the latter paper took two approaches, that is, the Fourier analysis and the combinatorial (path integral) approach. However both their results come mainly from Fourier analysis. The details on the derivation based on the combinatorial approach in Ambainis et al. (2001) are not so clear compared with this manuscript.

In another asymmetric case $\varphi = {}^T[e^{i\theta}, 0]$ where $\theta \in [0, 2\pi)$, a similar argument implies that if $-1/\sqrt{2} \le a < b \le 1/\sqrt{2}$, then as $n \to \infty$,

$$P(a \le X_n^{\varphi}/n \le b) \to \int_a^b \frac{1}{\pi(1+x)\sqrt{1-2x^2}} dx.$$

Note that $f(-x; {}^T[e^{i\theta}, 0]) = f(x; {}^T[0, e^{i\theta}])$ for any $x \in (-1/\sqrt{2}, 1/\sqrt{2})$. The symmetry of the distribution gives the same result as in the previous case $\varphi = {}^T[0, e^{i\theta}]$. So the standard deviation of the limit distribution Z is given by $\sqrt{(\sqrt{2}-1)/2} = 0.45508\ldots$. Simulation result 0.4544 ± 0.0012 in Mackay et al. (2002) (their case is $\theta = 0$) is consistent with our rigorous result.

Definition of Quantum Walk

In this subsection, we give a precise definition of the quantum walk. The important point is that P (resp. Q) represents that the particle moves to the left (resp. right). By using P and Q, we define the dynamics of the quantum walk in one dimension. To do so, we introduce the following $(2N+1) \times (2N+1)$ matrix $\overline{U}_N : (\mathbb{C}^2)^{2N+1} \to (\mathbb{C}^2)^{2N+1}$:

$$\overline{U}_N = \begin{bmatrix} 0 & P & 0 & \ldots & \ldots & 0 & Q \\ Q & 0 & P & 0 & \ldots & \ldots & 0 \\ 0 & Q & 0 & P & 0 & \ldots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ldots & 0 & Q & 0 & P & 0 \\ 0 & \ldots & \ldots & 0 & Q & 0 & P \\ P & 0 & \ldots & \ldots & 0 & Q & 0 \end{bmatrix} \qquad \text{with} \qquad 0 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

Let

$$\Psi_n(x) = \begin{bmatrix} \Psi_n^L(x) \\ \Psi_n^R(x) \end{bmatrix} = \Psi_n^L(x)|L\rangle + \Psi_n^R(x)|R\rangle \in \mathbb{C}^2$$

be the two component vector of amplitudes of the particle being at site x and at time n with the chirality being left (upper component) and right (lower component), and

$$\Psi_n = {}^T[\Psi_n(-N), \Psi_n(-(N-1)), \ldots, \Psi_n(N)]$$

be the qubit states at time n. Here the initial qubit state is given by

$$\Psi_0 = {}^T[\overbrace{0, \ldots, 0}^{N}, \varphi, \overbrace{0, \ldots, 0}^{N}] \in \mathbb{C}^{2(2N+1)},$$

where

$$0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad \varphi = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}.$$

The following equation defines the time evolution of the quantum walk:

$$\Psi_{n+1}(x) = (\overline{U}_N \Psi_n)_x = P\Psi_n(x+1) + Q\Psi_n(x-1),$$

where $(\Psi_n)_x = \Psi_n(x), -N \leq x \leq N$ and $1 \leq n < N$. Note that P and Q satisfy

$$PP^* + QQ^* = P^*P + Q^*Q = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad PQ^* = QP^* = Q^*P = P^*Q = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

The above relations imply that $\overline{U}_N$ becomes also unitary matrix.

For initial state $\overline{\varphi} = {}^T[\overbrace{0, \ldots, 0}^{N}, \varphi, \overbrace{0, \ldots, 0}^{N}]$, we have

$$\begin{aligned}
\overline{U}_N \overline{\varphi} &= {}^T[\overbrace{0, \ldots, 0}^{N-1}, P\varphi, 0, Q\varphi, \overbrace{0, \ldots, 0}^{N-1}], \\
\overline{U}_N^2 \overline{\varphi} &= {}^T[\overbrace{0, \ldots, 0}^{N-2}, P^2\varphi, 0, (PQ+QP)\varphi, 0, Q^2\varphi, \overbrace{0, \ldots, 0}^{N-2}], \\
\overline{U}_N^3 \overline{\varphi} &= {}^T[\overbrace{0, \ldots, 0}^{N-3}, P^3\varphi, 0, (P^2Q + PQP + QP^2)\varphi, 0, \\
&\qquad (Q^2P + QPQ + PQ^2)\varphi, 0, Q^3\varphi, \overbrace{0, \ldots, 0}^{N-3}].
\end{aligned}$$

This shows that expansion of $U^n = (P+Q)^n$ for the quantum walk corresponds to that of $1^n = (p+q)^n$ for the classical Bernoulli random walk.

By using $\Psi_n(x)$, the probability of $X_n = x$ is defined by

$$P(X_n = x) = \|\Psi_n(x)\|^2 = |\Psi_n^L(x)|^2 + |\Psi_n^R(x)|^2.$$

It is noted that the quantum walk X_n is not a stochastic process. It is a sequence of distributions arising from products of the unitary matrix $\overline{U}_N$. The unitarity of $\overline{U}_N$ ensures

$$\sum_{x=-n}^{n} P(X_n = x) = \|\overline{U}_N^n \overline{\varphi}\|^2 = \|\overline{\varphi}\|^2 = |\alpha|^2 + |\beta|^2 = 1,$$

for any $1 \leq n \leq N$. That is, the amplitude always defines a probability distribution for the location.

The system considered here belongs to the Hilbert space $H_p \otimes H_c$, where $H_p = \ell^2(\mathbb{Z})$ is associated with the position and $H_c = \mathbb{C}^2$ with the internal degree of freedom (coin space).

Let $|x\rangle \in H_p (x \in \mathbb{Z})$ be the position states of the quantum walk. A unitary shift operator is defined by

$$\hat{S} = \sum_{x\in\mathbb{Z}} |x+1\rangle\langle x|, \quad \hat{S}^{-1} = \hat{S}^* = \sum_{x\in\mathbb{Z}} |x-1\rangle\langle x|.$$

Then

$$\hat{S}|x\rangle = |x+1\rangle, \quad \hat{S}^{-1}|x\rangle = |x-1\rangle.$$

Remark that

$$\hat{S} = \begin{bmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \ldots & 0 & 0 & 0 & 0 & 0 & \ldots \\ \ldots & 1 & 0 & 0 & 0 & 0 & \ldots \\ \ldots & 0 & 1 & 0 & 0 & 0 & \ldots \\ \ldots & 0 & 0 & 1 & 0 & 0 & \ldots \\ \ldots & 0 & 0 & 0 & 1 & 0 & \ldots \\ \ldots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}, \qquad \hat{S}^{-1} = \begin{bmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \ldots & 0 & 1 & 0 & 0 & 0 & \ldots \\ \ldots & 0 & 0 & 1 & 0 & 0 & \ldots \\ \ldots & 0 & 0 & 0 & 1 & 0 & \ldots \\ \ldots & 0 & 0 & 0 & 0 & 1 & \ldots \\ \ldots & 0 & 0 & 0 & 0 & 0 & \ldots \\ \ldots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}.$$

If $\hat{P} = |L\rangle\langle L|$ and $\hat{Q} = |R\rangle\langle R|$ are operations onto the two states of the coin, then one step of the quantum walk is given by the following unitary operator:

$$\overline{U} = (\hat{S} \otimes \hat{Q} + \hat{S}^{-1} \otimes \hat{P})\,(I \otimes U).$$

Noting that $\hat{P}U = P$ and $\hat{Q}U = Q$, we see

$$\overline{U} = \begin{bmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \ldots & O & P & O & O & O & \ldots \\ \ldots & Q & O & P & O & O & \ldots \\ \ldots & O & Q & O & P & O & \ldots \\ \ldots & O & O & Q & O & P & \ldots \\ \ldots & O & O & O & Q & O & \ldots \\ \ldots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \quad \text{with} \quad O = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

Then after n steps of the walk, the state is

$$\Psi_n = \overline{U}^n \Psi_0.$$

In the next subsection, we will obtain an explicit form for $\Psi_n(x)$.

Combinatorial Approach

This subsection gives a combinatorial expression for the characteristic function of the quantum walk X_n. As a corollary, we obtain the m-th moment of X_n. As we explained in the previous subsection, we need to know the following combinatorial expression to study $P(X_n = x)$ for $n + x =$ even. For fixed l and m with $l + m = n$ and $-l + m = x$, we consider

$$\Xi_n(l, m) = \sum_{l_j, m_j} P^{l_1} Q^{m_1} P^{l_2} Q^{m_2} \cdots P^{l_n} Q^{m_n}$$

summed over all $l_j, m_j \geq 0$ satisfying $l_1 + \cdots + l_n = l$, $m_1 + \cdots + m_n = m$ and $l_j + m_j = 1$. We should note that

$$\Psi_n(x) = \Xi_n(l, m)\varphi,$$

since $\Psi_n(x) = {}^T[\Psi_n^L(x), \Psi_n^R(x)] (\in \mathbb{C}^2)$ is a two component vector of amplitudes of the particle being at site x at time n for initial qubit state $\varphi \in \Phi$ and $\Xi_n(l, m)$ is the sum of all possible paths in the trajectory consisting of l steps left and m steps right with $l = (n - x)/2$ and $m = (n + x)/2$. For example, in the case of $P(X_4 = -2)$, we have the following expression:

$$\Xi_4(3, 1) = QP^3 + PQP^2 + P^2QP + P^3Q.$$

Here we find a next nice relation:

$$P^2 = aP.$$

By using this, the above example becomes

$$\Xi_4(3, 1) = a^2QP + aPQP + aPQP + a^2PQ.$$

In general, we obtain the next table of products of the matrices P, Q, R and S:

	P	Q	R	S
P	aP	bR	aR	bP
Q	cS	dQ	cQ	dS
R	cP	dR	cR	dP
S	aS	bQ	aQ	bS

Table 1

where $PQ = bR$, for example. Since P, Q, R and S form an orthonormal basis of the vector space of complex 2×2 matrices with respect to the trace inner product $\langle A|B \rangle = \mathrm{tr}(A^*B)$, $\Xi_n(l, m)$ has the following form:

$$\Xi_n(l, m) = p_n(l, m)P + q_n(l, m)Q + r_n(l, m)R + s_n(l, m)S.$$

Next problem is to obtain explicit forms of $p_n(l, m), q_n(l, m), r_n(l, m)$ and $s_n(l, m)$. In the above example of $n = l + m = 4$ case, we have

$$\Xi_4(4,0) = a^3P, \quad \Xi_4(3,1) = 2abcP + a^2bR + a^2cS,$$
$$\Xi_4(2,2) = bcdP + abcQ + b(ad+bc)R + c(ad+bc)S,$$
$$\Xi_4(1,3) = 2bcdQ + bd^2R + cd^2S, \quad \Xi_4(2,2) = d^3Q.$$

So, for example,

$$p_4(3,1) = 2abc, \quad q_4(3,1) = 0, \quad r_4(3,1) = a^2b, \quad s_4(3,1) = a^2c.$$

In a general case, the next key lemma is obtained.

Lemma 1.1. *We consider quantum walks in one dimension with* $abcd \neq 0$. *Let*

$$P = \begin{bmatrix} a & b \\ 0 & 0 \end{bmatrix}, \quad Q = \begin{bmatrix} 0 & 0 \\ c & d \end{bmatrix}, \quad R = \begin{bmatrix} c & d \\ 0 & 0 \end{bmatrix}, \quad S = \begin{bmatrix} 0 & 0 \\ a & b \end{bmatrix}.$$

and $\triangle = \det U$ *with* $U = P + Q$. *Suppose that* $l, m \geq 0$ *with* $l + m = n$, *then we have*
(i) for $l \wedge m (= \min\{l, m\}) \geq 1$,

$$\Xi_n(l,m) = a^l \overline{a}^m \triangle^m \sum_{\gamma=1}^{l\wedge m} \left(-\frac{|b|^2}{|a|^2} \right)^{\gamma} \binom{l-1}{\gamma-1} \binom{m-1}{\gamma-1} \times \left[\frac{l-\gamma}{a\gamma} P + \frac{m-\gamma}{\triangle \overline{a} \gamma} Q - \frac{1}{\triangle \overline{b}} R + \frac{1}{b} S \right],$$

(ii) for $l (= n) \geq 1, m = 0$,

$$\Xi_n(l,0) = a^{n-1}P,$$

(iii) for $l = 0, m (= n) \geq 1$,

$$\Xi_n(0,m) = \triangle^{n-1} \overline{a}^{n-1} Q.$$

Proof. (a) $p_n(l,m)$ case : First we assume $l \geq 2$ and $m \geq 1$. From Table 1, it is sufficient to consider only the following case in order to compute $p_n(l,m)$:

$$C(P,w)_n^{(2\gamma+1)}(l,m) = \overbrace{PP\cdots P}^{w_1}\overbrace{QQ\cdots Q}^{w_2}\overbrace{PP\cdots P}^{w_3}\cdots\overbrace{QQ\cdots Q}^{w_{2\gamma}}\overbrace{PP\cdots P}^{w_{2\gamma+1}},$$

where $w = (w_1, w_2, \ldots, w_{2\gamma+1}) \in \mathbb{Z}_+^{2\gamma+1}$ with $w_1, w_2, \ldots, w_{2\gamma+1} \geq 1$ and $\gamma \geq 1$. For example, PQP case is $w_1 = w_2 = w_3 = 1$ and $\gamma = 1$. We should remark that l is the number of P's and m is the number of Q's, so we have

$$l = w_1 + w_3 + \cdots + w_{2\gamma+1}, \qquad m = w_2 + w_4 + \cdots + w_{2\gamma}.$$

Moreover $2\gamma+1$ is the number of clusters of P's and Q's. Next we consider the range of γ. The minimum is $\gamma=1$, that is, 3 clusters. This case is

$$P\cdots PQ\cdots QP\cdots P.$$

The maximum is $\gamma=(l-1)\wedge m$. This case is

$$\begin{aligned}&PQPQPQ\cdots PQPQPP\cdots PP\ \ (l-1\geq m),\\&PQPQPQ\cdots PQPQQ\cdots QQP\ \ (l-1\leq m),\end{aligned}$$

for example. Here we introduce a set of sequences with $2\gamma+1$ components: for fixed $\gamma\in[1,(l-1)\wedge m]$

$$\begin{aligned}W(P,2\gamma+1)=\{w=(w_1,w_2,\cdots,w_{2\gamma+1})\in\mathbb{Z}^{2\gamma+1}:w_1+w_3+\cdots+w_{2\gamma+1}=l,\\ w_2+w_4+\cdots+w_{2\gamma}=m,\ w_1,w_2,\ldots,w_{2\gamma},w_{2\gamma+1}\geq 1\}.\end{aligned}$$

By using Table 1, we have

$$\begin{aligned}C(P,w)_n^{(2\gamma+1)}(l,m)&=a^{w_1-1}Pd^{w_2-1}Qa^{w_3-1}P\cdots d^{w_{2\gamma}-1}Qa^{w_{2\gamma+1}-1}P\\&=a^{l-(\gamma+1)}d^{m-\gamma}(PQ)^{\gamma}P\\&=a^{l-(\gamma+1)}d^{m-\gamma}b^{\gamma}R^{\gamma}P\\&=a^{l-(\gamma+1)}d^{m-\gamma}b^{\gamma}c^{\gamma-1}RP\\&=a^{l-(\gamma+1)}d^{m-\gamma}b^{\gamma}c^{\gamma}P,\end{aligned}$$

where $w\in W(P,2\gamma+1)$. For $l\geq 2,m\geq 1$, that is, $\gamma\geq 1$, we obtain

$$C(P,w)_n^{(2\gamma+1)}(l,m)=a^{l-(\gamma+1)}b^{\gamma}c^{\gamma}d^{m-\gamma}P.$$

Note that the right-hand side of the above equation does not depend on $w\in W(P,2\gamma+1)$. So we write $C(P)_n^{(2\gamma+1)}(l,m)=C(P,w)_n^{(2\gamma+1)}(l,m)$ for $w\in W(P,2\gamma+1)$. Finally we compute the number of $w=(w_1,w_2,\ldots,w_{2\gamma},w_{2\gamma+1})$ satisfying $w\in W(P,2\gamma+1)$ by a standard combinatorial argument as follows:

$$|W(P,2\gamma+1)|=\binom{l-1}{\gamma}\binom{m-1}{\gamma-1}.$$

From the above observation, we obtain

$$\begin{aligned}p_n(l,m)P&=\sum_{\gamma=1}^{(l-1)\wedge m}\ \sum_{w\in W(P,2\gamma+1)}C(P,w)_n^{(2\gamma+1)}(l,m)\\&=\sum_{\gamma=1}^{(l-1)\wedge m}|W(P,2\gamma+1)|C(P)_n^{(2\gamma+1)}(l,m)\\&=\sum_{\gamma=1}^{(l-1)\wedge m}\binom{l-1}{\gamma}\binom{m-1}{\gamma-1}a^{l-(\gamma+1)}b^{\gamma}c^{\gamma}d^{m-\gamma}P.\end{aligned}$$

So we conclude that

$$p_n(l,m) = \sum_{\gamma=1}^{(l-1)\wedge m} \binom{l-1}{\gamma}\binom{m-1}{\gamma-1} a^{l-(\gamma+1)} b^{\gamma} c^{\gamma} d^{m-\gamma}.$$

When $l \geq 1$ and $m = 0$, it is easy to see that

$$p_n(l,0)P = P^l = a^{l-1}P.$$

Furthermore, when $l = 1, m \geq 1$ and $l = 0, m \geq 0$, it is clear that $p_n(l,m) = 0$.
(b) $q_n(l,m)$ case : We begin with $l \geq 1$ and $m \geq 2$. In this case, it is enough to study only the following case:

$$\overbrace{QQ\cdots Q}^{w_1}\overbrace{PP\cdots P}^{w_2}\overbrace{QQ\cdots Q}^{w_3}\cdots\overbrace{PP\cdots P}^{w_{2\gamma}}\overbrace{QQ\cdots Q}^{w_{2\gamma+1}},$$

where $w = (w_1, w_2, \ldots, w_{2\gamma+1}) \in \mathbb{Z}_+^{2\gamma+1}$ with $w_1, w_2, \ldots, w_{2\gamma+1} \geq 1$ and $\gamma \geq 1$. Note that

$$l = w_2 + w_4 + \cdots + w_{2\gamma}, \qquad m = w_1 + w_3 + \cdots + w_{2\gamma+1}.$$

Then $2\gamma + 1$ is the number of clusters of P's and Q's. As in the part (a), we obtain

$$q_n(l,m) = \sum_{\gamma=1}^{l\wedge(m-1)} \binom{l-1}{\gamma-1}\binom{m-1}{\gamma} a^{l-\gamma} b^{\gamma} c^{\gamma} d^{m-(\gamma+1)}.$$

When $l = 0$ and $m \geq 1$, this case is

$$q_n(0,m)Q = Q^m = d^{m-1}Q.$$

Furthermore, when $m = 1, l \geq 1$ and $m = 0, l \geq 0$, we see that $q_n(l,m) = 0$.
(c) $r_n(l,m)$ case : Suppose $l \geq 1$ and $m \geq 1$. In this case, it is sufficient to consider only the following case:

$$\overbrace{PP\cdots P}^{w_1}\overbrace{QQ\cdots Q}^{w_2}\overbrace{PP\cdots P}^{w_3}\cdots\overbrace{QQ\cdots Q}^{w_{2\gamma}},$$

where $w = (w_1, w_2, \ldots, w_{2\gamma+1}) \in \mathbb{Z}_+^{2\gamma}$ with $w_1, w_2, \ldots, w_{2\gamma} \geq 1$ and $\gamma \geq 1$. For example, $PQPQ$ case is $w_1 = w_2 = w_3 = w_4 = 1$ and $\gamma = 2$. It should be noted that l is the number of P's and m is the number of Q's, so we have

$$l = w_1 + w_3 + \cdots + w_{2\gamma-1}, \qquad m = w_2 + w_4 + \cdots + w_{2\gamma}.$$

Then 2γ is the number of clusters of P's and Q's. The range of γ is determined by the following observation. The minimum is $\gamma = 1$, that is, 2 clusters. This case is

$$P \cdots PQ \cdots Q.$$

The maximum is $\gamma = l \wedge m$. This case is

$$PQPQPQ \cdots PQPP \cdots PPQ \ \ (l \geq m),$$
$$PQPQPQ \cdots PQPQQ \cdots QQ \ \ (m \geq l),$$

for examples. As in the part (a), we get

$$r_n(l,m) = \sum_{\gamma=1}^{l \wedge m} \binom{l-1}{\gamma-1} \binom{m-1}{\gamma-1} a^{l-\gamma} b^{\gamma} c^{\gamma-1} d^{m-\gamma}.$$

If $l \wedge m = 0$, then $r_n(l,m) = 0$.
(d) $s_n(l,m)$ case : To begin, we assume $l \geq 1$ and $m \geq 1$. To compute $s_n(l,m)$, it is enough to consider only the following case:

$$\overbrace{QQ \cdots Q}^{w_1}\overbrace{PP \cdots P}^{w_2}\overbrace{QQ \cdots Q}^{w_3} \cdots \overbrace{PP \cdots P}^{w_{2\gamma}},$$

where $w = (w_1, w_2, \ldots, w_{2\gamma+1}) \in \mathbb{Z}_+^{2\gamma}$ with $w_1, w_2, \ldots, w_{2\gamma} \geq 1$ and $\gamma \geq 1$. Then

$$l = w_2 + w_4 + \cdots + w_{2\gamma}, \qquad m = w_1 + w_3 + \cdots + w_{2\gamma-1}.$$

As in the case of part (c), we obtain

$$s_n(l,m) = \sum_{\gamma=1}^{l \wedge m} \binom{l-1}{\gamma-1} \binom{m-1}{\gamma-1} a^{l-\gamma} b^{\gamma-1} c^{\gamma} d^{m-\gamma}.$$

When $l \wedge m = 0$, this case is $s_n(l,m) = 0$.

We assume $abcd \neq 0$. When $l \wedge m \geq 1$, combining the above results (a) - (d) gives

$$\Xi_n(l,m) = a^l d^m \sum_{\gamma=1}^{l \wedge m} \left(\frac{bc}{ad}\right)^{\gamma} \binom{l-1}{\gamma-1} \binom{m-1}{\gamma-1} \times \left[\frac{l-\gamma}{a\gamma} P + \frac{m-\gamma}{d\gamma} Q + \frac{1}{c} R + \frac{1}{b} S \right].$$

From $c = -\triangle \overline{b}, d = \triangle \overline{a}$, the proof of Lemma 1.1 (i) is complete. Furthermore, parts (ii) and (iii) are easily shown, so we will omit the proofs of them.

Then the distribution of X_n can be derived from Lemma 1.1 by direct computation.

Lemma 1.2. *For $k = 1, 2, \ldots, [n/2]$, we have*

$$P(X_n = n - 2k)$$
$$= |a|^{2(n-1)} \sum_{\gamma=1}^{k} \sum_{\delta=1}^{k} \left(-\frac{|b|^2}{|a|^2}\right)^{\gamma+\delta} \binom{k-1}{\gamma-1} \binom{k-1}{\delta-1} \binom{n-k-1}{\gamma-1} \binom{n-k-1}{\delta-1}$$
$$\times \left(\frac{1}{\gamma\delta}\right) \Bigg[\{k^2|a|^2 + (n-k)^2|b|^2 - (\gamma+\delta)(n-k)\}|\alpha|^2$$
$$+\{k^2|b|^2 + (n-k)^2|a|^2 - (\gamma+\delta)k\}|\beta|^2$$
$$+\frac{1}{|b|^2}\Bigg[\{(n-k)\gamma - k\delta + n(2k-n)|b|^2\}a\alpha\overline{b\beta}$$
$$+\{-k\gamma + (n-k)\delta + n(2k-n)|b|^2\}\overline{a\alpha}b\beta + \gamma\delta\Bigg]\Bigg],$$

$$P(X_n = -(n - 2k))$$
$$= |a|^{2(n-1)} \sum_{\gamma=1}^{k} \sum_{\delta=1}^{k} \left(-\frac{|b|^2}{|a|^2}\right)^{\gamma+\delta} \binom{k-1}{\gamma-1} \binom{k-1}{\delta-1} \binom{n-k-1}{\gamma-1} \binom{n-k-1}{\delta-1}$$
$$\times \left(\frac{1}{\gamma\delta}\right) \Bigg[\{k^2|b|^2 + (n-k)^2|a|^2 - (\gamma+\delta)k\}|\alpha|^2$$
$$+\{k^2|a|^2 + (n-k)^2|b|^2 - (\gamma+\delta)(n-k)\}|\beta|^2$$
$$+\frac{1}{|b|^2}\Bigg[\{k\gamma - (n-k)\delta - n(2k-n)|b|^2\}a\alpha\overline{b\beta}$$
$$+\{-(n-k)\gamma + k\delta - n(2k-n)|b|^2\}\overline{a\alpha}b\beta + \gamma\delta\Bigg]\Bigg],$$

$$P(X_n = n) = |a|^{2(n-1)}\{|b|^2|\alpha|^2 + |a|^2|\beta|^2 - (a\alpha\overline{b\beta} + \overline{a\alpha}b\beta)\},$$
$$P(X_n = -n) = |a|^{2(n-1)}\{|a|^2|\alpha|^2 + |b|^2|\beta|^2 + (a\alpha\overline{b\beta} + \overline{a\alpha}b\beta)\},$$

where $[x]$ is the integer part of x.

By using Lemma 1.2, we obtain a combinatorial expression for the characteristic function of X_n as follows. This result will be used in order to obtain a limit theorem of X_n.

Theorem 1.3. *(i) When $abcd \neq 0$, we have* $E(e^{i\xi X_n}) =$

$$|a|^{2(n-1)} \Bigg[\Big[\cos(n\xi) - \big\{ \left(|a|^2 - |b|^2\right) \left(|\alpha|^2 - |\beta|^2\right) + 2(a\alpha\overline{b\beta} + \overline{a\alpha}b\beta) \big\} \, i \sin(n\xi) \Big]$$

$$+ \sum_{k=1}^{\left[\frac{n-1}{2}\right]} \sum_{\gamma=1}^{k} \sum_{\delta=1}^{k} \left(-\frac{|b|^2}{|a|^2} \right)^{\gamma+\delta} \binom{k-1}{\gamma-1} \binom{k-1}{\delta-1} \binom{n-k-1}{\gamma-1} \binom{n-k-1}{\delta-1}$$

$$\times \left(\frac{1}{\gamma\delta} \right) \left[\left\{ (n-k)^2 + k^2 - n(\gamma+\delta) + \frac{2\gamma\delta}{|b|^2} \right\} \cos((n-2k)\xi) \right.$$

$$+ (n-2k) \Bigg\{ -\{n(|a|^2 - |b|^2) + \gamma + \delta\}(|\alpha|^2 - |\beta|^2)$$

$$\left. + \left(\frac{\gamma+\delta}{|b|^2} - 2n \right) (a\alpha\overline{b\beta} + \overline{a\alpha}b\beta) \Bigg\} i \sin((n-2k)\xi) \right]$$

$$+ I\left(\frac{n}{2} - \left[\frac{n}{2} \right], 0 \right) \times \sum_{\gamma=1}^{\frac{n}{2}} \sum_{\delta=1}^{\frac{n}{2}} \left(-\frac{|b|^2}{|a|^2} \right)^{\gamma+\delta} \binom{\frac{n}{2}-1}{\gamma-1}^2 \binom{\frac{n}{2}-1}{\delta-1}^2$$

$$\times \left(\frac{1}{4\gamma\delta} \right) \left[n^2 - 2n(\gamma+\delta) + \frac{4\gamma\delta}{|b|^2} \right] \Bigg],$$

where $I(x,y) = 1$ (resp. $= 0$) if $x = y$ (resp. $x \neq y$).
(ii) When $b = 0$, that is,

$$U = \begin{bmatrix} e^{i\theta} & 0 \\ 0 & \triangle e^{-i\theta} \end{bmatrix},$$

where $\theta \in \mathbb{R}$ and $\triangle = \det U \in \mathbb{C}$ with $|\triangle| = 1$, then we have

$$E(e^{i\xi X_n}) = \cos(n\xi) + i(|\beta|^2 - |\alpha|^2)\sin(n\xi).$$

(iii) When $a = 0$, that is,

$$U = \begin{bmatrix} 0 & e^{i\theta} \\ -\triangle e^{-i\theta} & 0 \end{bmatrix},$$

where $\theta \in \mathbb{R}$ and $\triangle = \det U \in \mathbb{C}$ with $|\triangle| = 1$, then we have

$$E(e^{i\xi X_n}) = \begin{cases} \cos\xi + i(|\alpha|^2 - |\beta|^2)\sin\xi & \text{if } n \text{ is odd,} \\ 1 & \text{if } n \text{ is even.} \end{cases}$$

From this theorem, we have the m-th moment of X_n in the standard fashion. The following result can be used in order to study symmetry of distribution of X_n.

Corollary 1.4. *(i) We assume that $abcd \neq 0$. When m is odd, we have*

$$E((X_n)^m) = |a|^{2(n-1)} \Bigg[\Bigg[-n^m \left\{ \left(|a|^2 - |b|^2\right) \left(|\alpha|^2 - |\beta|^2\right) + 2(a\alpha\overline{b\beta} + \overline{a\alpha}b\beta) \right\} \Bigg]$$

$$+ \sum_{k=1}^{\left[\frac{n-1}{2}\right]} \sum_{\gamma=1}^{k} \sum_{\delta=1}^{k} \left(-\frac{|b|^2}{|a|^2} \right)^{\gamma+\delta} \binom{k-1}{\gamma-1} \binom{k-1}{\delta-1} \binom{n-k-1}{\gamma-1} \binom{n-k-1}{\delta-1}$$

$$\times \frac{(n-2k)^{m+1}}{\gamma\delta} \Bigg[-\{n(|a|^2 - |b|^2) + \gamma + \delta\}(|\alpha|^2 - |\beta|^2)$$

$$+ \left(\frac{\gamma+\delta}{|b|^2} - 2n \right) (a\alpha\overline{b\beta} + \overline{a\alpha}b\beta) \Bigg] \Bigg].$$

We assume that $abcd \neq 0$. When m is even, we have

$$E((X_n)^m) = |a|^{2(n-1)} \Bigg[n^m$$

$$+ \sum_{k=1}^{\left[\frac{n-1}{2}\right]} \sum_{\gamma=1}^{k} \sum_{\delta=1}^{k} \left(-\frac{|b|^2}{|a|^2} \right)^{\gamma+\delta} \binom{k-1}{\gamma-1} \binom{k-1}{\delta-1} \binom{n-k-1}{\gamma-1} \binom{n-k-1}{\delta-1}$$

$$\times \frac{(n-2k)^m}{\gamma\delta} \left\{ (n-k)^2 + k^2 - n(\gamma+\delta) + \frac{2\gamma\delta}{|b|^2} \right\} \Bigg].$$

(ii) When $b = 0$, that is,

$$U = \begin{bmatrix} e^{i\theta} & 0 \\ 0 & \triangle e^{-i\theta} \end{bmatrix},$$

where $\theta \in [0, 2\pi)$ and $\triangle = \det U \in \mathbb{C}$ with $|\triangle| = 1$, then we have

$$E((X_n)^m) = \begin{cases} n^m(|\beta|^2 - |\alpha|^2) & \text{if } m \text{ is odd,} \\ n^m & \text{if } m \text{ is even.} \end{cases}$$

(iii) When $a = 0$, that is,

$$U = \begin{bmatrix} 0 & e^{i\theta} \\ -\triangle e^{-i\theta} & 0 \end{bmatrix},$$

where $\theta \in [0, 2\pi)$ and $\triangle = \det U \in \mathbb{C}$ with $|\triangle| = 1$, then we have

$$E((X_n)^m) = \begin{cases} |\alpha|^2 - |\beta|^2 & \text{if } n \text{ and } m \text{ are odd,} \\ 1 & \text{if } n \text{ is odd and } m \text{ is even,} \\ 0 & \text{if } n \text{ is even.} \end{cases}$$

For any case, when m is even, $E((X_n)^m)$ is independent of initial qubit state φ. Therefore a parity law of the m-th moment can be derived from the above theorem.

Symmetry of Distribution

In this subsection, the following necessary and sufficient condition for symmetry of distribution of X_n is given.

Theorem 1.5. *We assume* $abcd \neq 0$. *Then we have*

$$\Phi_s = \Phi_0 = \Phi_\perp,$$

where

$$\begin{aligned}
\Phi_s &= \{\varphi \in \Phi : \ P(X_n = x) = P(X_n = -x) \ \textit{for any}\, n \in \mathbb{Z}_+ \ \textit{and}\, x \in \mathbb{Z}\}, \\
\Phi_0 &= \{\varphi \in \Phi : \ E(X_n) = 0 \ \textit{for any}\, n \in \mathbb{Z}_+\}, \\
\Phi_\perp &= \left\{\varphi = {}^T[\alpha, \beta] \in \Phi : |\alpha| = |\beta|, \ a\alpha\overline{b\beta} + \overline{a\alpha}b\beta = 0\right\}.
\end{aligned}$$

This result is a generalization of Konno, Namiki, and Soshi (2004) for the Hadamard walk.

Proof. (i) $\Phi_s \subset \Phi_0$. This is obvious by the definitions of Φ_s and Φ_0.
(ii) $\Phi_0 \subset \Phi_\perp$. By Corollary 1.4 (i) ($m = 1$ case), we see that

$$E(X_1) = E(X_2) = 0$$

if and only if

$$\left(|a|^2 - |b|^2\right)\left(|\alpha|^2 - |\beta|^2\right) + 2(a\alpha\overline{b\beta} + \overline{a\alpha}b\beta) = 0. \tag{1.1.1}$$

Then (1.1.1) implies that for $n \geq 3$, Corollary 1.4 (i) ($m = 1$ case) can be rewritten as

$$\begin{aligned}
E(X_n) = &-(|\alpha|^2 - |\beta|^2)\frac{|a|^{2(n-1)}}{2|b|^2} \\
&\times \sum_{k=1}^{\left[\frac{n-1}{2}\right]} \sum_{\gamma=1}^{k} \sum_{\delta=1}^{k} \left(-\frac{|b|^2}{|a|^2}\right)^{\gamma+\delta} \binom{k-1}{\gamma-1}\binom{k-1}{\delta-1}\binom{n-k-1}{\gamma-1} \\
&\times \binom{n-k-1}{\delta-1}\frac{(n-2k)^2(\gamma+\delta)}{\gamma\delta}.
\end{aligned}$$

Therefore $E(X_n) = 0$ $(n \geq 3)$ gives $|\alpha| = |\beta|$. Combining $|\alpha| = |\beta|$ with (1.1.1), we have the desired result.
(iii) $\Phi_{\perp} \subset \Phi_s$. We assume that

$$|\alpha| = |\beta|, \qquad a\alpha\overline{b\beta} + \overline{a\alpha}b\beta = 0. \tag{1.1.2}$$

By using Lemma 1.2 and (1.1.2), we see that for $k = 1, 2, \ldots, [n/2]$,

$$\begin{aligned}
&P(X_n = n - 2k) = P(X_n = -(n-2k)) \\
&= |a|^{2(n-1)} \sum_{\gamma=1}^{k} \sum_{\delta=1}^{k} \left(-\frac{|b|^2}{|a|^2} \right)^{\gamma+\delta} \binom{k-1}{\gamma-1} \binom{k-1}{\delta-1} \binom{n-k-1}{\gamma-1} \binom{n-k-1}{\delta-1} \\
&\qquad \times \left[\frac{|\alpha|^2}{\gamma\delta} \{(n-k)^2 + k^2 - n(\gamma+\delta)\} + \frac{1}{|b|^2} \right],
\end{aligned}$$

and

$$P(X_n = n) = P(X_n = -n) = |a|^{2(n-1)} |\alpha|^2.$$

So the desired conclusion is obtained.

Weak Limit Theorem

In the subsection, we give a new type of limit theorems for X_n with $abcd \neq 0$ as follows.

Theorem 1.6. *If $n \to \infty$, then*

$$\frac{X_n}{n} \quad \Rightarrow \quad Z,$$

where Z has a density

$$\begin{aligned}
f(x) &= f(x; \varphi = {}^T[\alpha, \beta]) \\
&= \frac{\sqrt{1 - |a|^2}}{\pi(1 - x^2)\sqrt{|a|^2 - x^2}} \left\{ 1 - \left(|\alpha|^2 - |\beta|^2 + \frac{a\alpha\overline{b\beta} + \overline{a\alpha}b\beta}{|a|^2} \right) x \right\},
\end{aligned}$$

for $x \in (-|a|, |a|)$ and $f(x) = 0$ for $|x| \geq |a|$ with

$$\begin{aligned}
E(Z) &= -\left(|\alpha|^2 - |\beta|^2 + \frac{a\alpha\overline{b\beta} + \overline{a\alpha}b\beta}{|a|^2} \right) \times (1 - \sqrt{1 - |a|^2}), \\
E(Z^2) &= 1 - \sqrt{1 - |a|^2},
\end{aligned}$$

and $Y_n \Rightarrow Y$ means that Y_n converges weakly to a limit Y.

Proof. We begin with introducing the Jacobi polynomial $P_n^{\nu,\mu}(x)$, where $P_n^{\nu,\mu}(x)$ is orthogonal on $[-1,1]$ with respect to $(1-x)^\nu(1+x)^\mu$ with $\nu,\mu > -1$. Then the following relation holds:

$$P_n^{\nu,\mu}(x) = \frac{\Gamma(n+\nu+1)}{\Gamma(n+1)\Gamma(\nu+1)} {}_2F_1(-n, n+\nu+\mu+1; \nu+1; (1-x)/2), \tag{1.1.3}$$

where ${}_2F_1(a,b;c;z)$ is the hypergeometric series and $\Gamma(z)$ is the gamma function. In general, as for orthogonal polynomials, see Andrews, Askey, and Roy (1999). Then we see that

$$\begin{aligned}
&\sum_{\gamma=1}^{k} \left(-\frac{|b|^2}{|a|^2}\right)^{\gamma-1} \frac{1}{\gamma}\binom{k-1}{\gamma-1}\binom{n-k-1}{\gamma-1} \\
&= {}_2F_1(-(k-1), -\{(n-k)-1\}; 2; -|b|^2/|a|^2) \\
&= |a|^{-2(k-1)} {}_2F_1(-(k-1), n-k+1; 2; 1-|a|^2) \\
&= \frac{1}{k}|a|^{-2(k-1)} P_{k-1}^{1,n-2k}(2|a|^2-1).
\end{aligned}$$

The first equality is given by the definition of the hypergeometric series. The second equality comes from the following relation:

$${}_2F_1(a,b;c;z) = (1-z)^{-a} {}_2F_1(a, c-b; c; z/(z-1)).$$

The last equality follows from (1.1.3). In a similar way, we have

$$\sum_{\gamma=1}^{k} \left(-\frac{|b|^2}{|a|^2}\right)^{\gamma-1} \binom{k-1}{\gamma-1}\binom{n-k-1}{\gamma-1} = |a|^{-2(k-1)} P_{k-1}^{0,n-2k}(2|a|^2-1).$$

By using the above relations and Theorem 1.3, we obtain the next asymptotics of characteristic function $E(e^{i\xi X_n/n})$:

Lemma 1.7. *if* $n \to \infty$ *with* $k/n = x \in (-(1-|a|)/2, (1+|a|)/2)$, *then*

$$\begin{aligned}
E(e^{i\xi X_n/n}) \sim &\sum_{k=1}^{[(n-1)/2]} |a|^{2n-4k-2}|b|^4 \\
\times \Bigg[&\left\{ \frac{2x^2-2x+1}{x^2}(P_{k-1}^{1,n-2k})^2 - \frac{2}{x}P_{k-1}^{1,n-2k}P_{k-1}^{0,n-2k} + \frac{2}{|b|^2}(P_{k-1}^{0,n-2k})^2 \right\} \\
&\qquad \times \cos((1-2x)\xi) \\
&+ \left(\frac{1-2x}{x}\right)\left\{ -\frac{1}{x}\{(|a|^2-|b|^2)(|\alpha|^2-|\beta|^2) + 2(a\alpha\overline{b\beta} + \overline{a\alpha}b\beta)\}(P_{k-1}^{1,n-2k})^2 \right. \\
&\left. -2\left\{ |\alpha|^2 - |\beta|^2 - \frac{a\alpha\overline{b\beta} + \overline{a\alpha}b\beta}{|b|^2} \right\} P_{k-1}^{0,n-2k}P_{k-1}^{1,n-2k} \right\} i\sin((1-2x)\xi) \Bigg],
\end{aligned}$$

where $f(n) \sim g(n)$ *means* $f(n)/g(n) \to 1$ $(n \to \infty)$, *and* $P^{i,n-2k}_{k-1} = P^{i,n-2k}_{k-1}(2|a|^2-1)$ $(i = 0, 1)$.

Next we use an asymptotic result on the Jacobi polynomial $P_n^{\alpha+an,\beta+bn}(x)$ derived by Chen and Ismail (1991). By using (2.16) in their paper with $\alpha \to 0$ or $1, a \to 0, \beta = b \to (1-2x)/x, x \to 2|a|^2-1$ and $\triangle \to 4(1-|a|^2)(4x^2 - 4x + 1 - |a|^2)/x^2$, we have the following lemma. It should be noted that there are some minor errors in (2.16) in that paper, for example, $\sqrt{(-\triangle)} \to \sqrt{(-\triangle)}^{\,-1}$.

Lemma 1.8. *If* $n \to \infty$ *with* $k/n = x \in (-(1-|a|)/2, (1+|a|)/2)$, *then*

$$P^{0,n-2k}_{k-1} \sim \frac{2|a|^{2k-n}}{\sqrt{\pi n \sqrt{-\Lambda}}} \cos(An+B),$$
$$P^{1,n-2k}_{k-1} \sim \frac{2|a|^{2k-n}}{\sqrt{\pi n \sqrt{-\Lambda}}} \sqrt{\frac{x}{(1-x)(1-|a|^2)}} \cos(An+B+\theta),$$

where $\Lambda = (1-|a|^2)(4x^2-4x+1-|a|^2)$, A *and* B *are some constants (which are independent of* n*), and* $\theta \in [0, \pi/2]$ *is determined by* $\cos\theta = \sqrt{(1-|a|^2)/4x(1-x)}$.

From the Riemann-Lebesgue lemma (see Durrett (2004), for example) and Lemmas 1.7 and 1.8, we see that, if $n \to \infty$, then

$$\begin{aligned}
&E(e^{i\xi X_n/n}) \quad \to \\
&\frac{1-|a|^2}{\pi} \int_{\frac{1-|a|}{2}}^{\frac{1}{2}} dx \, \frac{1}{x(1-x)\sqrt{(|a|^2-1)(4x^2-4x+1-|a|^2)}} \\
&\times \left[\cos((1-2x)\xi) - (1-2x)\left\{ |\alpha|^2 - |\beta|^2 + \frac{a\alpha\overline{b\beta} + \overline{a\alpha}b\beta}{|a|^2} \right\} i\sin((1-2x)\xi) \right] \\
&= \frac{\sqrt{1-|a|^2}}{\pi} \int_{-|a|}^{|a|} dx \, \frac{1}{(1-x^2)\sqrt{|a|^2-x^2}} \\
&\qquad \times \left[\cos(x\xi) - x\left\{ |\alpha|^2 - |\beta|^2 + \frac{a\alpha\overline{b\beta} + \overline{a\alpha}b\beta}{|a|^2} \right\} i\sin(x\xi) \right] \\
&= \int_{-|a|}^{|a|} \frac{\sqrt{1-|a|^2}}{\pi(1-x^2)\sqrt{|a|^2-x^2}} \left\{ 1 - \left(|\alpha|^2 - |\beta|^2 + \frac{a\alpha\overline{b\beta} + \overline{a\alpha}b\beta}{|a|^2} \right) x \right\} e^{i\xi x} \, dx \\
&= \phi(\xi).
\end{aligned}$$

Then $\phi(\xi)$ is continuous at $\xi = 0$, so the continuity theorem implies that X_n/n converges weakly to a limit Z with characteristic function ϕ. Moreover the density function of Z is given by

$$f(x; {}^T[\alpha,\beta]) = \frac{\sqrt{1-|a|^2}}{\pi(1-x^2)\sqrt{|a|^2-x^2}} \left\{1 - \left(|\alpha|^2 - |\beta|^2 + \frac{a\alpha\overline{b\beta} + \overline{a\alpha}b\beta}{|a|^2}\right) x\right\},$$

for $x \in (-|a|, |a|)$. So the proof of Theorem 1.6 is complete.

It can be confirmed that $f(x; {}^T[\alpha,\beta])$ satisfies the property of a density function as follows: It is easily checked that $f(x; {}^T[\alpha,\beta]) \geq 0$, since

$$1 \geq \pm \left(|\alpha|^2 - |\beta|^2 + \frac{a\alpha\overline{b\beta} + \overline{a\alpha}b\beta}{|a|^2}\right) |a|. \tag{1.1.4}$$

On the other hand,

$$\begin{aligned}\int_{-|a|}^{|a|} f(x; {}^T[\alpha,\beta])\, dx &= \frac{\sqrt{1-|a|^2}}{\pi} \int_0^1 t^{-1/2}(1-t)^{-1/2}(1-|a|^2t)^{-1}\, dt \\ &= \frac{\sqrt{1-|a|^2}}{\pi} \Gamma(1/2)^2 {}_2F_1(1/2, 1; 1; |a|^2) \\ &= 1.\end{aligned}$$

The last equality comes from $\Gamma(1/2) = \sqrt{\pi}$ and ${}_2F_1(1/2, 1; 1; |a|^2) = 1/\sqrt{1-|a|^2}$.

Moreover, using (1.1.4), we see that for any $m \geq 1$,

$$|E(Z^m)| \leq 2|a|^m.$$

In the symmetric case of the Hadamard walk, we have the following result.

Proposition 1.9. *For $n \geq 1$,*

$$E(Z^{2n}) = 1 - \frac{1}{\sqrt{2}} \sum_{k=0}^{n-1} \frac{1}{2^{3k}} \binom{2k}{k}, \qquad E(Z^{2n-1}) = 0.$$

Proof. We begin with

$$E(Z^{2n}) = \int_{-1/\sqrt{2}}^{1/\sqrt{2}} \frac{x^{2n}}{\pi(1-x^2)\sqrt{1-2x^2}} dx = \frac{2^{(3-2n)/2}}{\pi} \times I_{2n},$$

where

$$I_n = \int_0^1 \frac{y^n}{(2-y^2)\sqrt{1-y^2}} dy = \int_0^{\pi/2} \frac{\sin^n\theta}{1+\cos^2\theta} d\theta.$$

It should be noted that

$$\begin{aligned}I_{2n+2} &= \int_0^{\pi/2} \frac{\{2-(1+\cos^2\theta)\}\sin^{2n}\theta}{1+\cos^2\theta} d\theta \\ &= 2I_{2n} - \frac{(2n-1)(2n-3)\cdots 1}{2n(2n-2)\cdots 2} \times \frac{\pi}{2}.\end{aligned}$$

Let $J_n = I_{2n}/2^n$. Then we see that for $n \geq 0$

$$J_{n+1} - J_n = -\frac{\pi}{2^{3n+2}}\binom{2n}{n},$$

where

$$J_0 = \frac{\pi}{2\sqrt{2}}, \qquad J_1 = \frac{2-\sqrt{2}}{4\sqrt{2}}\pi.$$

So we have

$$I_{2n} = 2^n J_n = 2^n \left[\frac{1}{2\sqrt{2}} - \sum_{k=0}^{n-1} \frac{1}{2^{3k+2}}\binom{2k}{k}\right]\pi.$$

Therefore for $n \geq 1$,

$$E(Z^{2n}) = 1 - \frac{1}{\sqrt{2}}\sum_{k=0}^{n-1}\frac{1}{2^{3k}}\binom{2k}{k}.$$

So the proof is complete.

Fourier Analysis

The two-component wave function of the quantum walk was given by

$$\Psi_n(x) = \begin{bmatrix} \Psi_n^L(x) \\ \Psi_n^R(x) \end{bmatrix}.$$

Following the definition of the model, we have

$$\Psi_{n+1}(x) = \begin{bmatrix} a\Psi_n^L(x+1) + b\Psi_n^R(x+1) \\ c\Psi_n^L(x-1) + d\Psi_n^R(x-1) \end{bmatrix}, \tag{1.1.5}$$

where $U = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \in \mathrm{U}(2)$. If we set

$$\hat{\Psi}_n(k) = \begin{bmatrix} \hat{\Psi}_n^L(k) \\ \hat{\Psi}_n^R(k) \end{bmatrix},$$

and assume the relations

$$\Psi_n^j(x) = \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{ikx}\hat{\Psi}_n^j(k),$$
$$\hat{\Psi}_n^j(k) = \sum_{x\in\mathbb{Z}} e^{-ikx}\Psi_n^j(x),$$

for $j = L, R$, then (1.1.5) is rewritten in the wave-number space (k-space) of the Fourier transformation, $k \in [-\pi, \pi)$ as

$$\hat{\Psi}_{n+1}(k) = U(k)\hat{\Psi}_n(k), \quad n = 0, 1, 2, \cdots,$$

where $U(k)$ is given by

$$U(k) = \begin{bmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{bmatrix} U.$$

The state at time step n is then obtained from the initial state $\hat{\Psi}_0(k) = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$, $\alpha, \beta \in \mathbb{C}$, $|\alpha|^2 + |\beta|^2 = 1$, by

$$\hat{\Psi}_n(k) = U(k)^n \hat{\Psi}_0(k), \tag{1.1.6}$$

whose Fourier transformation gives the wave function at time step n as

$$\begin{aligned} \Psi_n(x) &= \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{ikx} \hat{\Psi}_n(k) \\ &= \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{ikx} U(k)^n \hat{\Psi}_0(k). \end{aligned}$$

The probability distribution function in the real space at time step n is given by

$$\begin{aligned} P_n(x) &= ||\Psi_n(x)||^2 \\ &= \int_{-\pi}^{\pi} \frac{dk'}{2\pi} \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{i(k-k')x} \left(\hat{\Psi}_0^*(k') U^*(k')^n\right) \left(U(k)^n \hat{\Psi}_0(k)\right). \end{aligned} \tag{1.1.7}$$

Let X_n denote the position of the one-dimensional quantum walk at time step $n = 0, 1, 2, \cdots$ and consider a function f of $x \in \mathbb{Z}$. The expectation of $f(X_n)$ is defined by

$$\begin{aligned} E(f(X_n)) &= \sum_{x \in \mathbb{Z}} f(x) P_n(x) \\ &= \sum_{x \in \mathbb{Z}} f(x) \int_{-\pi}^{\pi} \frac{dk'}{2\pi} e^{-ik'x} \hat{\Psi}_n^*(k') \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{ikx} \hat{\Psi}_n(k). \end{aligned}$$

If $f(x) = x^r, r = 0, 1, 2, \cdots$, it is written as

$$E(X_n^r) = \sum_{x \in \mathbb{Z}} \int_{-\pi}^{\pi} \frac{dk'}{2\pi} e^{-ik'x} \hat{\Psi}_n^*(k') \int_{-\pi}^{\pi} \frac{dk}{2\pi} \left\{ \left(-i \frac{d}{dk}\right)^r e^{ikx} \right\} \hat{\Psi}_n(k).$$

We note that $\hat{\Psi}_n(k)$ should be a periodic function of $k \in [-\pi, \pi)$, and then by partial integrations, we will have

$$\int_{-\pi}^{\pi} \frac{dk}{2\pi} \left\{ \left(-i \frac{d}{dk} \right)^r e^{ikx} \right\} \hat{\Psi}_n(k) = \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{ikx} \left(i \frac{d}{dk} \right)^r \hat{\Psi}_n(k),$$

and thus

$$E(X_n^r) = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \hat{\Psi}_n^*(k) \left(i \frac{d}{dk} \right)^r \hat{\Psi}_n(k), \tag{1.1.8}$$

where we have used the summation formula $\sum_{x\in\mathbb{Z}} e^{ikx} = 2\pi\delta(k)$. Then, if $f(x)$ is analytic around $x = 0$, that is, if it has a converging Taylor expansion in the form $f(x) = \sum_{j=0}^{\infty} a_j x^j$, we will have the formula

$$E(f(X_n)) = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \hat{\Psi}_n^*(k) f\left(i \frac{d}{dk} \right) \hat{\Psi}_n(k). \tag{1.1.9}$$

Method of Grimmett, Janson, and Scudo (2004)

The unitary matrix $U(k)$ has two eigenvalues $\lambda_1(k)$ and $\lambda_2(k)$ and has corresponding eigenvectors $v_1(k)$ and $v_2(k)$ that define an orthonormal basis for $H = L^2(\mathbb{K}) \otimes H_c$, where $\mathbb{K} = [-\pi, \pi)$ and $H_c = \mathbb{C}^2$. Put $D = id/dk$. Then

$$D^r \Psi_n(k) = \sum_{j=1}^{2} (n)_r \lambda_j(k)^{n-r} (D\lambda_j(k))^r \langle v_j(k), \Psi_0(k) \rangle v_j(k) + O(n^{r-1}), \tag{1.1.10}$$

where $(n)_r = n(n-1)\cdots(n-r+1)$. On the other hand, (1.1.8) becomes

$$E(X_n^r) = \int_{-\pi}^{\pi} \hat{\Psi}_n^*(k) D^r \hat{\Psi}_n(k) \frac{dk}{2\pi}. \tag{1.1.11}$$

Combining (1.1.10) with (1.1.11) yields

$$\begin{aligned} E(X_n^r) &= \int_{-\pi}^{\pi} \sum_{j=1}^{2} (n)_r \lambda_j(k)^{n-r} (D\lambda_j(k))^r \langle v_j(k), \Psi_0(k) \rangle \langle \Psi_0(k), v_j(k) \rangle \frac{dk}{2\pi} \\ &\qquad + O(n^{-1}) \\ &= \int_{-\pi}^{\pi} \sum_{j=1}^{2} (n)_r \left(\frac{D\lambda_j(k)}{\lambda_j(k)} \right)^r |\langle v_j(k), \Psi_0(k) \rangle|^2 \frac{dk}{2\pi} + O(n^{-1}). \end{aligned} \tag{1.1.12}$$

Therefore let $\Omega = \mathbb{K} \times \{1, 2\}$ and μ denote the probability measure on Ω given by $dk/2\pi \times |\langle v_j(k), \Psi_0(k) \rangle|^2$ on $\mathbb{K} \times \{j\}$. Put

$$h_j(k) = \frac{D\lambda_j(k)}{\lambda_j(k)}.$$

Define $h : \Omega \to \mathbb{R}$ by $h(k,j) = h_j(k)$. By (1.1.12),

$$\lim_{n\to\infty} E((X_n/n)^r) = \int_\Omega h^r \, d\mu.$$

Therefore Grimmett, Janson, and Scudo (2004) obtained

Theorem 1.10. *If $n \to \infty$, then*

$$\frac{X_n}{n} \quad \Rightarrow \quad Y = h(Z),$$

where Z is a random variable of Ω with distribution μ.

Here we consider the Hadamard walk case. In this case,

$$U(k) = \frac{1}{\sqrt{2}} \begin{bmatrix} e^{ik} & e^{ik} \\ e^{-ik} & -e^{-ik} \end{bmatrix}.$$

The eigenvalues are

$$\lambda_1(k) = \frac{1}{\sqrt{2}}(\sqrt{I} + i\sin k), \quad \lambda_2(k) = \frac{1}{\sqrt{2}}(-\sqrt{I} + i\sin k), \tag{1.1.13}$$

where $I = 1 + \cos^2 k$. Then

$$h_1(k) = -\frac{\cos k}{\sqrt{I}}, \quad h_2(k) = \frac{\cos k}{\sqrt{I}},$$

and

$$v_1(k) = \sqrt{\frac{\sqrt{I} + \cos k}{2\sqrt{I}}} \begin{bmatrix} e^{ik} \\ \sqrt{I} - \cos k \end{bmatrix}, \quad v_2(k) = \sqrt{\frac{\sqrt{I} - \cos k}{2\sqrt{I}}} \begin{bmatrix} e^{ik} \\ -\sqrt{I} - \cos k \end{bmatrix},$$

with $\langle v_j(k), v_j(k) \rangle = 1$ $(j = 1, 2)$. Let $p_j(k) = |\langle v_j(k), \Psi_0(k) \rangle|^2$ for $j = 1, 2$. Note that $p_1(k) + p_2(k) = 1$ $(k \in [-\pi, \pi))$. From Theorem 1.10, we have

$$P(Y \le y) = \int_{\{k\in[-\pi,\pi):h_1(k)\le y\}} p_1(k)\,\frac{dk}{2\pi} + \int_{\{k\in[-\pi,\pi):h_2(k)\le y\}} p_2(k)\,\frac{dk}{2\pi}.$$

Let $k = k(y) \in [0, \pi)$ denote the unique solution of $h_1(k) = -\cos k/\sqrt{I} = y$ for $-1/\sqrt{2} < y < 1/\sqrt{2}$. Therefore

$$P(Y \le y) = \int_{-k(y)}^{k(y)} p_1(k)\,\frac{dk}{2\pi} + \left(\int_{-\pi}^{-\pi+k(y)} + \int_{\pi-k(y)}^{\pi} \right) p_2(k)\,\frac{dk}{2\pi}.$$

Then we have

$$
\begin{aligned}
f(y) &= \frac{d}{dy} P(Y \le y) \\
&= \frac{1}{2\pi} \left\{ p_1(k(y)) + p_1(-k(y)) + p_2(-\pi + k(y)) + p_2(\pi - k(y)) \right\} \, \frac{dk(y)}{dy}.
\end{aligned}
\tag{1.1.14}
$$

Noting that

$$
\cos(k(y)) = -\frac{y}{\sqrt{1-y^2}}, \tag{1.1.15}
$$

we have

$$
\frac{dk(y)}{dy} = \frac{1}{(1-y^2)\sqrt{1-2y^2}}. \tag{1.1.16}
$$

On the other hand, from (1.1.15) and

$$
\sin(k(y)) = \sqrt{\frac{1-2y^2}{1-y^2}}, \quad I = 1 + \cos^2(k(y)) = \frac{1}{1-y^2},
$$

we get

$$
\begin{aligned}
v_1(k(y)) &= \frac{1}{\sqrt{2(1+y)}} \begin{bmatrix} -y + i\sqrt{1-2y^2} \\ 1+y \end{bmatrix}, \\
v_1(-k(y)) &= \frac{1}{\sqrt{2(1+y)}} \begin{bmatrix} -y - i\sqrt{1-2y^2} \\ 1+y \end{bmatrix}, \\
v_2(-\pi + k(y)) &= \frac{1}{\sqrt{2(1+y)}} \begin{bmatrix} y - i\sqrt{1-2y^2} \\ -1-y \end{bmatrix}, \\
v_2(\pi - k(y)) &= \frac{1}{\sqrt{2(1+y)}} \begin{bmatrix} y + i\sqrt{1-2y^2} \\ -1-y \end{bmatrix}.
\end{aligned}
$$

Combining these with (1.1.14) and (1.1.16) yields

$$
f(y) = \frac{1}{\pi(1-y^2)\sqrt{1-2y^2}} \{1 - (|\alpha|^2 - |\beta|^2 + \alpha\overline{\beta} + \overline{\alpha}\beta)y\} I_{(-1/\sqrt{2},1/\sqrt{2})}(y). \tag{1.1.17}
$$

In Katori, Fujino, and Konno (2005), the time-evolution equation of a one-dimensional quantum walker is exactly mapped to the three-dimensional Weyl equation for a zero-mass particle with spin 1/2, in which each wave number k of walker's wave function is mapped to a point $\mathbf{q}(k)$ in the three-dimensional momentum space and $\mathbf{q}(k)$ makes a planar orbit as k changes its value in $[-\pi, \pi)$. The integration over k providing the real-space wave function for a quantum walker corresponds to considering an orbital state of a Weyl particle, which is defined as a superposition (curvilinear integration) of the energy-momentum eigenstates of a free Weyl equation along the orbit. The above density function (1.1.17) of quantum-walker's pseudo-velocities in the long-time limit is fully controlled by the shape of the orbit and how the orbit is embedded in the three-dimensional momentum space. The family of orbital states can b e regarded as a geometrical representation of the unitary group U(2).

1.2 Three-State Case

Introduction

In this section we consider the three-state Grover walk. The Hadamard walk plays a key role in studies of the quantum walk and it has been analyzed in detail. Thus the generalization of the Hadamard walk is a fascinating challenge. The simplest classical random walker on a one-dimensional lattice moves to the left or to the right with probability 1/2. On the other hand, the quantum walker according to the Hadamard walk on a line moves both to the left and to the right. It is well known that the spatial distribution of the probability of finding a particle governed by the Hadamard walk after long time is quite different from that of the classical random walk. However there are some common properties. In both walks the probability of finding the particle at a fixed lattice site converges to zero as time goes to infinity.

Let us consider a classical random walker that can stay at the same position with non-zero probability in a single time-evolution. In the limit of long time, does the probability of finding the walker at a fixed position converge to a positive value ? If the probability of staying at the same position in a single step is very close to 1, the walker diffuses very slowly. However the probability of existence at a fixed position surely converges to zero if the jumping probability is not zero. The classical random walker who can remain at the same position is essentially regarded as the same process as a walk that jumps right or left with probability 1/2, by scaling the time. Is the same conclusion valid for a quantum walk ? The answer is "No". We show that the profile of the Hadamard walk changes drastically by appending only one degree of freedom to the inner states.

If the quantum particle in a three-state Grover walk exists at only one site initially, the particle is trapped with high probability near the initial position. Similar localization has already been seen in other quantum walks. The first simulation showing the localization was presented by Mackay et al. (2002) in studying the two-dimensional Grover walk. After that, more refined simulations were performed by Tregenna et al. (2003) and an exact proof on the localization was given by Inui, Konishi, and Konno (2004). The second is found in the four-state Grover walk (Inui and Konno (2005)). In this walk, a particle moves not only to the nearest sites but also the second nearest sites according to the four inner states. The four-state Grover walk is also a generalized Hadamard walk, and it is similar to the three-state Grover walk. The significant difference between them is that the wave function of the four-state Grover walk does not converge, but that of the three-state Grover walk converges as time tends to infinity. We focus on localized stationary distribution of the three-state quantum particle and calcul ate it rigorously. On the other hand, Konno (2005c) proved that a weak limit distribution of a continuous-time rescaled two-state quantum walk has a similar form to that of the discrete-time one. In fact, both limit density functions for two-state quantum walks have two peaks at the two end points of the supports. As a corollary, it is easily shown that a weak limit distribution of the corresponding continuous-time three-state quantum walk has the same shape as that of the two-state walk. So the localization does not occur in the continuous-time case in contrast with the discrete-time case. In this situation the main aim of this section is to show rigorously that the localization occurs for a discrete-time three-state Grover walk. The results in this section are based on Inui, Konno, and Segawa (2005). Furthermore, we give a weak limit theorem for the three-state Grover walk and clarify the relation between the localization and the limit theorem.

Definition of the Three-state Grover Walk

The three-state quantum walk considered here is a kind of generalized Hadamard walk on a line. The particle ruled by three-state quantum walk is characterized in the Hilbert space which is defined by a direct product of a chirality state space $\{|L\rangle, |0\rangle, |R\rangle\}$ and a position space $\{|x\rangle : x \in \mathbb{Z}\}$. The chirality states are transformed at each time step by the following unitary transformation:

$$|L\rangle = \frac{1}{3}(-|L\rangle + 2|0\rangle + 2|R\rangle),$$
$$|0\rangle = \frac{1}{3}(2|L\rangle - |0\rangle + 2|R\rangle),$$
$$|R\rangle = \frac{1}{3}(2|L\rangle + 2|0\rangle - |R\rangle).$$

Let $\Psi_n(x) = {}^T[\Psi_n^L(x), \Psi_n^0(x), \Psi_n^R(x)]$ be the amplitude of the wave function of the particle corresponding to the chiralities "L", "0" and "R" at the position $x \in \mathbb{Z}$ and the time $n \in \{0, 1, 2, \ldots\}$. We assume that a particle exists initially at the origin. Then the initial quantum states are determined by $\Psi_0(0) = {}^T[\alpha, \beta, \gamma]$, where $\alpha, \beta, \gamma \in \mathbb{C}$ with $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$.

Before we define the time evolution of the wave function, we introduce the following three operators:

$$U_L = \frac{1}{3}\begin{bmatrix} -1 & 2 & 2 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad U_0 = \frac{1}{3}\begin{bmatrix} 0 & 0 & 0 \\ 2 & -1 & 2 \\ 0 & 0 & 0 \end{bmatrix}, \quad U_R = \frac{1}{3}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 2 & 2 & -1 \end{bmatrix}.$$

The three-state quantum walk considered here given by

$$U^{(G,3)} = U_L + U_0 + U_R = \frac{1}{3}\begin{bmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{bmatrix}$$

is often called three-state Grover walk. In general, n-state Grover walk is defined by a unitary matrix $U^{(G,n)} = [u^{(G,n)}(i,j) : 1 \le i,j \le n]$, where $u^{(G,n)}(i,j)$ is the (i,j) component of the matrix $U^{(G,n)}$ and

$$u^{(G,n)}(i,i) = 2/n - 1, \quad u^{(G,n)}(i,j) = 2/n \text{ if } i \neq j.$$

If the matrix U_L is applied to the function $\Psi_n(x)$, the "L"-component is selected after carrying out the superimposition between $\Psi_n^L(x), \Psi_n^0(x)$, and $\Psi_n^R(x)$. Similarly the "0"-component and "R"-component are selected in $U_0\Psi_n(x)$ and $U_R\Psi_n(x)$.

We now define the time evolution of the wave function by

$$\Psi_{n+1}(x) = U_L\Psi_n(x+1) + U_0\Psi_n(x) + U_R\Psi_n(x-1).$$

One finds clearly that the chiralities "L" and "R" correspond to the left and the right, and the chirality "0" corresponds to the neutral state for the motion.

Using the Fourier analysis, which is often used in the calculations of quantum walks, we obtain the wave function. The spatial Fourier transformation of $\Psi_n(x)$ is defined by

$$\hat{\Psi}_n(k) = \sum_{x\in\mathbb{Z}} e^{-ikx}\Psi_n(x).$$

The dynamics of the wave function in the Fourier domain is given by

$$\begin{aligned} \hat{\Psi}_{n+1}(k) &= \frac{1}{3}\begin{bmatrix} e^{ik} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-ik} \end{bmatrix}\begin{bmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{bmatrix}\hat{\Psi}_n(k) \\ &\equiv U(k)\hat{\Psi}_n(k). \end{aligned} \tag{1.2.18}$$

Thus the solution of (1.2.18) is $\hat{\Psi}_n(k) = U(k)^n\hat{\Psi}_0(k)$. Let $e^{i\theta_{j,k}}$ and $|v_j(k)\rangle$ be the eigenvalues of $U(k)$ and the orthonormal eigenvector corresponding to $e^{i\theta_{j,k}}$ $(j = 1,2,3)$. Since the matrix $U(k)$ is a unitary matrix, it is diagonalizable. Therefore the wave unction $\hat{\Psi}_n(k)$ is expressed by

$$\hat{\Psi}_n(k) = \left(\sum_{j=1}^{3} e^{i\theta_{j,k} n} |v_j(k)\rangle\langle v_j(k)| \right) \hat{\Psi}_0(k),$$

where $\hat{\Psi}_0(k) = {}^T[\alpha, \beta, \gamma] \in \mathbb{C}^3$ with $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$. The eigenvalues are given by

$$\begin{aligned} \theta_{j,k} &= \begin{cases} 0, & j = 1, \\ \theta_k, & j = 2, \\ -\theta_k, & j = 3, \end{cases} \\ \cos\theta_k &= -\frac{1}{3}(2 + \cos k), \\ \sin\theta_k &= \frac{1}{3}\sqrt{(5 + \cos k)(1 - \cos k)}, \end{aligned} \tag{1.2.19}$$

for $k \in [-\pi, \pi)$. The eigenvectors of $U(k)$ which form an orthonormal basis are obtained after some algebra:

$$|v_j(k)\rangle = \sqrt{c_k(\theta_{j,k})} \begin{bmatrix} \frac{1}{1+e^{i(\theta_{j,k}-k)}} \\ \frac{1}{1+e^{i\theta_{j,k}}} \\ \frac{1}{1+e^{i(\theta_{j,k}+k)}} \end{bmatrix}, \tag{1.2.20}$$

where

$$c_k(\theta) = 2\left\{ \frac{1}{1 + \cos(\theta - k)} + \frac{1}{1 + \cos\theta} + \frac{1}{1 + \cos(\theta + k)} \right\}^{-1}.$$

In the above calculation, it is most important to emphasize that there is the eigenvalue "1" independently on the value of k. The eigenvalues of the Hadamard walk are given by $e^{i\theta_k}$ and $e^{i(\pi-\theta_k)}$ with the arguments satisfying $\sin\theta_k = \sin k/\sqrt{2}$ (see (1.1.13)). Therefore the eigenvalues do not take the value "1" except the special case $k = 0$. We have shown the existence of strongly degenerated eigenvalue such as "1" in (1.2.19) is necessary condition in the quantum walks showing the localization (see also Inui, Konishi, and Konno (2004)).

Let us number each chirality "L","0", and "R" using $l = 1$, 2, and 3, respectively. Then the wave function in real space is obtained by the inverse Fourier transform: for $\alpha, \beta, \gamma \in \mathbb{C}$ with $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$,

$$\begin{aligned} \Psi_n(x) &= \Psi_n(x; \alpha, \beta, \gamma) \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \hat{\Psi}_n(k) e^{ikx} dk \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \left(\sum_{j=1}^{3} e^{i\theta_{j,k} n} |v_j(k)\rangle\langle v_j(k)|\hat{\Psi}_0(k) \right) e^{ikx} dk \end{aligned}$$

$$= {}^T\left[\Psi_n(x;1;\alpha,\beta,\gamma),\Psi_n(x;2;\alpha,\beta,\gamma),\Psi_n(x;3;\alpha,\beta,\gamma)\right]$$
$$= \sum_{j=1}^{3} {}^T\left[\Psi_n^j(x;1;\alpha,\beta,\gamma),\Psi_n^j(x;2;\alpha,\beta,\gamma),\Psi_n^j(x;3;\alpha,\beta,\gamma)\right], \tag{1.2.21}$$

where

$$\Psi_n^j(x;l;\alpha,\beta,\gamma) = \frac{1}{2\pi}\int_{-\pi}^{\pi} c_k(\theta_{j,k})\varphi_k(\theta_{j,k},l)e^{i(\theta_{j,k}n+kx)}dk \quad (l=1,2,3), \tag{1.2.22}$$

with

$$\varphi_k(\theta,l) = \zeta_{l,k}(\theta)[\alpha\overline{\zeta_{1,k}(\theta)}+\beta\overline{\zeta_{2,k}(\theta)}+\gamma\overline{\zeta_{3,k}(\theta)}] \quad (l=1,2,3),$$
$$\zeta_{1,k}(\theta) = (1+e^{i(\theta-k)})^{-1},\ \zeta_{2,k}(\theta) = (1+e^{i\theta})^{-1},\ \zeta_{3,k}(\theta) = (1+e^{i(\theta+k)})^{-1}, \tag{1.2.23}$$

where $\overline{z}$ is conjugate of $z \in \mathbb{C}$. Sometimes we omit the initial qubit state $[\alpha,\beta,\gamma]$ such as $\Psi_n^j(x;l) = \Psi_n^j(x;l;\alpha,\beta,\gamma)$. The probability of finding the particle at the position x and time n with the chirality l is given by $P_n(x;l) = |\Psi_n(x;l)|^2$. Thus the probability of finding the particle at the position x and time n is $P_n(x) = \sum_{l=1}^{3} P_n(x;l)$.

Time-averaged Probability

We focus our attention on the spatial distribution of the probability of finding the particle after long time. Then (1.2.21) is rather complicated, but the value of $\lim_{n\to\infty} P_n(x)$ can be calculated in following subsections. We start by showing a numerical result for the probability of finding the particle at the origin before carrying out an analytical calculation. The value at the origin of the time-averaged probability is defined by

$$\bar{P}_\infty(0;\alpha,\beta,\gamma) = \lim_{N\to\infty}\left(\lim_{T\to\infty}\frac{1}{T}\sum_{l=1}^{3}\sum_{n=0}^{T-1} P_{n,N}(0;l;\alpha,\beta,\gamma)\right),$$

where $P_{n,N}(x;l;\alpha,\beta,\gamma)$ is the probability of finding a particle with the chirality l at the position x and time n on a cyclic lattice containing N sites. The time-averaged probability introduced here was already used to study the quantum walk. In the case of the Hadamard walk on a cycle containing odd sites, the time-averaged probability takes a value $1/N$ independently of the initial states (see Aharonov et al. (2001), Inui, Konishi, Konno, and Soshi (2005)). Therefore the time-averaged probability converges to zero in the limit $N \to \infty$. On the other hand, the time-averaged probability of quantum walks which exhibit the localization converges to a non-zero value. For this reason, we first calculate the time-averaged probability of three-state Grover walk, and we will show in the next subsection that the probability $P_n(x)$ itself converges as well.

We calculate the time-averaged probability at the origin in three-state Grover walk on a cycle with N sites. We assume that the number N is odd. The argument of eigenvalues of three-state Grover walk with a finite N is $\theta_{j,2m\pi/N}$ for $m \in [-(N-1)/2, (N-1)/2]$. Since the eigenvalue corresponding to m is the same as the eigenvalues corresponding to $-m$, the wave function is formally expressed by

$$\Psi_{n,N}(0;l;\alpha,\beta,\gamma) = \sum_{j=1}^{3} \sum_{m=0}^{(N-1)/2} c_{j,m,l}(N) e^{i\theta_{N,j,m} n},$$

where $\theta_{N,j,m}$ is $\theta_{j,2m\pi/N}$. We note here that the coefficients $c_{j,m,l}(N)$ depend on the initial state $[\alpha,\beta,\gamma]$, but we omit to describe the dependence. Then the probability $P_{n,N}(0;\alpha,\beta,\gamma)$ at the origin is given by

$$\begin{aligned} &P_{n,N}(0;\alpha,\beta,\gamma) \\ &\quad = \sum_{l_1,l_2,j_1,j_2=1}^{3} \sum_{m_1,m_2=0}^{(N-1)/2} c^*_{j_1,m_1,l_1}(N) c_{j_2,m_2,l_2}(N) e^{i(\theta_{N,j_2,m_2} - \theta_{N,j_1,m_1})n}. \end{aligned}$$

The coefficients $c_{j,m,l}(N)$ are determined from the product of eigenvectors. Although lengthy calculations are required to express the coefficients $c_{j,m,l}(N)$ explicitly, it is shown below that coefficients $c_{j,m,l}(N)$ except $j=1$ do not contribute $P_{n,N}(x)$. Noting that the following equation

$$\lim_{T\to\infty} \frac{1}{T} \sum_{n=0}^{T-1} e^{i\theta n} = \begin{cases} 1, & \theta = 0, \\ 0, & \theta \neq 0, \end{cases}$$

we have

$$\begin{aligned} \bar{P}_N(0;\alpha,\beta,\gamma) = \sum_{l=1}^{3} \Bigg(& \left| \sum_{m=0}^{(N-1)/2} c_{1,m,l}(N) \right|^2 \\ & + \left| \sum_{j=2}^{3} c_{j,0,l}(N) \right|^2 + \sum_{j=2}^{3} \sum_{m=1}^{(N-1)/2} |c_{j,m,l}(N)|^2 \Bigg). \end{aligned} \quad (1.2.24)$$

The difference between the first term and the other terms is caused by the difference of the degree of degenerate eigenvalues.

Let $\phi_{j,k}(N)$ be the eigenvectors corresponding to the eigenvalue $e^{i\theta_{j,k} n}$ of the time-evolution matrix of the three-state Grover walk with a matrix size $3N \times 3N$. They are easily obtained from $|v_j(k)\rangle$ by

$$|\phi_{j,k}(N)\rangle = \frac{1}{\sqrt{3N}}[|v_j(k)\rangle, \omega|v_j(k)\rangle, \omega^2|v_j(k)\rangle, \ldots, \omega^{N-1}|v_j(k)\rangle],$$

where $\omega = e^{2\pi i/N}$. Since the coefficients $c_{j,m,l}(N)$ are proportional to the product of eigenvectors, the orders with respect to N of the first term and the second term in (1.2.24) are $O(1)$ and $O(N^{-1})$, respectively. Thus we can neglect the second term in the limit of $N \to \infty$. Using the eigenvectors in (1.2.20), we have

$$\bar{P}_\infty(0;\alpha,\beta,\gamma) = (5-2\sqrt{6})(1+|\alpha+\beta|^2+|\beta+\gamma|^2-2|\beta|^2).$$

The time-averaged probability takes the maximum value $2(5-2\sqrt{6})$ at $\beta = 0$. The component of $\bar{P}_\infty(0;\alpha,\beta,\gamma)$ corresponding to $l = 1,2,3$ are respectively given by

$$\begin{aligned}\bar{P}_\infty(0;1;\alpha,\beta,\gamma) &= \frac{|\sqrt{6}\alpha - 2(\sqrt{6}-3)\beta + (12-5\sqrt{6})\gamma|^2}{36},\\ \bar{P}_\infty(0;2;\alpha,\beta,\gamma) &= \frac{(\sqrt{6}-3)^2|\alpha+\beta+\gamma|^2}{9},\\ \bar{P}_\infty(0;3;\alpha,\beta,\gamma) &= \frac{|\sqrt{6}\gamma - 2(\sqrt{6}-3)\beta + (12-5\sqrt{6})\alpha|^2}{36}.\end{aligned} \quad (1.2.25)$$

We stress here that the time-averaged probability is not always positive. If $\alpha = 1/\sqrt{6}$, $\beta = -2/\sqrt{6}$ and $\gamma = 1/\sqrt{6}$, then the time-averaged probability becomes zero, that is, $\bar{P}_\infty(0;1/\sqrt{6},-2/\sqrt{6},1/\sqrt{6}) = 0$.

Stationary Distribution of the Particle

We showed that the time-averaged probability of three-state Grover walk converges to non-zero values except special initial states. In this subsection we calculate the limit $P_*(x) \equiv \lim_{n\to\infty} P_n(x) (= \lim_{n\to\infty} P_n(x;\alpha,\beta,\gamma))$ rigorously and consider the dependence of $P_*(x)$ on the position x.

The wave function given by (1.2.21) is infinite superposition of the wave function $e^{i(\theta_{j,k}n+kx)}$. If the argument $\theta_{j,k}$ given in (1.2.19) for $j = 2,3$ is not absolute zero, then the $e^{i\theta_{j,k}n}$ oscillates with high frequency in k-space for large n. On the other hand, $c_k(\theta_{j,k})\varphi_k(\theta_{j,k},l)$ in (1.2.22) changes smoothly with respect to k. Therefore we expect that the integration for $j = 2,3$ in (1.2.22) becomes small as the time increases due to cancellation and converges to zero in the limit of $n \to \infty$. That is,

Lemma 1.11. *For fixed $x \in \mathbb{Z}$,*

$$\lim_{n\to\infty} \sum_{j=2}^{3} \Psi_n^j(x;l;\alpha,\beta,\gamma) = 0, \quad (1.2.26)$$

for $l = 1,2,3$ and $\alpha,\beta,\gamma \in \mathbb{C}$ with $|\alpha|^2+|\beta|^2+|\gamma|^2 = 1$.

Proof. Here we give an outline of the proof. A direct computation gives

$$\sum_{j=2}^{3} \begin{bmatrix} \Psi_n^j(x;1;\alpha,\beta,\gamma) \\ \Psi_n^j(x;2;\alpha,\beta,\gamma) \\ \Psi_n^j(x;3;\alpha,\beta,\gamma) \end{bmatrix} = M \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix},$$

where $M = (m_{ij})_{1 \le i,j \le 3}$ with

$$m_{11} = 3J_{x,n} + \frac{1}{2}\left\{J_{x-1,n} + J_{x+1,n} + (K_{x-1,n} - K_{x+1,n})\right\},$$
$$m_{33} = 3J_{x,n} + \frac{1}{2}\left\{J_{x-1,n} + J_{x+1,n} - (K_{x-1,n} - K_{x+1,n})\right\},$$
$$m_{12} = -\left\{J_{x,n} + J_{x+1,n} + (K_{x,n} - K_{x+1,n})\right\},$$
$$m_{32} = -\left\{J_{x,n} + J_{x-1,n} + (K_{x,n} - K_{x-1,n})\right\},$$
$$m_{13} = -2J_{x+1,n}, \qquad m_{31} = -2J_{x-1,n},$$
$$m_{21} = -\left\{J_{x,n} + J_{x-1,n} + (K_{x-1,n} - K_{x,n})\right\},$$
$$m_{23} = -\left\{J_{x,n} + J_{x+1,n} + (K_{x+1,n} - K_{x,n})\right\},$$
$$m_{22} = 4J_{x,n},$$

and

$$J_{x,n} = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{\cos(kx)}{5+\cos k}\cos(\theta_k n)dk,$$
$$K_{x,n} = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{\cos(kx)}{\sqrt{(5+\cos k)(1-\cos k)}}\sin(\theta_k n)dk.$$

From the Riemann-Lebesgue lemma, we can show that

$$\lim_{n\to\infty} J_{x,n} = 0, \qquad \lim_{n\to\infty}(K_{x,n} - K_{x+1,n}) = 0,$$

for any $x \in \mathbb{Z}$. Therefore we have the desired conclusion.

From this lemma, the probability $P_*(x) = P_*(x;\alpha,\beta,\gamma)$ is determined from the eigenvectors corresponding to the eigenvalue “1”, that is, $\theta_{1,k} = 0$ (see (1.2.19)), and l-th component of $P_*(x;l) = P_*(x;l;\alpha,\beta,\gamma)$ is given by

$$P_*(x;l;\alpha,\beta,\gamma) = \left|\Psi_n^1(x;l;\alpha,\beta,\gamma)\right|^2. \qquad (1.2.27)$$

Note that $\Psi_n^1(x;l;\alpha,\beta,\gamma)$ does not depend on time n, since $\theta_{1,k} = 0$. By transforming integration in the left-hand side in (1.2.27) into complex integral, we have

$$
\begin{aligned}
P_*(x;1;\alpha,\beta,\gamma) &= \left|2\alpha I(x) + \beta J_+(x) + 2\gamma K_+(x)\right|^2, \\
P_*(x;2;\alpha,\beta,\gamma) &= \left|\alpha J_-(x) + \frac{\beta}{2} L(x) + \gamma J_+(x)\right|^2, \\
P_*(x;3;\alpha,\beta,\gamma) &= \left|2\alpha K_-(x) + \beta J_-(x) + 2\gamma I(x)\right|^2,
\end{aligned} \tag{1.2.28}
$$

where $c = -5 + 2\sqrt{6}$ $(\in (-1,0))$ and

$$
\begin{aligned}
& I(x) = \frac{2c^{|x|+1}}{c^2 - 1}, \quad L(x) = I(x-1) + 2I(x) + I(x+1), \\
& J_+(x) = I(x) + I(x+1), \quad J_-(x) = I(x-1) + I(x), \\
& K_+(x) = I(x+1), \quad K_-(x) = I(x-1),
\end{aligned} \tag{1.2.29}
$$

for any $x \in \mathbb{Z}$. Therefore we have

Theorem 1.12.

$$
P_*(x;\alpha,\beta,\gamma) = \sum_{l=1}^{3} P_*(x;l;\alpha,\beta,\gamma) \qquad (x \in \mathbb{Z}).
$$

We should remark that it is confirmed $\bar{P}_\infty(0;l;\alpha,\beta,\gamma) = P_*(0;l;\alpha,\beta,\gamma)$ for $l = 1,2,3$ by using (1.2.25), (1.2.28) and (1.2.29).

Here we give an example. From (1.2.28) and (1.2.29), we obtain

$$
P_*(0; i/\sqrt{2}, 0, 1/\sqrt{2}) = \frac{4c^2(5c^2 + 2c + 5)}{(1-c^2)^2} = 2(5 - 2\sqrt{6}) = 0.202\ldots, \tag{1.2.30}
$$

$$
P_*(x; i/\sqrt{2}, 0, 1/\sqrt{2}) = \frac{2(5c^4 + 2c^3 + 10c^2 + 2c + 5)}{(1-c^2)^2} c^{2|x|}, \tag{1.2.31}
$$

for any x with $|x| \geq 1$. Furthermore,

$$
0 < \sum_{x \in \mathbb{Z}} P_*(x; i/\sqrt{2}, 0, 1/\sqrt{2}) = 1/\sqrt{6} = 0.408\ldots < 1. \tag{1.2.32}
$$

That is, $P_*(x; i/\sqrt{2}, 0, 1/\sqrt{2})$ is not a probability measure. The above value depends on the initial qubit state, for example,

$$
\begin{aligned}
& \sum_{x \in \mathbb{Z}} P_*(x; 1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3}) = 3 - \sqrt{6} = 0.550\ldots, \\
& \sum_{x \in \mathbb{Z}} P_*(x; 1/\sqrt{3}, -1/\sqrt{3}, 1/\sqrt{3}) = (3 - \sqrt{6})/9 = 0.061\ldots.
\end{aligned}
$$

We should remark that in the case of the classical symmetric random walk starting from the origin, it is known that $P_*(x) = 0$ for any $x \in \mathbb{Z}$, therefore we have $\sum_{x\in\mathbb{Z}} P_*(x) = 0$. The same conclusion can be obtained for the discrete-time and continuous-time two-state quantum walks.

Weak Limit Theorem

In this subsection we give a weak limit theorem for the three-state Grover walk for any initial state $\varphi = {}^T[\alpha, \beta, \gamma]$ by using the method of Grimmett, Janson, and Scudo (2004). The unitary matrix of the walk is

$$U = \frac{1}{3}\begin{bmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{bmatrix}.$$

So we have

$$U(k) = \frac{1}{3}\begin{bmatrix} -e^{ik} & 2e^{ik} & 2e^{ik} \\ 2 & -1 & 2 \\ 2e^{-ik} & 2e^{-ik} & -e^{-ik} \end{bmatrix}.$$

The eigenvalues and corresponding eigenvectors of $U(k)$ are

$$\lambda_1(k) = 1, \quad \lambda_2(k) = e^{i\theta_k}, \quad \lambda_3(k) = e^{-i\theta_k},$$

where

$$\cos\theta_k = -\frac{1}{3}(\cos k + 2), \quad \sin\theta_k = \frac{1}{3}\sqrt{(5+\cos k)(1-\cos k)},$$

and

$$v_1(k) = \frac{2}{5+\cos k}\begin{bmatrix} 1 \\ (1+e^{-ik})/2 \\ e^{-ik} \end{bmatrix},$$

$$v_2(k) = \frac{1}{\sqrt{|1/w_1(k)|^2 + |1/w_2(k)|^2 + |1/w_3(k)|^2}}\begin{bmatrix} 1/w_1(k) \\ 1/w_2(k) \\ 1/w_3(k) \end{bmatrix},$$

$$v_3(k) = \frac{1}{\sqrt{|1/w_1(k)|^2 + |1/w_2(k)|^2 + |1/w_3(k)|^2}}\begin{bmatrix} 1/\overline{w_3(k)} \\ 1/\overline{w_2(k)} \\ 1/\overline{w_1(k)} \end{bmatrix},$$

where

$$w_1(k) = 1 + e^{i(\theta_k - k)}, \quad w_2(k) = 1 + e^{i\theta_k}, \quad w_3(k) = 1 + e^{i(\theta_k + k)}.$$

Then we have

$$h_1(k) = 0, \quad h_2(k) = \frac{\sin k}{\sqrt{(5+\cos k)(1-\cos k)}},$$
$$h_3(k) = -\frac{\sin k}{\sqrt{(5+\cos k)(1-\cos k)}}.$$

From Theorem 1.10, we obtain

$$P(Y \le y) = \sum_{j=1}^{3} \int_{\{k \in [-\pi,\pi): h_j(k) \le y\}} p_j(k) \frac{dk}{2\pi}.$$

Let $k(y) \in (0, \pi]$ be the unique solution of $h_2(k)$ for $y \ge 0$. Then we get

$$P(Y \le y) = \int_{-\pi}^{\pi} p_1(k) \frac{dk}{2\pi} + \left(\int_{-\pi}^{0} + \int_{k(y)}^{\pi} \right) p_2(k) \frac{dk}{2\pi} + \left(\int_{-\pi}^{-k(y)} + \int_{0}^{\pi} \right) p_3(k) \frac{dk}{2\pi}.$$

Let $\tilde{k}(y)(= -k(y)) \in [-\pi, 0)$ be the unique solution of $h_2(k)$ for $y \le 0$. Similarly we have

$$P(Y \le y) = \int_{\tilde{k}(y)}^{0} p_2(k) \frac{dk}{2\pi} + \int_{0}^{-\tilde{k}(y)} p_3(k) \frac{dk}{2\pi}.$$

Therefore the limit measure is given by

$$f(y) = \frac{d}{dy} P(Y \le y) = \Delta\delta_0(y) - \frac{1}{2\pi} \left\{ p_2(k(y)) + p_3(-k(y)) \right\} \frac{dk(y)}{dy},$$

where

$$\cos k(y) = \frac{5y^2 - 1}{1 - y^2}, \quad \sin k(y) = \frac{2y\sqrt{2(1-3y^2)}}{1-y^2},$$
$$\cos \theta_{k(y)} = -\frac{1+3y^2}{3(1-y^2)}, \quad \sin \theta_{k(y)} = \frac{2\sqrt{2(1-3y^2)}}{3(1-y^2)}.$$

Moreover

$$v_2(k(y)) = \frac{1}{2\sqrt{3}} \begin{bmatrix} \sqrt{2(1-3y^2)} + i(1-3y) \\ \sqrt{2(1-3y^2)} - 2i \\ \sqrt{2(1-3y^2)} + i(1+3y) \end{bmatrix},$$

$$v_3(-k(y)) = \frac{1}{2\sqrt{3}} \begin{bmatrix} \sqrt{2(1-3y^2)} - i(1-3y) \\ \sqrt{2(1-3y^2)} + 2i \\ \sqrt{2(1-3y^2)} - i(1+3y) \end{bmatrix}.$$

Remark that

$$\frac{dk(y)}{dy} = -\frac{2\sqrt{2}}{(1-y^2)\sqrt{1-3y^2}}.$$

Therefore we have

Theorem 1.13. *If $n \to \infty$, then*

$$\frac{X_n}{n} \quad \Rightarrow \quad Z,$$

where Z has the following measure:

$$f(y) = \Delta(\alpha,\beta,\gamma)\,\delta_0(y) + \frac{\sqrt{2}(c_0 + c_1 y + c_2 y^2)}{2\pi(1-y^2)\sqrt{1-3y^2}}\, I_{(-1/\sqrt{3},1/\sqrt{3})}(y),$$

where

$$\begin{aligned}\Delta(\alpha,\beta,\gamma) &= \int_{-\pi}^{\pi} p_1(k)\frac{dk}{2\pi} \\ &= \left(\left|\alpha + \frac{\beta}{2}\right|^2 + \left|\gamma + \frac{\beta}{2}\right|^2\right)\frac{\sqrt{6}}{6} \\ &\quad + \Re\left((2\alpha+\beta)(2\overline{\gamma}+\overline{\beta})\right)\left(1 - \frac{5}{12}\sqrt{6}\right),\end{aligned}$$

and

$$\begin{aligned} c_0 &= |\alpha+\gamma|^2 + 2|\beta|^2, \\ c_1 &= 2\left(-|\alpha-\beta|^2 + |\gamma-\beta|^2\right), \\ c_2 &= |\alpha-\gamma|^2 - 2\Re((2\alpha+\beta)(2\overline{\gamma}+\overline{\beta})).\end{aligned}$$

Here $\Re(z)$ is the real part of $z \in \mathbb{C}$.

Therefore by Theorem 1.13 we check

$$\begin{aligned}\Delta(i/\sqrt{2},0,1/\sqrt{2}) &= \sum_{x\in\mathbb{Z}} P_*(x; i/\sqrt{2},0,1/\sqrt{2}) = 1/\sqrt{6}, \\ \Delta(1/\sqrt{3},1/\sqrt{3},1/\sqrt{3}) &= \sum_{x\in\mathbb{Z}} P_*(x; 1/\sqrt{3},1/\sqrt{3},1/\sqrt{3}) = 3 - \sqrt{6}, \\ \Delta(1/\sqrt{3},-1/\sqrt{3},1/\sqrt{3}) &= \sum_{x\in\mathbb{Z}} P_*(x; 1/\sqrt{3},-1/\sqrt{3},1/\sqrt{3}) = (3-\sqrt{6})/9.\end{aligned}$$

In general, we see that

$$\Delta(\alpha,\beta,\gamma) = \sum_{x\in\mathbb{Z}} P_*(x;\alpha,\beta,\gamma).$$

Conclusions and Discussions

Some properties which are not observed in two-state quantum walks were found in three-state Grover walk. The particle which exists at the origin splits in a superposition of three pieces. Two of the three parts leave for points at infinity and the remainder stays at the origin. In contrast with the ordinary Hadamard walk, the probability of finding the particle at the origin does not vanish for large time, and its maximum probability is $2(5-2\sqrt{6}) = 0.202\ldots$.

A simple reason why the three-state Grover walk is different from two-state quantum walks is the difference in the degree of degenerate eigenvalues. The necessary condition of the localization is the existence of degenerate eigenvalues. And furthermore, each degree of degeneration must be proportional to the dimension of the Hilbert space. In addition, if the degenerate eigenvalue is 1 only, then the probability of finding the particle can converges in the limit of $n \to \infty$. The four-state Grover walk exhibits the localization, but the probability of finding the particle oscillates, because there are degenerate eigenvalues with values "1" and "-1". On the other hand, the degenerated eigenvalue in three-state Grover walk unrelated to the wave number is only "1", therefore the probability converges. Although no experiment exists about the quantum walks yet, the stationary properties of three-state Grover walk may be useful for comparison wit h theoretical results.

We discuss a relation between the limit distribution for the original three-state Grover walk X_n as time $n \to \infty$ and that of the rescaled X_n/n in the same limit. When we consider the three-state Grover walk starting from a mixture of three pure states ${}^T[1,0,0]$, ${}^T[0,1,0]$, and ${}^T[0,0,1]$ with probability 1/3 respectively, we can obtain a weak limit probability distribution $f(x)$ for the rescaled three-state quantum walk X_n/n as $n \to \infty$:

$$f(x) = \frac{1}{3}\delta_0(x) + \frac{\sqrt{8}}{3\pi(1-x^2)\sqrt{1-3x^2}}\, I_{(-1/\sqrt{3},1/\sqrt{3})}(x), \qquad (1.2.33)$$

for $x \in \mathbb{R}$, where $\delta_0(x)$ denotes the pointmass at the origin and $I_{(a,b)}(x) = 1$, if $x \in (a,b)$, $= 0$, otherwise. The above derivation is due to the method by Grimmett, Janson, and Scudo (2004). We should note that the first term in the right-hand side of (1.2.33) corresponds to the localization for the original three-state quantum walk. In fact, we have

$$\frac{1}{3}\sum_{x\in\mathbb{Z}} [P_*(x;1,0,0) + P_*(x;0,1,0) + P_*(x;0,0,1)] = \frac{1}{3}.$$

The last value 1/3 is nothing but the coefficient 1/3 of $\delta_0(x)$. Moreover, the second term in the right-hand side of (1.2.33) has a similar weak limit density function for the same rescaled Hadamard walk with two inner states starting from a uniform random mixture of two pure states ${}^T[1,0]$ and ${}^T[0,1]$:

$$f_H(x) = \frac{1}{\pi(1-x^2)\sqrt{1-2x^2}} I_{(-1/\sqrt{2},1/\sqrt{2})}(x),$$

for $x \in \mathbb{R}$. This case does not have a delta measure term corresponding to a localization.

1.3 Multi-State Case

Rigorous results for multi-state quantum walks are very limited. Localization of one-dimensional four-state Grover walk (Inui and Konno (2005)) and two-dimensional four-state quantum walks (Inui, Konishi, and Konno (2004)) was investigated. Moreover, Miyazaki, Katori, and Konno (2007) obtained weak limit theorems for a class of multi-state quantum walks in one dimension.

2 Disordered Case

2.1 Introduction

A unitary matrix corresponding to the evolution of the quantum walk is usually deterministic and independent of the time step. In this chapter we study a random unitary matrix case motivated by numerical results of Mackay et al. (2002) and Ribeiro, Milman, and Mosseri (2004). We obtain a classical random walk from the quantum walk by introducing an independent random fluctuation at each time step and performing an ensemble average in a rigorous way based on a combinatorial approach. The time evolution of the quantum walk is given by the following random unitary matrices $\{U_n : n = 1, 2, \ldots\}$:

$$U_n = \begin{bmatrix} a_n & b_n \\ c_n & d_n \end{bmatrix},$$

where $a_n, b_n, c_n, d_n \in \mathbb{C}$. The subscript n indicates the time step. The unitarity of U_n gives

$$\begin{aligned} &|a_n|^2 + |c_n|^2 = |b_n|^2 + |d_n|^2 = 1, \\ &a_n\overline{c_n} + b_n\overline{d_n} = 0,\ c_n = -\triangle_n\overline{b_n},\ d_n = \triangle_n\overline{a_n}, \end{aligned} \tag{2.1.1}$$

where $\overline{z}$ is the complex conjugate of $z \in \mathbb{C}$ and $\triangle_n = \det U_n = a_n d_n - b_n c_n$ with $|\triangle_n| = 1$. Put $w_n = (a_n, b_n, c_n, d_n)$. Let $\{w_n : n = 1, 2, \ldots\}$ be independent and identically distributed (or i.i.d. for short) on some space, (for example, $[0, 2\pi)$) with

$$E(|a_1|^2) = E(|b_1|^2) = 1/2, \tag{2.1.2}$$

$$E(a_1\overline{c_1}) = 0. \tag{2.1.3}$$

Remark that (2.1.2) implies $E(|c_1|^2) = E(|d_1|^2) = 1/2$, and (2.1.3) gives $E(b_1\overline{d_1}) = 0$ by using (2.1.1). The set of initial qubit states for the quantum walk is given by

$$\Phi = \left\{\varphi = {}^T[\alpha, \beta] \in \mathbb{C}^2 : |\alpha|^2 + |\beta|^2 = 1\right\}.$$

Moreover we assume that $\{w_n : n = 1, 2, \ldots\}$ and $\{\alpha, \beta\}$ are independent. We call the above process a *disordered quantum walk* in this chapter. Let $\mathbb{R}$ be the set of the real numbers. Then we consider the following two cases:

Case I: $a_n, b_n, c_n, d_n \in \mathbb{R}$ $(n = 1, 2, \ldots)$ and $E(\alpha\overline{\beta} + \overline{\alpha}\beta) = 0$.

Case II: $E(|\alpha|^2) = 1/2$ and $E(\alpha\overline{\beta}) = 0$.

We should note that Case I corresponds to an example given by Ribeiro, Milman, and Mosseri (2004) and Case II corresponds to an example given by Mackay et al. (2002), respectively. The numerical simulations by two groups suggest that the probability distribution of a disordered quantum walk converges to a binomial distribution by averaging over many trials. So the main purpose of this chapter is to prove the above numerical results by using a combinatorial (path integral) approach. Results in this chapter are based on Konno (2005b). Main result here (Theorem 2.1) shows that the expectation of the probability distribution for the disordered quantum walk becomes the probability distribution of a classical symmetric random walk. However our result does not treat a crossover from quantum to classical walks.

2.2 Definition of Disordered Quantum Walk

First we divide U_n into two matrices:

$$P_n = \begin{bmatrix} a_n & b_n \\ 0 & 0 \end{bmatrix}, \quad Q_n = \begin{bmatrix} 0 & 0 \\ c_n & d_n \end{bmatrix},$$

with $U_n = P_n + Q_n$. The important point is that P_n (resp. Q_n) represents that the particle moves to the left (resp. right) at each time step n. By using P_n and Q_n, we define the dynamics of the disordered quantum walk on the line. To do so, we define a $(4N+2) \times (4N+2)$ matrix $\overline{U}_n$ by

$$\overline{U}_n = \begin{bmatrix} 0 & P_n & 0 & \ldots & \ldots & 0 & Q_n \\ Q_n & 0 & P_n & 0 & \ldots & \ldots & 0 \\ 0 & Q_n & 0 & P_n & 0 & \ldots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ldots & 0 & Q_n & 0 & P_n & 0 \\ 0 & \ldots & \ldots & 0 & Q_n & 0 & P_n \\ P_n & 0 & \ldots & \ldots & 0 & Q_n & 0 \end{bmatrix},$$

where $0 = O_2$ is the 2×2 zero matrix. Note that P_n and Q_n satisfy

$$P_n P_n^* + Q_n Q_n^* = P_n^* P_n + Q_n^* Q_n = I_2,$$
$$P_n Q_n^* = Q_n P_n^* = Q_n^* P_n = P_n^* Q_n = O_2,$$

where $*$ means the adjoint operator and I_2 is the 2×2 unit matrix. The above relations imply that $\overline{U}_n$ is also a unitary matrix. Using $\overline{U}_n$, we can define a disordered quantum walk X_n at time n starting from $\varphi \in \Phi$. Let $\Psi_n(x)$ be the two component vector of amplitudes of the particle being at site x and at time n. Then the probability of $\{X_n = x\}$ is defined by

$$P(X_n = x) = \|\Psi_n(x)\|^2.$$

Remark that $\{X_n = x\}$ is an event generated by $\{w_i : i = 1, 2, \dots, n\}$ and $\{\alpha, \beta\}$. The unitarity of $\overline{U}_m (m = 1, 2, \dots, n)$ ensures

$$\sum_{x=-n}^{n} P(X_n = x) = \|\overline{U}_n \overline{U}_{n-1} \cdots \overline{U}_1 \overline{\varphi}\|^2 = \|\overline{\varphi}\|^2 = |\alpha|^2 + |\beta|^2 = 1,$$

for any $1 \le n \le N$. That is, the amplitude always defines a probability distribution for the location.

2.3 Result

We now give a combinatorial expression for the probability distribution of the disordered quantum walk. For fixed l and m with $l + m = n$ and $-l + m = x$, we introduce

$$\Xi_n(l, m) = \sum_{l_j, m_j} P^{l_n} Q^{m_n} P^{l_{n-1}} Q^{m_{n-1}} \cdots P^{l_1} Q^{m_1}$$

summed over all $l_j, m_j \ge 0$ satisfying $l_1 + \cdots + l_n = l$, $m_1 + \cdots + m_n = m$ and $l_j + m_j = 1$. We should note that

$$\Psi_n(x) = \Xi_n(l, m)\varphi.$$

For example, in the case of $P(X_4 = 0)$, we have

$$\Xi_4(2, 2) = P_4 Q_3 Q_2 P_1 + Q_4 P_3 P_2 Q_1 + P_4 P_3 Q_2 Q_1$$
$$+ P_4 Q_3 P_2 Q_1 + Q_4 P_3 Q_2 P_1 + Q_4 Q_3 P_2 P_1.$$

To compute $\Xi_n(l, m)$, we introduce the following useful random matrices:

$$R_n = \begin{bmatrix} c_n & d_n \\ 0 & 0 \end{bmatrix}, \quad S_n = \begin{bmatrix} 0 & 0 \\ a_n & b_n \end{bmatrix}.$$

In general, we obtain the following table of products of the matrices P_j, Q_j, R_j and S_j $(j = 1, 2, \ldots)$: for any $m, n \geq 1$,

	P_n	Q_n	R_n	S_n
P_m	$a_m P_n$	$b_m R_n$	$a_m R_n$	$b_m P_n$
Q_m	$c_m S_n$	$d_m Q_n$	$c_m Q_n$	$d_m S_n$
R_m	$c_m P_n$	$d_m R_n$	$c_m R_n$	$d_m P_n$
S_m	$a_m S_n$	$b_m Q_n$	$a_m Q_n$	$b_m S_n$

where $P_m Q_n = b_m R_n$, for example. From this table, we obtain

$$\Xi_4(2,2) = b_4 d_3 c_2 P_1 + c_4 a_3 b_2 Q_1 + (a_4 b_3 d_2 + b_4 c_3 b_2) R_1 + (c_4 b_3 c_2 + d_4 c_3 a_2) S_1.$$

We should note that P_1, Q_1, R_1 and S_1 form an orthonormal basis of the vector space of complex 2×2 matrices with respect to the trace inner product $\langle A|B \rangle = \mathrm{tr}(A^* B)$. So $\Xi_n(l,m)$ has the following form:

$$\Xi_n(l,m) = p_n(l,m) P_1 + q_n(l,m) Q_1 + r_n(l,m) R_1 + s_n(l,m) S_1. \quad (2.3.4)$$

In general, explicit forms for $p_n(l,m), q_n(l,m), r_n(l,m)$ and $s_n(l,m)$ are complicated. From (2.3.4), we have

$$\Xi_n(l,m) = \begin{bmatrix} p_n(l,m)a_1 + r_n(l,m)c_1 & p_n(l,m)b_1 + r_n(l,m)d_1 \\ q_n(l,m)c_1 + s_n(l,m)a_1 & q_n(l,m)d_1 + s_n(l,m)b_1 \end{bmatrix}.$$

Remark that $p_n(l,m), q_n(l,m), r_n(l,m), s_n(l,m)$ depend only on $\{w_i : i = 2, 3, \ldots n\}$, so they are independent of w_1, where $w_i = (a_i, b_i, c_i, d_i)$. Moreover it should be noted that $\{w_i : i = 1, 2, \ldots\}$ and $\{\alpha, \beta\}$ are independent. Therefore we obtain

$$\begin{aligned} P(X_n = x) &= ||\Xi_n(l,m)\varphi||^2 \\ &= \left\{ |p_n(l,m)a_1 + r_n(l,m)c_1|^2 + |q_n(l,m)c_1 + s_n(l,m)a_1|^2 \right\} |\alpha|^2 \\ &\quad + \left\{ |p_n(l,m)b_1 + r_n(l,m)d_1|^2 + |q_n(l,m)d_1 + s_n(l,m)b_1|^2 \right\} |\beta|^2 \\ &\quad + \Big\{ \overline{(p_n(l,m)a_1 + r_n(l,m)c_1)} (p_n(l,m)b_1 + r_n(l,m)d_1) \\ &\quad + \overline{(q_n(l,m)c_1 + s_n(l,m)a_1)} (q_n(l,m)d_1 + s_n(l,m)b_1) \Big\} \overline{\alpha}\beta \\ &\quad + \Big\{ (p_n(l,m)a_1 + r_n(l,m)c_1) \overline{(p_n(l,m)b_1 + r_n(l,m)d_1)} \\ &\quad + (q_n(l,m)c_1 + s_n(l,m)a_1) \overline{(q_n(l,m)d_1 + s_n(l,m)b_1)} \Big\} \alpha\overline{\beta} \\ &= C_1 |\alpha|^2 + C_2 |\beta|^2 + C_3 \overline{\alpha}\beta + C_4 \alpha \overline{\beta}. \end{aligned}$$

Then we see that

$$E(C_1|\alpha|^2) = \frac{1}{2} E\big[|p_n(l,m)|^2 + |s_n(l,m)|^2 + |q_n(l,m)|^2 + |r_n(l,m)|^2 \big] E(|\alpha|^2),$$

since $\{p_n(l,m), q_n(l,m), r_n(l,m), s_n(l,m)\}$ and w_1 are independent, $\{w_i : i = 1, 2, \ldots\}$ and $\{\alpha, \beta\}$ are independent, (2.1.2) and (2.1.3). Similarly, we have

$$E(C_2|\beta|^2) = \frac{1}{2}E\left[|p_n(l,m)|^2 + |s_n(l,m)|^2 + |q_n(l,m)|^2 + |r_n(l,m)|^2\right]E(|\beta|^2).$$

Case I: First we note that $C_4 = \overline{C_3}$. So $a_n, b_n, c_n, d_n \in \mathbb{R}$ gives $C_3 = C_4$. Then the condition $\alpha\overline{\beta} + \overline{\alpha}\beta = 0$ implies $C_3\overline{\alpha}\beta + C_4\alpha\overline{\beta} = 0$. Therefore we obtain

$$\begin{aligned}
&E(P(X_n = x)) \\
&= E(||\Xi_n(l,m)\varphi||^2) \\
&= \frac{1}{2}E\left[|p_n(l,m)|^2 + |s_n(l,m)|^2 + |q_n(l,m)|^2 + |r_n(l,m)|^2\right] E(|\alpha|^2) \\
&+ \frac{1}{2}E\left[|p_n(l,m)|^2 + |s_n(l,m)|^2 + |q_n(l,m)|^2 + |r_n(l,m)|^2\right] E(|\beta|^2) \\
&= \frac{1}{2}\left\{E(|p_n(l,m)|^2) + E(|q_n(l,m)|^2) + E(|r_n(l,m)|^2) + E(|s_n(l,m)|^2)\right\},
\end{aligned}$$

since $|\alpha|^2 + |\beta|^2 = 1$.
Case II: $E(\alpha\overline{\beta}) = E(\overline{\alpha}\beta) = 0$ gives the same conclusion as above in a similar fashion.

To get a feel for the following main result, we will look at the concrete case where $n = 4$ and $l = m = 2$.

$$\begin{aligned}
&E(P(X_4^{\varphi} = 0)) \\
&= E(||\Xi_4(2,2)\varphi||^2) \\
&= \frac{1}{2}\left\{E(|p_4(2,2)|^2) + E(|q_4(2,2)|^2) + E(|r_4(2,2)|^2) + E(|s_4(2,2)|^2)\right\} \\
&= \frac{1}{2}\left\{E(|b_4|^2)E(|d_3|^2)E(|c_2|^2) + E(|c_4|^2)E(|a_3|^2)E(|b_2|^2)\right. \\
&\quad + E(|a_4|^2)E(|b_3|^2)E(|d_2|^2) + E(|b_4|^2)E(|c_3|^2)E(|b_2|^2) \\
&\quad + E(a_4\overline{b_4})E(b_3\overline{c_3})E(d_2\overline{b_2}) + E(\overline{a_4}b_4)E(\overline{b_3}c_3)E(\overline{d_2}b_2) \\
&\quad + E(|c_4|^2)E(|b_3|^2)E(|c_2|^2) + E(|d_4|^2)E(|c_3|^2)E(|a_2|^2) \\
&\quad \left. + E(c_4\overline{d_4})E(b_3\overline{c_3})E(c_2\overline{a_2}) + E(\overline{c_4}d_4)E(\overline{b_3}c_3)E(\overline{c_2}a_2)\right\} \\
&= \frac{1}{16} + \frac{1}{16} + \frac{2}{16} + \frac{2}{16} = \frac{1}{2^4}\binom{4}{2},
\end{aligned}$$

since $E(|a_1|^2) = E(|b_1|^2) = E(|c_1|^2) = E(|d_1|^2) = 1/2$, and $E(a_1\overline{c_1}) = E(b_1\overline{d_1}) = 0$. This result corresponds to $P(Y_4^o = 0) = \binom{4}{2}/2^4$, where Y_n^o denotes the classical symmetric random walk starting from the origin. We generalize the above example as follows:

Theorem 2.1. *We assume that a disordered quantum walk starting from φ satisfies Case I or Case II. For $n = 0, 1, 2, \ldots,$ and $x = -n, -(n-1), \ldots, n-1, n$, with $n + x$ is even, we have*

$$E(P(X_n = x)) = P(Y_n^o = x) = \frac{1}{2^n}\binom{n}{(n+x)/2}.$$

Proof. For $n = 0, 1, 2, \ldots$, and $x = -n, -(n-1), \ldots, n-1, n$, with $n + x$ is even, let $l = (n-x)/2$, $m = (n+x)/2$ and $M = \binom{n}{(n+x)/2}$. In general, as in the case of $n = 4$ with $l = m = 2$, we have

$$\begin{aligned} P(X_n = x) &= E(||\Xi_n(l,m)\varphi||^2) \\ &= \frac{1}{2}\sum_{j=1}^{M} E(|u_n^{(j)}|^2)E(|u_{n-1}^{(j)}|^2)\cdots E(|u_2^{(j)}|^2) + R(w_1, w_2, \ldots, w_n), \end{aligned}$$

where $u_i^{(j)} \in \{a_i, b_i, c_i, d_i\}$ for any $i = 2, 3, \ldots, n$, $j = 1, 2, \ldots, M$ and $w_k = (a_k, b_k, c_k, d_k)$ for any $k = 1, 2, \ldots, n$. Then $E(|a_1|^2) = E(|b_1|^2) = E(|c_1|^2) = E(|d_1|^2) = 1/2$ gives

$$E(P(X_n = x)) = \frac{M}{2^n} + R(w_1, w_2, \ldots, w_n).$$

To get the desired conclusion, it suffices to show that $R(w_1, w_2, \ldots, w_n) = 0$. When there are more than two terms in $p_n(l,m)$ or $s_n(l,m)$, we have to consider two cases: there is a k such that

$$\cdots P_{k+1}P_kP_{k-1}\cdots P_1, \qquad \cdots Q_{k+1}P_kP_{k-1}\cdots P_1.$$

For example, $s_4(2,2) = d_4c_3a_2 + c_4b_3c_2$ case is $k = 1$, since

$$Q_4Q_3P_2P_1, \qquad Q_4P_3Q_2P_1.$$

Then the corresponding $p_n(l,m)$ or $s_n(l,m)$ are given by

$$\cdots a_{k+1}a_ka_{k-1}\cdots a_2, \qquad \cdots c_{k+1}a_ka_{k-1}\cdots a_2.$$

Therefore we have

$$\begin{aligned} &E\left[\overline{(\cdots a_{k+1}a_ka_{k-1}\cdots a_2)}(\cdots c_{k+1}a_ka_{k-1}\cdots a_2)\right] \\ &= E(\cdots)\, E(\overline{a_{k+1}}c_{k+1})\, E(|a_k|^2)\, E(|a_{k-1}|^2)\cdots E(|a_2|^2) = 0, \end{aligned}$$

since $E(\overline{a_1}c_1) = 0$. When there are more than two terms in $q_n(l,m)$ or $r_n(l,m)$, we have to consider two cases: there is a k such that

$$\cdots Q_{k+1}Q_kQ_{k-1}\cdots Q_1, \qquad \cdots P_{k+1}Q_kQ_{k-1}\cdots Q_1.$$

Therefore, a similar argument holds. So the proof is complete.

The above theorem implies that the expectation of the probability distribution for the disordered quantum walk is nothing but the probability distribution of a classical symmetric random walk.

2.4 Examples

The first example was introduced and studied by Ribeiro, Milman, and Mosseri (2004). This corresponds to Case I:

$$U_n = \begin{bmatrix} \cos(\theta_n) & \sin(\theta_n) \\ \sin(\theta_n) & -\cos(\theta_n) \end{bmatrix},$$

where $\{\theta_n : n = 1, 2, \ldots\}$ are i.i.d. on $[0, 2\pi)$ with

$$E(\cos^2(\theta_1)) = E(\sin^2(\theta_1)) = 1/2, \quad E(\cos(\theta_1)\sin(\theta_1)) = 0.$$

Here we give two concrete cases:
 (i) θ_1 is the uniform distribution on $[0, 2\pi)$,
 (ii) $P(\theta_1 = \xi) = P(\theta_1 = \pi/2 + \xi) = 1/2$ for some $\xi \in [0, \pi)$.
For an initial qubit state, we choose a non-random $\varphi = {}^T[\alpha, \beta] \in \Psi$ with $|\alpha| = |\beta| = 1/\sqrt{2}$, and $\alpha\overline{\beta} + \overline{\alpha}\beta = 0$.

The second example was given by Mackay et al. (2002). This corresponds to Case II:

$$U_n = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & e^{i\theta_n} \\ e^{-i\theta_n} & -1 \end{bmatrix},$$

where $\{\theta_n : n = 1, 2, \ldots\}$ are i.i.d. on $[0, 2\pi)$ with

$$E(\cos(\theta_1)) = E(\sin(\theta_1)) = 0.$$

Moreover an initial qubit state is chosen as $\varphi = {}^T[\alpha, \beta] \in \Psi$ with $E(|\alpha|^2) = 1/2$ and $E(\alpha\overline{\beta}) = 0$. For example, both θ_1 and θ_* are uniform distributions on $[0, 2\pi)$, and they are independent of each other. Let $\alpha = \cos(\theta_*)$ and $\beta = \cos(\theta_*)$. So the above conditions hold.

Finally we discuss an example studied by Shapira et al. (2003). Let $W_n = \{X_n, Y_n, Z_n\}$, where $\{W_n : n = 1, 2, \ldots\}$ is i.i.d., and $\{X_n, Y_n, Z_n\}$ is also i.i.d., moreover, X_n is normally distributed with mean zero and variance σ^2, for some $\sigma > 0$. Their case is

$$U_n = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \times V_n,$$

where

$$V_n = \frac{1}{\sqrt{2}} \begin{bmatrix} \cos(R_n) + iZ_n \frac{\sin(R_n)}{R_n} & (Y_n + iX_n)\frac{\sin(R_n)}{R_n} \\ (-Y_n + iX_n)\frac{\sin(R_n)}{R_n} & \cos(R_n) - iZ_n \frac{\sin(R_n)}{R_n} \end{bmatrix},$$

and $R_n = \sqrt{X_n^2 + Y_n^2 + Z_n^2}$. Then a direct computation gives

$$E(|a_1|^2) = E(|b_1|^2) = 1/2,$$
$$E(a_1\overline{c_1}) = \frac{1}{6} + \frac{1}{3}(1-4\sigma^2)e^{-2\sigma^2} \equiv \mu(\sigma). \qquad (2.4.5)$$

We see that (2.4.5) implies $0 < \mu(\sqrt{3}/2) = 0.0179\ldots \leq \mu(\sigma) \leq 1/2(= \lim_{\sigma\downarrow 0}\mu(\sigma))$ for any $\sigma > 0$. Note that the limit $\sigma \downarrow 0$ corresponds to the Hadamard walk case. So their example does not satisfy our condition (2.1.3).

3 Reversible Cellular Automata

3.1 Introduction

In this chapter we consider some properties of a one-dimensional reversible cellular automaton (RCA) derived from a quantum walk on a line. Results in this chapter are based on Konno, Mitsuda, Soshi, and Yoo (2004). We present necessary and sufficient conditions on the initial state for the existence of some conserved quantities of the RCA. One is the expectation of the distribution (the 1st moment), and the other is the squared norm of the distribution (the 0th moment). The former corresponds to the symmetry of the distribution, one of the results below (see Theorem 3.2) implies that the distribution is symmetric for any time step if and only if its expectation is zero for any time step. We should note that our RCA is different from the quantum cellular automaton studied by Grössing and Zeilinger (1988a, 1988b). In Grössing and Zeilinger (1988b), they found a conservation law which connects the strength of the mixing of locally interacting states and the periodicity of the global structures. Their conservation law also differs from ours. For a recent review on quantum cellular automata, see Aoun and Tarifi (2004), and Schumacher and Wernerfor (2004), for examples. It is well known that cellular automata are models based on simple rules which upon deterministic time evolution exhibit various complex behavior (Wolfram (2002)). Our investigation of the RCA might shed some additional light on the analysis of this complex behavior. Moreover, by applying our results to the quantum walk case, we may obtain more detailed information on quantum walks. The purpose of this chapter is to investigate some correspondence relation between quantum walks and RCAs. Then, we analyze some properties and conserved quantities of a quantum walk by examining a RCA. Thus, properties that are hidden or less obvious in a quantum walk may be more obvious when studying the RCA. This method then provides a useful tool for studying quantum walks.

In this chapter, we consider an extension of the Hadamard walk as follows:

$$H(\theta) = \begin{bmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{bmatrix},$$

where $\theta \in [0, 2\pi)$. Here we study mainly the case of $\theta \in [0, \pi/2)$ for the sake of simplicity. Remark that when $\theta = \pi/4$ it becomes the Hadamard walk, that is, $H(\pi/4) = H$.

The definition of the quantum walk gives

$$\Psi_{n+1}^{L}(x) = a\Psi_n^L(x+1) + b\Psi_n^R(x+1),$$
$$\Psi_{n+1}^{R}(x) = c\Psi_n^L(x-1) + d\Psi_n^R(x-1),$$

for

$$U = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \in \mathrm{U}(2).$$

Furthermore, we can rewrite the above equations to uncouple both chirality components:

$$\Psi_{n+2}^{L}(x) = a\Psi_{n+1}^L(x+1) + d\Psi_{n+1}^L(x-1) - (ad-bc)\Psi_n^L(x),$$
$$\Psi_{n+2}^{R}(x) = a\Psi_{n+1}^R(x+1) + d\Psi_{n+1}^R(x-1) - (ad-bc)\Psi_n^R(x).$$

That is, the left and right chiralities both satisfy the following partial difference equation:

$$\eta_{n+2}(x) = a\eta_{n+1}(x+1) + d\eta_{n+1}(x-1) - (ad-bc)\eta_n(x), \qquad (3.1.1)$$

where $\eta_n(x) \in \mathbb{C}$ stands for the probability amplitudes of left or right chirality at time $n \in \mathbb{Z}_+$ at location $x \in \mathbb{Z}$, where $\mathbb{Z}_+$ is the set of non-negative integers. The above argument appeared in Knight, Roldán, and Sipe (2003a, 2003b) (see also page 279 in Gudder (1988)). In other words, (3.1.1) implies a dynamical independence of the evolution of the two chiralities L and R. Thus there are two essentially independent walks, coupled only by the first two steps. After that the two walks can behave independently of each other. In this chapter, we call (3.1.1) a *reversible cellular automata* (RCA), since (3.1.1) implies that $\eta_n(x)$ can also be determined by $\eta_{n+1}(\cdot)$ and $\eta_{n+2}(\cdot)$.

It should be noted that if we put $(\eta_0(0), \eta_1(-1), \eta_1(1)) = (\Psi_0^L(0), a\Psi_0^L(0) + b\Psi_0^R(0), 0)$ on the initial state of (3.1.1), then $\eta_n(x) = \Psi_n^L(x)$, that is, $\eta_n(x)$ represents the left chirality of the quantum walk. Similarly, an initial qubit state of (3.1.1), that is, $(\eta_0(0), \eta_1(-1), \eta_1(1)) = (\Psi_0^R(0), 0, c\Psi_0^L(0) + d\Psi_0^R(0))$ gives the right chirality of the quantum walk, namely, $\eta_n(x) = \Psi_n^R(x)$.

Here we consider a more general setting concerning initial states. The study on the dependence of some important quantities on the initial state is one of the essential parts, so we define the set of initial states for the RCA as follows:

$$\widetilde{\Phi} = \{\widetilde{\varphi} = (\eta_0(0), \eta_1(-1), \eta_1(1)) \equiv (\alpha, \beta, \gamma) : \alpha, \beta, \gamma \in \mathbb{C}\}.$$

To distinguish our initial state for the RCA considered here from the initial qubit state for quantum walks in our previous chapters, we put "$\sim$" in Φ etc. From now on we consider only RCA's defined by $H(\theta)$:

$$\eta_{n+2}(x) = \cos\theta[\eta_{n+1}(x+1) - \eta_{n+1}(x-1)] + \eta_n(x). \tag{3.1.2}$$

McGuigan (2003) studied some classes of quantum cellular automata. In his setting, (3.1.2) belongs to a class of fermionic quantum cellular automata whose update equation is given by

$$\eta_{n+2}(x) = f(\eta_{n+1}(x+1), \eta_n(x), \eta_{n+1}(x-1)) + \eta_n(x). \tag{3.1.3}$$

Our case is $f(x,y,z) = (x-z)\cos\theta$. By using (3.1.2), Romanelli et al. (2004) analyzed in detail discrete-time one-dimensional quantum walks by separating the quantum evolution into Markovian and interference terms.

Now we define a distribution (in general, non-probability distribution) of RCA η_n at time $n \in \mathbb{Z}_+$ by

$$\{|\eta_n(x)|^2 : x \in \mathbb{Z}\}.$$

In this chapter, we call $\{|\eta_n(x)|^2 : x \in \mathbb{Z}\}$ the distribution of η_n.

One of the main results of this chapter is to give the following necessary and sufficient conditions of the symmetry of distribution of η_n for any time step n.

3.2 Symmetry of Distribution

First we present the following useful lemma to prove Theorem 3.2.

Lemma 3.1. (i) *We suppose that the initial state is*

$$\widetilde{\varphi} = (\eta_0(0), \eta_1(-1), \eta_1(1)) \equiv (\alpha, \beta, -\beta),$$

where $\alpha, \beta \in \mathbb{C}$. Then we have

$$\eta_n(x) = (-1)^n \eta_n(-x), \tag{3.2.4}$$

for any $x \in \mathbb{Z}$ and $n \in \mathbb{Z}_+$.
(ii) *We suppose that the initial state is*

$$\widetilde{\varphi} = (\eta_0(0), \eta_1(-1), \eta_1(1)) \equiv (0, \beta, e^{i\xi}\beta),$$

where $\beta \in \mathbb{R}$, $\xi \in \mathbb{R}$. Then we have

$$\eta_n(x) = (-1)^{n+1} e^{i\xi} \overline{\eta_n(-x)}, \tag{3.2.5}$$

for any $x \in \mathbb{Z}_+$ and $n \in \mathbb{Z}_+$.

Proof. We prove the Lemma by induction on the time step n. The proof of part (ii) is essentially the same as that of part (i), so we omit it.

First we consider $n = 0$, 1 case. We can easily check that (3.2.4) holds for $n = 0$, 1. Next we assume that (3.2.4) holds for time $n = m$ and $m + 1$ $(m \geq 0)$. Then we have

$$\begin{aligned}
\eta_{m+2}(x) &= \cos\theta[\eta_{m+1}(x+1) - \eta_{m+1}(x-1)] + \eta_m(x) \\
&= \cos\theta[(-1)^{m+1}\eta_{m+1}(-x-1) - (-1)^{m+1}\eta_{m+1}(-x+1)] \\
&\qquad\qquad\qquad\qquad\qquad\qquad + (-1)^m\eta_m(-x) \\
&= (-1)^{m+1}\cos\theta[\eta_{m+1}(-x-1) - \eta_{m+1}(-x+1)] + (-1)^m\eta_m(-x) \\
&= (-1)^{m+2}\{\cos\theta[\eta_{m+1}(-x+1) - \eta_{m+1}(-x-1)] + \eta_m(-x)\} \\
&= (-1)^{m+2}\eta_{m+2}(-x).
\end{aligned}$$

Remark that the first and last equalities come from (3.1.2). The second equality uses the induction hypothesis. So we have shown that (3.2.4) is also correct for time $n = m + 2$. The proof is complete.

We introduce the following three classes:

$$\begin{aligned}
\widetilde{\Phi}_\perp = \{\widetilde{\varphi} \in \widetilde{\Phi} : \beta + \gamma = 0 & \quad (3.2.6) \\
\text{or } |\beta| = |\gamma|(>0), \text{ and } \alpha = 0 & \quad (3.2.7) \\
\text{or } |\beta| = |\gamma|(>0), \alpha \neq 0, \text{ and } \theta_\beta + \theta_\gamma - 2\theta_\alpha = \pi \pmod{2\pi}\}, & \quad (3.2.8)
\end{aligned}$$

$$\widetilde{\Phi}_s = \{\widetilde{\varphi} \in \widetilde{\Phi} : |\eta_n(x)| = |\eta_n(-x)| \text{ for any } n \in \mathbb{Z}_+ \text{ and } x \in \mathbb{Z}\},$$

$$\widetilde{\Phi}_0 = \left\{\widetilde{\varphi} \in \widetilde{\Phi} : \sum_{x=-\infty}^{\infty} x|\eta_n(x)|^2 = 0 \text{ for any } n \in \mathbb{Z}_+\right\}.$$

Here θ_z is the argument of $z \in \mathbb{C}$ with $z \neq 0$. It is noted that if $\widetilde{\varphi} \in \widetilde{\Phi}_s$, then the distribution (in general, non-probability distribution) of η_n becomes symmetric for any time $n \in \mathbb{Z}_+$.

Theorem 3.2. *For the RCA defined by (3.1.2), we have*

$$\widetilde{\Phi}_\perp = \widetilde{\Phi}_s = \widetilde{\Phi}_0.$$

Proof. First we see that the definitions of $\widetilde{\Phi}_s$ and $\widetilde{\Phi}_0$ give immediately

$$\widetilde{\Phi}_s \subset \widetilde{\Phi}_0. \tag{3.2.9}$$

Next, we prove $\widetilde{\Phi}_\perp \subset \widetilde{\Phi}_s$. The proof is divided into the following three cases.

Case 1. If the initial states are satisfying (3.2.6), then we can obtain the following relation from Lemma 3.1 (i):

$$|\eta_n(x)| = |\eta_n(-x)|. \tag{3.2.10}$$

Case 2. We assume that the initial states satisfy (3.2.7). By using Lemma 3.1 (ii), we can obtain (3.2.10).
Case 3. We assume that the initial states satisfy (3.2.8). Let

$$\widetilde{\varphi}_1 = (|\alpha|e^{i\theta_\alpha}, |\beta|e^{i\theta_\beta}, |\beta|e^{i(\pi-\theta_\beta+2\theta_\alpha)}).$$

Then

$$\widetilde{\varphi}_2 = e^{-i\theta_\alpha}\widetilde{\varphi}_1 = (|\alpha|, |\beta|e^{i(\theta_\beta-\theta_\alpha)}, |\beta|e^{i(\pi-\theta_\beta+\theta_\alpha)}).$$

We put $\theta = \theta_\alpha - \theta_\beta$, then $\widetilde{\varphi}_2 = (|\alpha|, |\beta|e^{i\theta}, |\beta|e^{i(\pi-\theta)})$. Therefore, real and imaginary parts of $\widetilde{\varphi}_2$ become

$$\begin{aligned}\Re(\widetilde{\varphi}_2) &= (|\alpha|, |\beta|\cos\theta, -|\beta|\cos\theta),\\ \Im(\widetilde{\varphi}_2) &= (0, |\beta|\sin\theta, |\beta|\sin\theta),\end{aligned}$$

respectively. Here if we take $\Re(\widetilde{\varphi}_2)$ as an initial state of the RCA, then we can see that the distribution of η_n is symmetric by using Lemma 3.1 (i). Similarly, using Lemma 3.1 (ii), the initial state $\Im(\widetilde{\varphi}_2)$ also gives a symmetric distribution. From $\widetilde{\varphi}_2 = \Re(\widetilde{\varphi}_2) + \Im(\widetilde{\varphi}_2) \in \widetilde{\Phi}_s$, we can get $\widetilde{\varphi}_1 \in \widetilde{\Phi}_s$. Therefore for any $\widetilde{\varphi} \in \widetilde{\Phi}_\perp$, we have $|\eta_n(x)| = |\eta_n(-x)|$ for any $x \in \mathbb{Z}$ and $n \in \mathbb{Z}_+$. Then we conclude

$$\widetilde{\Phi}_\perp \subset \widetilde{\Phi}_s. \tag{3.2.11}$$

Finally, a direct computation gives

$$\begin{aligned}m(1) &= |\gamma|^2 - |\beta|^2,\\ m(2) &= 2\cos^2\theta(|\gamma|^2 - |\beta|^2),\\ m(3) &= \frac{1}{2}(3\cos^2 2\theta + 2\cos 2\theta + 1)(|\gamma|^2 - |\beta|^2)\\ &\qquad -\frac{1}{2}\sin\theta\,\sin 2\theta\,\{\alpha(\overline{\beta}+\overline{\gamma}) + \overline{\alpha}(\beta+\gamma)\},\end{aligned}$$

where $m(n) \equiv \sum_{x=-\infty}^{\infty} x|\eta_n(x)|^2$. The above equations imply that if $\widetilde{\varphi} \in \widetilde{\Phi}_0$ then $\widetilde{\varphi} \in \widetilde{\Phi}_\perp$. So we have

$$\widetilde{\Phi}_0 \subset \widetilde{\Phi}_\perp. \tag{3.2.12}$$

Combining (3.2.10) - (3.2.12) gives

$$\widetilde{\Phi}_\perp \subset \widetilde{\Phi}_s \subset \widetilde{\Phi}_0 \subset \widetilde{\Phi}_\perp,$$

so the proof is complete.

3.3 Conserved Quantity for RCA

From now on we assume that $0 < \theta < \pi/2$ for simplicity. First we let

$$||\eta_n||^2 = \sum_{x=-\infty}^{\infty} |\eta_n(x)|^2.$$

Here we consider the necessary and sufficient conditions on initial states for a conserved quantity. That is, there exists $c \geq 0$ such that $||\eta_n||^2 = c$ for any $n \in \mathbb{Z}_+$. To do so, we introduce the following two subsets of $\widetilde{\Phi}$:

$$\widetilde{\Phi}_*(c) = \{\widetilde{\varphi} \in \widetilde{\Phi} : \ |\alpha|^2 = c, \tag{3.3.13}$$
$$|\beta|^2 + |\gamma|^2 = c, \tag{3.3.14}$$
$$\beta\overline{\gamma} + \overline{\beta}\gamma = 0, \tag{3.3.15}$$
$$\alpha(\overline{\beta} - \overline{\gamma}) + \overline{\alpha}(\beta - \gamma) = 2c\,\cos\theta\,\}, \tag{3.3.16}$$

and

$$\widetilde{\Phi}(c) = \left\{\widetilde{\varphi} \in \widetilde{\Phi} : ||\eta_n||^2 = c \text{ for any } n \in \mathbb{Z}_+\right\},$$

where $\widetilde{\Phi}(c)$ stands for the set of initial states satisfying that $||\eta_n||$ becomes a conserved quantity. When $c = 0$, it is easily shown that

$$\widetilde{\Phi}_*(0) = \widetilde{\Phi}(0) = \left\{\widetilde{\varphi} \in \widetilde{\Phi} : \alpha = \beta = \gamma = 0\right\}.$$

So we assume that $c > 0$. Then we have

Theorem 3.3. *For any $c > 0$,*

$$\widetilde{\Phi}_*(c) = \widetilde{\Phi}(c).$$

The above theorem implies that $\widetilde{\Phi}_*(c)$ gives the necessary and sufficient conditions we want to know.

Proof. Case 1: $\widetilde{\Phi}(c) \subset \widetilde{\Phi}_*(c)$. A little algebra reveals

$$||\eta_0||^2 = |\alpha|^2, \tag{3.3.17}$$
$$||\eta_1||^2 = |\beta|^2 + |\gamma|^2, \tag{3.3.18}$$
$$||\eta_2||^2 = |\alpha|^2 + 2\cos^2\theta(|\beta|^2 + |\gamma|^2) - \cos^2\theta(\beta\overline{\gamma} + \overline{\beta}\gamma) - \cos\theta(\alpha(\overline{\beta} - \overline{\gamma}) + \overline{\alpha}(\beta - \gamma)), \tag{3.3.19}$$
$$||\eta_3||^2 = 2\cos^2\theta|\alpha|^2 + \left\{2\cos^4\theta + (1 - 2\cos^2\theta)^2\right\}(|\beta|^2 + |\gamma|^2) + 2\cos^2\theta(1 - 2\cos^2\theta)(\beta\overline{\gamma} + \overline{\beta}\gamma) + \cos\theta(1 - 3\cos^2\theta)\{\alpha(\overline{\beta} - \overline{\gamma}) + \overline{\alpha}(\beta - \gamma)\}. \tag{3.3.20}$$

From (3.3.17) - (3.3.19), we have

$$\alpha(\overline{\beta}-\overline{\gamma})+\overline{\alpha}(\beta-\gamma)=\cos\theta\{2c-(\beta\overline{\gamma}+\overline{\beta}\gamma)\}. \tag{3.3.21}$$

Combining (3.3.21) with (3.3.17), (3.3.18), (3.3.20) implies

$$\sin\theta\cos\theta(\beta\overline{\gamma}+\overline{\beta}\gamma)=0,$$

so we have $\beta\overline{\gamma}+\overline{\beta}\gamma=0$, since $0<\theta<\pi/2$. Then (3.3.21) becomes $\alpha(\overline{\beta}-\overline{\gamma})+\overline{\alpha}(\beta-\gamma)=2c\,\cos\theta$. So we have the desired result.
Case 2: $\widetilde{\Phi}_*(c)\subset\widetilde{\Phi}(c)$. Let

$$\widetilde{\eta}_n(\xi)=\sum_{x=-\infty}^{\infty}e^{i\xi x}\eta_n(x),$$

where $\xi\in\mathbb{R}$. By using (3.1.2), we have

$$\widetilde{\eta}_{n+2}(\xi)=\cos\theta(e^{-i\xi}-e^{i\xi})\widetilde{\eta}_{n+1}(\xi)+\widetilde{\eta}_n(\xi),$$

where

$$\widetilde{\eta}_0(\xi)=\alpha,\qquad \widetilde{\eta}_1(\xi)=e^{-i\xi}\beta+e^{i\xi}\gamma.$$

So we obtain

$$\widetilde{\eta}_n(\xi)=A(\xi)\lambda_+^n(\xi)+B(\xi)\lambda_-^n(\xi),$$

where

$$A(\xi)=\frac{\alpha e^{-i\varphi}+C(\xi)}{e^{i\varphi}+e^{-i\varphi}},\quad B(\xi)=\frac{\alpha e^{i\varphi}-C(\xi)}{e^{i\varphi}+e^{-i\varphi}},\quad C(\xi)=\beta e^{-i\xi}+\gamma e^{i\xi},$$

and

$$\lambda_\pm(\xi)=-i\cos\theta\sin\xi\pm\sqrt{1-\cos^2\theta\sin^2\xi}.$$

Define

$$\langle f|g\rangle=\frac{1}{2\pi}\int_0^{2\pi}\overline{f(\xi)}g(\xi)d\xi.$$

In particular, $||f||_*^2=\langle f|f\rangle$. Then

$$\sum_{x=-\infty}^{\infty}|\eta_n(x)|^2=\frac{1}{2\pi}\int_0^{2\pi}|\widetilde{\eta}_n(\xi)|^2d\xi$$

implies

$$||\eta_n||=||\widetilde{\eta}_n||_*.$$

We define $\varphi = \varphi(\xi) \in \mathbb{R}$ by $\lambda_+(\xi) = e^{i\xi\varphi}$, that is,

$$\cos\varphi = \sqrt{1 - \cos^2\theta \sin^2\xi}, \qquad \sin\varphi = -\cos\theta \sin\xi.$$

So $\lambda_-(\xi) = -e^{-i\xi\varphi}$. In this setting, we have the following result: for any $n \in \mathbb{Z}_+$,

$$||\eta_n||^2 = ||A||_*^2 + ||B||_*^2 + (-1)^n \{\langle e^{in\varphi} A | e^{-in\varphi} B\rangle + \langle e^{-in\varphi} B | e^{in\varphi} A\rangle\}.$$

A direct computation gives

$$\begin{aligned} &||A||_*^2 = ||B||_*^2 \\ &= \frac{1}{4\sin\theta}\Bigg[(|\alpha|^2 + |\beta|^2 + |\gamma|^2) - \{\alpha(\overline{\beta} - \overline{\gamma}) + \overline{\alpha}(\beta - \gamma)\}\left(\frac{1-\sin\theta}{\cos\theta}\right) \\ &\qquad\qquad - (\beta\overline{\gamma} + \overline{\beta}\gamma)\left(\frac{1-\sin\theta}{\cos\theta}\right)^2\Bigg]. \end{aligned}$$

Moreover we have

$$\begin{aligned} &4\pi\{\langle e^{in\varphi} A | e^{-in\varphi} B\rangle + \langle e^{-in\varphi} B | e^{in\varphi} A\rangle\} \\ &= |\alpha|^2 \int_0^{2\pi} \frac{\cos(2(n-1)\varphi)}{\cos^2\varphi}\, d\xi \\ &+ (\overline{\alpha}\gamma - \alpha\overline{\beta}) i \left\{\int_0^{2\pi} \frac{\cos\xi \sin((2n-1)\varphi)}{\cos^2\varphi}\, d\xi + i \int_0^{2\pi} \frac{\sin\xi \sin((2n-1)\varphi)}{\cos^2\varphi}\, d\xi\right\} \\ &+ (\overline{\alpha}\beta - \alpha\overline{\gamma}) i \left\{\int_0^{2\pi} \frac{\cos\xi \sin((2n-1)\varphi)}{\cos^2\varphi}\, d\xi - i \int_0^{2\pi} \frac{\sin\xi \sin((2n-1)\varphi)}{\cos^2\varphi}\, d\xi\right\} \\ &- (|\beta|^2 + |\gamma|^2) \int_0^{2\pi} \frac{\cos(2n\varphi)}{\cos^2\varphi}\, d\xi \\ &- \beta\overline{\gamma}\left\{\int_0^{2\pi} \frac{\cos(2\xi)\cos(2n\varphi)}{\cos^2\varphi}\, d\xi - i \int_0^{2\pi} \frac{\sin(2\xi)\cos(2n\varphi)}{\cos^2\varphi}\, d\xi\right\} \\ &- \overline{\beta}\gamma\left\{\int_0^{2\pi} \frac{\cos(2\xi)\cos(2n\varphi)}{\cos^2\varphi}\, d\xi + i \int_0^{2\pi} \frac{\sin(2\xi)\cos(2n\varphi)}{\cos^2\varphi}\, d\xi\right\}, \end{aligned}$$

for any $n \in \mathbb{Z}_+$. Furthermore we have the following equation:

$$\begin{aligned} ||\eta_n||^2 = &\frac{1}{2\sin\theta}\Bigg[(|\alpha|^2 + |\beta|^2 + |\gamma|^2) - \{\alpha(\overline{\beta} - \overline{\gamma}) + \overline{\alpha}(\beta - \gamma)\}\left(\frac{1-\sin\theta}{\cos\theta}\right) \\ &\qquad - (\beta\overline{\gamma} + \overline{\beta}\gamma)\left(\frac{1-\sin\theta}{\cos\theta}\right)^2\Bigg] \\ &+ \frac{(-1)^n}{\pi}\Bigg[|\alpha|^2 \int_{\theta-\pi/2}^0 \frac{\cos(2(n-1)x)}{\cos x\sqrt{\cos^2 x - \sin^2\theta}}\, dx \end{aligned}$$

$$-\{\alpha(\overline{\beta}-\overline{\gamma})+\overline{\alpha}(\beta-\gamma)\}\frac{1}{\cos\theta}\int_{\theta-\pi/2}^{0}\frac{\sin x\sin((2n-1)x)}{\cos x\sqrt{\cos^2 x-\sin^2\theta}}\,dx$$
$$-(|\beta|^2+|\gamma|^2)\int_{\theta-\pi/2}^{0}\frac{\cos(2nx)}{\cos x\sqrt{\cos^2 x-\sin^2\theta}}\,dx$$
$$-(\beta\overline{\gamma}+\overline{\beta}\gamma)\left\{\frac{2}{\cos\theta}\int_{\theta-\pi/2}^{0}\frac{\cos(2nx)\sqrt{\cos^2 x-\sin^2\theta}}{\cos x}\,dx\right.$$
$$\left.\left.-\int_{\theta-\pi/2}^{0}\frac{\cos(2nx)}{\cos x\sqrt{\cos^2 x-\sin^2\theta}}\,dx\right\}\right], \qquad (3.3.22)$$

for any $n\in\mathbb{Z}_+$. The condition "$|\alpha|^2=|\beta|^2+|\gamma|^2=c$, $\alpha(\overline{\beta}-\overline{\gamma})+\overline{\alpha}(\beta-\gamma)=2c\cos\theta$, $\beta\overline{\gamma}+\overline{\beta}\gamma=0$" gives

$$||\eta_n||^2=c+\frac{(-1)^n c}{\pi}$$
$$\times\int_{\theta-\pi/2}^{0}\frac{\cos(2(n-1)x)-2\sin x\sin((2n-1)x)-\cos(2nx)}{\cos x\sqrt{\cos^2 x-\sin^2\theta}}\,dx,$$

for any $n\in\mathbb{Z}_+$. On the other hand, a little algebra reveals that

$$\cos(2(n-1)x)-2\sin x\sin((2n-1)x)-\cos(2nx)=0,$$

for any $n\in\mathbb{Z}_+$. Therefore we conclude that

$$||\eta_n||^2=c \qquad (n\in\mathbb{Z}_+),$$

that is, $\widetilde{\Phi}_*(c)\subset\widetilde{\Phi}(c)$. The proof of Theorem 3.3 is complete.

By (3.3.22) and the Riemann-Lebesgue lemma, we have

$$\lim_{n\to\infty}||\eta_n||^2=\frac{1}{2\sin\theta}\left[(|\alpha|^2+|\beta|^2+|\gamma|^2)-\{\alpha(\overline{\beta}-\overline{\gamma})+\overline{\alpha}(\beta-\gamma)\}\right.$$
$$\left.\times\left(\frac{1-\sin\theta}{\cos\theta}\right)-(\beta\overline{\gamma}+\overline{\beta}\gamma)\left(\frac{1-\sin\theta}{\cos\theta}\right)^2\right]. \quad (3.3.23)$$

The above equation will be used in the next section. As a corollary to Theorem 3.3, we can show that the quantity is not conserved in any RCA with a symmetric distribution.

Corollary 3.4. *For any* $c>0$,

$$\widetilde{\Phi}_s\cap\widetilde{\Phi}(c)=\phi.$$

Proof. We consider the following three cases.
Case 1. When $\beta+\gamma=0$, from $|\beta|^2+|\gamma|^2=c$, we have

$$\beta=\sqrt{\frac{c}{2}}\,e^{i\theta_\beta}, \qquad \gamma=-\sqrt{\frac{c}{2}}\,e^{i\theta_\beta}. \tag{3.3.24}$$

However (3.3.24) and $\beta\overline{\gamma}+\overline{\beta}\gamma=0$ contradict each other, since $\beta\overline{\gamma}+\overline{\beta}\gamma=-c\,(<0)$.
Case 2. "$|\beta|=|\gamma|(>0)$, and $\alpha=0$" and "$|\alpha|^2=c\,(>0)$" contradict each other.
Case 3. We assume that "$|\beta|=|\gamma|(>0), \alpha\neq 0$, and $\theta_\beta+\theta_\gamma-2\theta_\alpha=\pi \pmod{2\pi}$". From now on we omit "mod 2π". Then

$$\alpha(\overline{\beta}-\overline{\gamma})+\overline{\alpha}(\beta-\gamma)=2c\,\cos\theta$$

can be rewritten as

$$|\alpha|\{|\beta|\cos(\theta_\alpha-\theta_\beta)-|\gamma|\cos(\theta_\alpha-\theta_\gamma)\}=c\,\cos\theta. \tag{3.3.25}$$

On the other hand, $|\alpha|=\sqrt{c}$, $|\beta|=|\gamma|=\sqrt{c/2}$. So (3.3.25) becomes

$$\cos(\theta_\alpha-\theta_\beta)-\cos(\theta_\alpha-\theta_\gamma)=\sqrt{2}\,\cos\theta. \tag{3.3.26}$$

Combining (3.3.26) with $\theta_\beta+\theta_\gamma-2\theta_\alpha=\pi$ implies

$$\sin\left(\frac{\theta_\beta-\theta_\gamma}{2}\right)=-\frac{\cos\theta}{\sqrt{2}}. \tag{3.3.27}$$

We see that $\beta\overline{\gamma}+\overline{\beta}\gamma=0$ gives $\theta_\beta-\theta_\gamma=\pm\pi/2$, so (3.3.27) becomes $\cos\theta=\pm 1$. Then we have a contradiction, since we assumed that $0<\theta<\pi/2$. So the proof is complete.

3.4 Quantum Walk Case

In this section we return to the quantum walk given by $H(\theta)$. By using the correspondence between quantum walks and RCAs, non-trivial properties of the quantum walk can be derived. Let $\varphi={}^T[\alpha_l,\alpha_r]$ with $|\alpha_l|^2+|\alpha_r|^2=1$ be the initial qubit state at the origin for the quantum walk. Here we apply our result (Theorem 3.3) for the conserved quantity of the RCA to the quantum walk. First we consider the left chirality case; that is, $\alpha=\alpha_l$, $\beta=\cos\theta\,\alpha_l+\sin\theta\,\alpha_r$, and $\gamma=0$. Then (3.3.15) holds, since $\gamma=0$. (3.3.14) and (3.3.16) can be rewritten as

$$\cos^2\theta|\alpha_l|^2+\sin^2\theta|\alpha_r|^2+\cos\theta\sin\theta(\alpha_l\overline{\alpha_r}+\overline{\alpha_l}\alpha_r)=c, \tag{3.4.28}$$
$$2\cos\theta|\alpha_l|^2+\sin\theta(\alpha_l\overline{\alpha_r}+\overline{\alpha_l}\alpha_r)=2c\cos\theta, \tag{3.4.29}$$

respectively. By using $\sin\theta \neq 0$ (since $0 < \theta < \pi/2$) and (3.3.13) and (3.4.29), we have

$$\alpha_l \overline{\alpha_r} + \overline{\alpha_l}\alpha_r = 0. \tag{3.4.30}$$

Combining (3.4.28) with (3.4.30) gives

$$\cos^2\theta|\alpha_l|^2 + \sin^2\theta|\alpha_r|^2 = c. \tag{3.4.31}$$

On the other hand, it follows from $|\alpha_l|^2 + |\alpha_r|^2 = 1$ and (3.3.13) that $|\alpha_r|^2 = 1 - c$. By (3.4.31) and the last equation, we get

$$c = 1/2. \tag{3.4.32}$$

Moreover $|\alpha_l| = |\alpha_r| = 1/\sqrt{2}$ can be derived from (3.4.32). So combining this result and (3.4.30), we conclude that the initial state of the quantum walk with the corresponding RCA having the conserved quantity $c = 1/2$ is determined by

$$\varphi = \begin{bmatrix} \alpha_l \\ \alpha_r \end{bmatrix} = \pm\frac{e^{i\xi}}{\sqrt{2}}\begin{bmatrix} 1 \\ i \end{bmatrix}, \tag{3.4.33}$$

where $\xi \in \mathbb{R}$. Similarly, we consider the right chirality case, that is, $\alpha = \alpha_r$, $\beta = 0$, and $\gamma = \sin\theta\,\alpha_l - \cos\theta\,\alpha_r$. In this case also, a similar computation gives the same conclusions, i.e., (3.4.32) and (3.4.33).

On the other hand if we choose (3.4.33) as an initial qubit state for the quantum walk defined by $H(\theta)$, then the probability distribution becomes symmetric (see Theorem 1.5). Furthermore our result gives additional information on the conserved quantity:

$$||\Psi_n^L||^2 = ||\Psi_n^R||^2 = \frac{1}{2},$$

for any $n \in \mathbb{Z}_+$. In particular, when $\theta = \pi/4$ (the Hadamard walk), if $\varphi = {}^T[1/\sqrt{2}, i/\sqrt{2}]$, then $||\Psi_n^L||^2 = ||\Psi_n^R||^2 = 1/2$ for any $n \in \mathbb{Z}_+$. However Corollary 3.4 implies that the conserved quantity (in our case $c = 1/2$) is not compatible with the symmetry of the distribution. This gives an interesting result on the quantum walk: a symmetric probability distribution of the quantum walk can not be written as the sum of the symmetric distribution for each chirality of the quantum walk.

Finally we consider the general case. The unitary evolution of the quantum walk implies $||\Psi_n^L||^2 + ||\Psi_n^R||^2 = 1$ for any time step $n \in \mathbb{Z}_+$. Furthermore (3.3.23) gives

$$\lim_{n\to\infty} ||\Psi_n^L||^2 = \frac{1}{2\sin\theta}\Bigg[(1+\cos^2\theta)|\alpha_l|^2 + \sin^2\theta|\alpha_r|^2 + \sin\theta\cos\theta(\alpha_l\overline{\alpha_r} + \overline{\alpha_l}\alpha_r) \\ -\{2\cos\theta|\alpha_l|^2 + \sin\theta(\alpha_l\overline{\alpha_r} + \overline{\alpha_l}\alpha_r)\}\left(\frac{1-\sin\theta}{\cos\theta}\right)\Bigg],$$

$$\lim_{n\to\infty} ||\Psi_n^R||^2 = \frac{1}{2\sin\theta}\Bigg[(1+\cos^2\theta)|\alpha_r|^2 + \sin^2\theta|\alpha_l|^2 - \sin\theta\cos\theta(\alpha_l\overline{\alpha_r} + \overline{\alpha_l}\alpha_r)$$
$$-\{2\cos\theta|\alpha_r|^2 - \sin\theta(\alpha_l\overline{\alpha_r} + \overline{\alpha_l}\alpha_r)\}\left(\frac{1-\sin\theta}{\cos\theta}\right)\Bigg].$$

For example, if we choose $\theta \in (0, \pi/2)$ and $\varphi = {}^T[1, 0]$ (asymmetric case), then

$$\lim_{n\to\infty} ||\Psi_n^L||^2 = 1 - \frac{\sin\theta}{2} \in \left(\frac{1}{2}, 1\right), \quad \lim_{n\to\infty} ||\Psi_n^R||^2 = \frac{\sin\theta}{2} \in \left(0, \frac{1}{2}\right).$$

4 Quantum Cellular Automata

4.1 Introduction

Patel, Raghunathan, and Rungta (2005a) constructed a quantum walk on a line without using a coin toss instruction, and analyzed the asymptotic behavior of the walk on the line and its escape probability with an absorbing wall. In fact the quantum walk investigated by them can be considered as a class of quantum cellular automata on the line (see Meyer (1996, 1997, 1998), for examples), so we call their quantum walk a *quantum cellular automaton* (QCA) in this chapter. Results here are based on Hamada, Konno, and Segawa (2005).

At a first glance, the QCA looks different from the quantum walk. However, we show that there exists a one-to-one correspondence between them in a more general setting. The purpose of this chapter is to clarify this connection. Once the connection is well understood, the result by Patel, Raghunathan, and Rungta (2005a) is straightforwardly obtained.

4.2 Definition of QCA

We define the dynamics of a one-dimensional QCA including the model investigated by Patel, Raghunathan, and Rungta (2005a). Let $\eta_n^{(m)}(x)(\in \mathbb{C})$ be the amplitude of the QCA at time $n \in \mathbb{Z}_+$ and at location $x \in \mathbb{Z}$ starting from $m \in \mathbb{Z}$, that is, $\eta_0^{(m)}(m) = 1$ and $\eta_0^{(m)}(x) = 0$ if $x \neq m$. Moreover, let

$$\zeta_n^{(m:\pm)}(x) = |\alpha\eta_n^{(m)}(x) + \beta\eta_n^{(m\pm1)}(x)|^2,$$

and

$$\zeta_n^{(m:\pm)} = (\zeta_n^{(m:\pm)}(x) : x \in \mathbb{Z}),$$

where $\alpha, \beta \in \mathbb{C}$ with $|\alpha|^2 + |\beta|^2 = 1$. As we will show later, the $\zeta_n^{(m:\pm)}(x)$ is equivalent to a probability distribution of a quantum walk at time n, where the pair (α, β) corresponds to the initial qubit state of the quantum walk. The evolution of the QCA on the line is given by

$$\eta_{n+1}^{(m)} = \overline{U}\eta_n^{(m)},$$

where $\overline{U}$ is the unitary matrix

$$\overline{U} = \begin{array}{c} \\ \vdots \\ -3 \\ -2 \\ -1 \\ 0 \\ +1 \\ +2 \\ +3 \\ +4 \\ \vdots \end{array} \begin{array}{c} \begin{array}{cccccccccc} \ldots & -3 & -2 & -1 & 0 & +1 & +2 & +3 & +4 & \ldots \end{array} \\ \begin{pmatrix} \ddots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \ldots \\ \ldots & b & a & 0 & 0 & 0 & 0 & 0 & 0 & \ldots \\ \ldots & a & b & c & d & 0 & 0 & 0 & 0 & \ldots \\ \ldots & d & c & b & a & 0 & 0 & 0 & 0 & \ldots \\ \ldots & 0 & 0 & a & b & c & d & 0 & 0 & \ldots \\ \ldots & 0 & 0 & d & c & b & a & 0 & 0 & \ldots \\ \ldots & 0 & 0 & 0 & 0 & a & b & c & d & \ldots \\ \ldots & 0 & 0 & 0 & 0 & d & c & b & a & \ldots \\ \ldots & 0 & 0 & 0 & 0 & 0 & 0 & a & b & \ldots \\ \ldots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \ddots \end{pmatrix} \end{array},$$

with $a, b, c, d \in \mathbb{C}$ and $\eta_n^{(m)}$ is the configuration

$$\eta_n^{(m)} = {}^T[\ldots, \eta_n^{(m)}(-1), \eta_n^{(m)}(0), \eta_n^{(m)}(+1), \ldots],$$

for any $n \in \mathbb{Z}_+$. Let $||u||^2 = \sum_{x=-\infty}^{\infty} |u(x)|^2$. The unitarity of $\overline{U}$ ensures that if $||\eta_0^{(m)}|| = 1$, then $||\eta_n^{(m)}|| = 1$ for any $n \in \mathbb{Z}_+$. Furthermore, if $||\zeta_0^{(m:\pm)}|| = 1$, then $||\zeta_n^{(m:\pm)}|| = 1$ for any $n \in \mathbb{Z}_+$. A little algebra reveals that $\overline{U}$ is unitary if and only if

$$|a|^2 + |b|^2 + |c|^2 + |d|^2 = 1, \tag{4.2.1}$$
$$a\overline{d} + \overline{a}d + b\overline{c} + \overline{b}c = 0, \tag{4.2.2}$$
$$a\overline{c} + b\overline{d} = 0, \tag{4.2.3}$$
$$a\overline{b} + \overline{a}b = 0, \tag{4.2.4}$$
$$c\overline{d} + \overline{c}d = 0, \tag{4.2.5}$$

where $\overline{z}$ is a complex conjugate of $z \in \mathbb{C}$. Here we consider a, b, c, d satisfying (4.2.1) - (4.2.5). Trivial cases are "$|a| = 1, b = c = d = 0$", "$|b| = 1, a = c = d = 0$", "$|c| = 1, a = b = d = 0$", and "$|d| = 1, a = b = c = 0$". For other cases, we have the following five types:
Type I: $|b|^2 + |c|^2 = 1,\ b\overline{c} + \overline{b}c = 0,\ bc \neq 0,\ a = d = 0.$
Type II: $|a|^2 + |b|^2 = 1,\ a\overline{b} + \overline{a}b = 0,\ ab \neq 0,\ c = d = 0.$
Type III: $|c|^2 + |d|^2 = 1,\ c\overline{d} + \overline{c}d = 0,\ cd \neq 0,\ a = b = 0.$

Type IV: $|a|^2 + |d|^2 = 1$, $a\overline{d} + \overline{a}d = 0$, $ad \neq 0$, $b = c = 0$.
Type V: a, b, c, d satisfying (4.2.1) - (4.2.5) and $abcd \neq 0$.

Let $\mathrm{supp}[\zeta_n^{(m:\pm)}] = \{x \in \mathbb{Z} : \zeta_n^{(m:\pm)}(x) > 0\}$. Then, it is easily seen that for any $n \in \mathbb{Z}_+$, $\mathrm{supp}[\zeta_n^{(0:\pm)}] \subset \{-2, -1, 0, 1\}$ in Type I, and $\mathrm{supp}[\zeta_n^{(0:\pm)}] \subset \{-1, 0, 1, 2\}$ in Type II. So both Types I and II are also trivial cases. To investigate non-trivial Types III - V, we introduce a quantum walk in the next section.

We see that a direct computation implies that (a, b, c, d) satisfying (4.2.1) - (4.2.5) has the following form:

$$(a, b, c, d) = e^{i\delta}(\cos\theta\cos\phi, -i\cos\theta\sin\phi, \sin\theta\sin\phi, i\sin\theta\cos\phi), \qquad (4.2.6)$$

where $\theta, \phi, \delta \in [0, 2\pi)$. From now on, we assume that (a, b, c, d) has the above form. Remark that the case studied by Patel, Raghunathan, and Rungta (2005a) is $\delta = \pi/2$ and $\theta = \phi = \pi/4$, that is, $(a, b, c, d) = (i/2, 1/2, i/2, -1/2)$, which belongs to Type V.

4.3 Definition of A-type and B-type Quantum Walks

The time evolution of both one-dimensional A-type and B-type quantum walks is given by the following unitary matrix:

$$U = \begin{bmatrix} a' & b' \\ c' & d' \end{bmatrix},$$

where $a', b', c', d' \in \mathbb{C}$. So we have $|a'|^2 + |b'|^2 = |c'|^2 + |d'|^2 = 1$, $a'\overline{c'} + b'\overline{d'} = 0$, $c' = -\triangle\overline{b'}$, $d' = \triangle\overline{a'}$, where $\triangle = \det U = a'd' - b'c'$ with $|\triangle| = 1$.

Let $|L\rangle = {}^T[1, 0]$ and $|R\rangle = {}^T[0, 1]$. For an A-type quantum walk, each coin performs the evolution:

$$|L\rangle \;\rightarrow\; U|L\rangle = a'|L\rangle + c'|R\rangle, \qquad |R\rangle \;\rightarrow\; U|R\rangle = b'|L\rangle + d'|R\rangle,$$

at each time step for which that coin is active, where L and R can be respectively thought of as the head and tail states of the coin, or equivalently as an internal chirality state of the particle. The value of the coin controls the direction in which the particle moves. When the coin shows L, the particle moves one unit to the left, when it shows R, it moves one unit to the right. Then a B-type quantum walk is also defined in a similar way as we will state later. Thus the quantum walk can be considered as a quantum version of a classical random walk with an additional degree of freedom called the chirality which takes values left and right.

The amplitude of the location of the particle is defined by a 2-vector $\in \mathbb{C}^2$ at each location at any time n. The probability that the particle is at location x is given by the square of the modulus of the vector at x. For the j-type quantum walk ($j = A, B$), let $\Psi_{j,n}(x)$ denote the amplitude at time n at location x where

$$\Psi_{j,n}(x) = \begin{bmatrix} \Psi^L_{j,n}(x) \\ \Psi^R_{j,n}(x) \end{bmatrix},$$

with the chirality being left (upper component) or right (lower component). For each $j = A$ and B, the dynamics of $\Psi_{j,n}(x)$ for the j-type quantum walk starting from the origin with an initial qubit state $\varphi = {}^T[\alpha, \beta]$, (where $\alpha, \beta \in \mathbb{C}$ and $|\alpha|^2 + |\beta|^2 = 1$), is presented as the following transformation:

$$\Psi_{j,n+1}(x) = P_j \Psi_{j,n}(x+1) + Q_j \Psi_{j,n}(x-1), \tag{4.3.7}$$

where

$$P_A = \begin{bmatrix} a' & b' \\ 0 & 0 \end{bmatrix}, \quad Q_A = \begin{bmatrix} 0 & 0 \\ c' & d' \end{bmatrix} \quad \text{and} \quad P_B = \begin{bmatrix} a' & 0 \\ c' & 0 \end{bmatrix}, \quad Q_B = \begin{bmatrix} 0 & b' \\ 0 & d' \end{bmatrix}.$$

It is noted that $U = P_j + Q_j$ ($j = A, B$). The unitarity of U ensures that the amplitude always defines a probability distribution for the location. From (4.3.7), we see that the unitary matrix of the system is described as

$$\begin{bmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & O & P_j & O & O & O & \dots \\ \dots & Q_j & O & P_j & O & O & \dots \\ \dots & O & Q_j & O & P_j & O & \dots \\ \dots & O & O & Q_j & O & P_j & \dots \\ \dots & O & O & O & Q_j & O & \dots \\ \dots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \quad \text{with} \quad O = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix},$$

for $j = A$ and B. Remark that the A-type (resp. B-type) quantum walk is called an A-type (resp. a G-type) quantum walk in Konno (2002b).

4.4 Connection Between QCA and A-type Quantum Walk

To begin with, we investigate a relation between the QCA and the A-type quantum walk. To do so, the unitary matrix of the QCA

$$\overline{U} = \begin{array}{c} \\ \vdots \\ -3 \\ -2 \\ -1 \\ 0 \\ +1 \\ +2 \\ +3 \\ +4 \\ \vdots \end{array} \begin{array}{c} \begin{array}{cccccccccc} \dots & -3 & -2 & -1 & 0 & +1 & +2 & +3 & +4 & \dots \end{array} \\ \left(\begin{array}{cccccccccc} \ddots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \dots & b & a & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ \dots & a & b & c & d & 0 & 0 & 0 & 0 & \dots \\ \dots & d & c & b & a & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & a & b & c & d & 0 & 0 & \dots \\ \dots & 0 & 0 & d & c & b & a & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & a & b & c & d & \dots \\ \dots & 0 & 0 & 0 & 0 & d & c & b & a & \dots \\ \dots & 0 & 0 & 0 & 0 & 0 & 0 & a & b & \dots \\ \dots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \ddots \end{array} \right) \end{array}$$

is rewritten as

$$\overline{U} = \begin{array}{c} \\ \vdots \\ -1 \\ 0 \\ +1 \\ +2 \\ \vdots \end{array} \begin{array}{c} \begin{array}{cccccc} \dots & -1 & 0 & +1 & +2 & \dots \end{array} \\ \left(\begin{array}{cccccc} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & T_A & Q_A & O & O & \dots \\ \dots & P_A & T_A & Q_A & O & \dots \\ \dots & O & P_A & T_A & Q_A & \dots \\ \dots & O & O & P_A & T_A & \dots \\ \dots & \vdots & \vdots & \vdots & \vdots & \ddots \end{array} \right) \end{array},$$

where

$$P_A = \begin{bmatrix} d & c \\ 0 & 0 \end{bmatrix}, \quad T_A = \begin{bmatrix} b & a \\ a & b \end{bmatrix}, \quad Q_A = \begin{bmatrix} 0 & 0 \\ c & d \end{bmatrix}.$$

We consider a pair $(2x-1, 2x)$ in the QCA as a site x in the A-type quantum walk for any $x \in \mathbb{Z}$. Moreover we observe that $2x-1$ (resp. $2x$) site in the QCA corresponds to right (resp. left) chirality at a site x in the A-type quantum walk. We call the QCA a *generalized A-type quantum walk*. When T_A is not the zero matrix, the particle has non-zero amplitudes for maintaining its position during each time step. More precisely,

$$\Psi_{A,n}(x) = \begin{bmatrix} \Psi^R_{A,n}(x) \\ \Psi^L_{A,n}(x) \end{bmatrix}$$

and

$$\Psi_{A,n+1}(x) = Q_A \Psi_{A,n}(x+1) + T_A \Psi_{A,n}(x) + P_A \Psi_{A,n}(x-1).$$

From the above observation, we see that "Type V QCA $\longleftrightarrow$ generalized A-type quantum walk", where "$X \longleftrightarrow Y$" means that there is a one-to-one correspondence between X and Y; that is,

$$\Psi_{A,n}^{R}(x) = \beta\eta_n^{(-1)}(2x-1) + \alpha\eta_n^{(0)}(2x-1),$$
$$\Psi_{A,n}^{L}(x) = \beta\eta_n^{(-1)}(2x) + \alpha\eta_n^{(0)}(2x),$$
$$\zeta_n^{(0:-)}(2x-1) = |\Psi_{A,n}^{R}(x)|^2, \quad \zeta_n^{(0:-)}(2x) = |\Psi_{A,n}^{L}(x)|^2.$$

Here we recall Type III: $|c|^2 + |d|^2 = 1$, $c\overline{d} + \overline{c}d = 0$, $cd \neq 0$, $a = b = 0$. In this case, T_A becomes zero matrix. So we see that Type III is nothing but an A-type quantum walk by interchanging P_A and Q_A, and the roles of left and right chiralities with $c = b' = c'$, $d = a' = d'$. That is, "Type III QCA $\longleftrightarrow$ A-type quantum walk".

We should remark that as $\tan\phi$ increases (see (4.2.6)), the relative weight of T_A increases and the particle has greater probability of maintaining its position. This property also holds in a generalized B-type case introduced in the next section.

4.5 Connection Between QCA and B-type Quantum Walk

As in the case of the A-type quantum walk, we study a relation between the QCA and the B-type quantum walk; that is, "Type V QCA $\longleftrightarrow$ generalized B-type quantum walk". To do this, the unitary matrix of the QCA

$$\overline{U} = \begin{array}{c} \\ \vdots \\ -2 \\ -1 \\ 0 \\ +1 \\ +2 \\ +3 \\ +4 \\ +5 \\ \vdots \end{array} \begin{array}{c} \begin{array}{ccccccccccc} \dots & -2 & -1 & 0 & +1 & +2 & +3 & +4 & +5\dots & & \end{array} \\ \begin{pmatrix} \ddots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \dots & b & c & d & 0 & 0 & 0 & 0 & 0 & \dots \\ \dots & c & b & a & 0 & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & a & b & c & d & 0 & 0 & 0 & \dots \\ \dots & 0 & d & c & b & a & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & a & b & c & d & 0 & \dots \\ \dots & 0 & 0 & 0 & d & c & b & a & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & 0 & a & b & c & \dots \\ \dots & 0 & 0 & 0 & 0 & 0 & d & c & b & \dots \\ \dots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \ddots \end{pmatrix} \end{array}$$

is rewritten as

$$\overline{U} = \begin{array}{c} \\ \vdots \\ -1 \\ 0 \\ +1 \\ +2 \\ \vdots \end{array} \begin{array}{c} \begin{array}{cccccc} \dots & -1 & 0 & +1 & +2 & \dots \end{array} \\ \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & T_B & P_B & O & O & \dots \\ \dots & Q_B & T_B & P_B & O & \dots \\ \dots & O & Q_B & T_B & P_B & \dots \\ \dots & O & O & Q_B & T_B & \dots \\ \dots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \end{array},$$

where

$$P_B = \begin{bmatrix} d & 0 \\ a & 0 \end{bmatrix}, \quad T_B = \begin{bmatrix} b & c \\ c & b \end{bmatrix}, \quad Q_B = \begin{bmatrix} 0 & a \\ 0 & d \end{bmatrix}.$$

We consider a pair $(2x, 2x+1)$ in the QCA as a site x in the B-type quantum walk for any $x \in \mathbb{Z}$. Moreover we observe that $2x$ (resp. $2x+1$) site in the QCA corresponds to left (resp. right) chirality at site x in the B-type quantum walk. We call the QCA a *generalized B-type quantum walk*. When T_B is not the zero matrix, the particle has non-zero amplitudes for maintaining its position during each time step. As in the case of the A-type quantum walk, it is shown that "Type V QCA $\longleftrightarrow$ generalized B-type quantum walk", that is,

$$\begin{aligned} &\Psi^L_{B,n}(x) = \alpha\eta^{(0)}_x(2x) + \beta\eta^{(1)}_n(2x), \quad \Psi^R_{B,n}(x) = \alpha\eta^{(0)}_n(2x+1) + \beta\eta^{(1)}_n(2x+1), \\ &\zeta^{(0:+)}_n(2x) = |\Psi^L_{B,n}(x)|^2, \quad \zeta^{(0:+)}_n(2x+1) = |\Psi^R_{B,n}(x)|^2. \end{aligned}$$

We think of Type IV: $|a|^2 + |d|^2 = 1$, $a\overline{d} + \overline{a}d = 0$, $ad \neq 0$, $b = c = 0$. In this case, T_B is zero matrix. So Type IV becomes a B-type quantum walk with $d = a' = d'$, $a = b' = c'$; that is, "Type IV QCA $\longleftrightarrow$ B-type quantum walk".

Meyer (1996, 1997, 1998) has investigated the B-type quantum walks, which was called a *quantum lattice gas automaton*. His case (for example, (24) in his paper (1996)) can be obtained by $\delta \to 3\pi/2$, $\phi \to \rho$, and $\theta \to \pi/2 + \theta$ in (4.2.6).

4.6 Connection Between Type V QCA and Two-step Quantum Walk

In the previous two sections, we have clarified the following relations: "Type III QCA $\longleftrightarrow$ A-type quantum walk", "Type IV QCA $\longleftrightarrow$ B-type quantum walk", moreover "Type V QCA $\longleftrightarrow$ generalized A-type quantum walk $\longleftrightarrow$ generalized B-type quantum walk". This section gives a relation between Type V QCA and two-step quantum walk. The meaning of the "two-step" is that we identify the one-step transition of Type V QCA with the two-step transition of the quantum walk.

First "Type V QCA $\longleftrightarrow$ two-step A-type quantum walk" is given. Next "Type V QCA $\longleftrightarrow$ two-step B-type quantum walk" is also presented. Combining them all, we finally obtain the following relations:

"Type V QCA $\longleftrightarrow$ generalized A-type quantum walk $\longleftrightarrow$ two-step A-type quantum walk"

"Type V QCA $\longleftrightarrow$ generalized B-type quantum walk $\longleftrightarrow$ two-step B-type quantum walk"

Now we present "generalized A-type quantum walk $\longleftrightarrow$ two-step A-type quantum walk" in the following way. A direct computation implies that a generalized A-type quantum walk with

$$P_A = \begin{bmatrix} d & c \\ 0 & 0 \end{bmatrix}, \quad T_A = \begin{bmatrix} b & a \\ a & b \end{bmatrix}, \quad Q_A = \begin{bmatrix} 0 & 0 \\ c & d \end{bmatrix}$$

is equivalent to a two-step A-type quantum walk with

$$P_A(1) = \begin{bmatrix} i\cos\phi\, e^{i\theta_2} & \sin\phi\, e^{i\theta_2} \\ 0 & 0 \end{bmatrix}, \quad P_A(2) = e^{i\delta} \begin{bmatrix} \sin\theta\, e^{-i\theta_2} & -i\cos\theta\, e^{-i\theta_1} \\ 0 & 0 \end{bmatrix},$$

and

$$Q_A(1) = \begin{bmatrix} 0 & 0 \\ \sin\phi\, e^{i\theta_1} & i\cos\phi\, e^{i\theta_1} \end{bmatrix}, \quad Q_A(2) = e^{i\delta} \begin{bmatrix} 0 & 0 \\ -i\cos\theta\, e^{-i\theta_2} & \sin\theta\, e^{-i\theta_1} \end{bmatrix},$$

for any $\theta_1, \theta_2 \in [0, 2\pi)$ such that

$$P_A = P_A(2)P_A(1), \quad Q_A = Q_A(2)Q_A(1), \quad T_A = P_A(2)Q_A(1) + Q_A(2)P_A(1).$$

Note that (a, b, c, d) has the form given in (4.2.6) and $U(n) \equiv P_A(n) + Q_A(n)$ is unitary for $n = 1, 2$.

In a similar fashion, we show that "generalized B-type quantum walk $\longleftrightarrow$ two-step B-type quantum walk"; that is, a generalized B-type quantum walk with

$$P_B = \begin{bmatrix} d & 0 \\ a & 0 \end{bmatrix}, \quad T_B = \begin{bmatrix} b & c \\ c & b \end{bmatrix}, \quad Q_B = \begin{bmatrix} 0 & a \\ 0 & d \end{bmatrix}$$

corresponds to a two-step B-type quantum walk with

$$P_B(1) = \begin{bmatrix} i\cos\phi\, e^{i\theta_2} & 0 \\ \sin\phi\, e^{i\theta_1} & 0 \end{bmatrix}, \quad P_B(2) = e^{i\delta} \begin{bmatrix} \sin\theta\, e^{-i\theta_2} & 0 \\ -i\cos\theta\, e^{-i\theta_2} & 0 \end{bmatrix},$$

and

$$Q_B(1) = \begin{bmatrix} 0 & \sin\phi\, e^{i\theta_2} \\ 0 & i\cos\phi\, e^{i\theta_1} \end{bmatrix}, \quad Q_B(2) = e^{i\delta} \begin{bmatrix} 0 & -i\cos\theta\, e^{-i\theta_1} \\ 0 & \sin\theta\, e^{-i\theta_1} \end{bmatrix},$$

for any $\theta_1, \theta_2 \in [0, 2\pi)$ such that

$$P_B = P_B(2)P_B(1), \quad Q_B = Q_B(2)Q_B(1), \quad T_B = P_B(2)Q_B(1) + Q_B(2)P_B(1).$$

Remark that $P_B(n) + Q_B(n) = P_A(n) + Q_A(n)$ for $n = 1, 2$.

Finally we discuss the case given by Patel, Raghunathan, and Rungta (2005a). In their notation, we take general 2×2 blocks of U_e and U_o as

$$U_e = \begin{bmatrix} \cos\phi_1 & i\sin\phi_1 \\ i\sin\phi_1 & \cos\phi_1 \end{bmatrix}, \qquad U_o = \begin{bmatrix} \cos\phi_2 & i\sin\phi_2 \\ i\sin\phi_2 & \cos\phi_2 \end{bmatrix}.$$

Their special case is $\phi_1 = \phi_2 = \pi/4$, i.e.,

$$U_e = U_o = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix}. \tag{4.6.8}$$

By using U_e and U_o, the following matrices are defined:

$$\overline{U}_e = \begin{array}{c} \\ \vdots \\ -2 \\ -1 \\ 0 \\ +1 \\ +2 \\ +3 \\ \vdots \end{array} \begin{array}{c} \cdots \quad -2 \quad -1 \quad 0 \quad +1 \quad +2 \quad +3 \quad \cdots \\ \left(\begin{array}{cccccccc} \ddots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdots \\ \cdots & \cos\phi_1 & i\sin\phi_1 & 0 & 0 & 0 & 0 & \cdots \\ \cdots & i\sin\phi_1 & \cos\phi_1 & 0 & 0 & 0 & 0 & \cdots \\ \cdots & 0 & 0 & \cos\phi_1 & i\sin\phi_1 & 0 & 0 & \cdots \\ \cdots & 0 & 0 & i\sin\phi_1 & \cos\phi_1 & 0 & 0 & \cdots \\ \cdots & 0 & 0 & 0 & 0 & \cos\phi_1 & i\sin\phi_1 & \cdots \\ \cdots & 0 & 0 & 0 & 0 & i\sin\phi_1 & \cos\phi_1 & \cdots \\ \cdots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \ddots \end{array} \right) \end{array},$$

and

$$\overline{U}_o = \begin{array}{c} \\ \vdots \\ -2 \\ -1 \\ 0 \\ +1 \\ +2 \\ +3 \\ \vdots \end{array} \begin{array}{c} \cdots \quad -2 \quad -1 \quad 0 \quad +1 \quad +2 \quad +3 \quad \cdots \\ \left(\begin{array}{cccccccc} \ddots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdots \\ \cdots & \cos\phi_2 & 0 & 0 & 0 & 0 & 0 & \cdots \\ \cdots & 0 & \cos\phi_2 & i\sin\phi_2 & 0 & 0 & 0 & \cdots \\ \cdots & 0 & i\sin\phi_2 & \cos\phi_2 & 0 & 0 & 0 & \cdots \\ \cdots & 0 & 0 & 0 & \cos\phi_2 & i\sin\phi_2 & 0 & \cdots \\ \cdots & 0 & 0 & 0 & i\sin\phi_2 & \cos\phi_2 & 0 & \cdots \\ \cdots & 0 & 0 & 0 & 0 & 0 & \cos\phi_2 & \cdots \\ \cdots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \ddots \end{array} \right) \end{array}.$$

Noting that $\overline{U} = \overline{U}_e \overline{U}_o$, we have

$$(a, b, c, d) = (i \cos\phi_1 \sin\phi_2, \cos\phi_1 \cos\phi_2, i \sin\phi_1 \cos\phi_2, -\sin\phi_1 \sin\phi_2). \tag{4.6.9}$$

Therefore, by choosing $\theta = \phi_1, \phi = \pi/2 - \phi_2$, and $\delta = \pi/2$ in (4.2.6), we have (4.6.9).

Furthermore, we see that if $\theta + \phi = \pi/2, 3\pi/2$, $\theta_1 = \theta_2$, and $\delta = 2\theta_1 + \pi/2$, then $U(1) = U(2)$. To get the case of Patel, Raghunathan, and Rungta (2005a), we take $\theta = \phi = \pi/4$, $\theta_1 = \theta_2 = 0$, and $\delta = \pi/2$, so

$$U(1) = U(2) = \frac{1}{\sqrt{2}} \begin{bmatrix} i & 1 \\ 1 & i \end{bmatrix}. \tag{4.6.10}$$

Remark that $U_e = U_o$ is not equal to $U(1) = U(2)$ in their case (see (4.6.8) and (4.6.10)). To obtain their asymptotic result, we define their walk at time n with the initial qubit state $\varphi = {}^T[1/\sqrt{2}, 1/\sqrt{2}]$ by X_n. Note that if $\varphi = {}^T[\alpha, \beta]$

satisfies $\alpha\overline{\beta} = \overline{\alpha}\beta$, then the distribution is symmetric at any time, (see Theorem 1.5). Then, Theorem 1.6 implies that

$$P(a \le X_n^{\varphi}/n \le b) \to \int_a^b \frac{4}{\pi(4-x^2)\sqrt{4-2x^2}} dx \qquad (n \to \infty),$$

for $-\sqrt{2} \le a < b \le \sqrt{2}$. It should be noted that their case can be considered as a two-step quantum walk with $U(1) = U(2)$, so we make a change of variables; $x \to x/2$ in Theorem 1.6. The above limit density function corresponds to (34) at time $t = 1$ in their paper. Thus, their asymptotic result can be easily derived from the connection between the QCA and the two-step quantum walk that is given in this section. Moreover, it would be shown that a similar convergence theorem holds for any general model with $U(1) = U(2)$ as in the above case.

5 Cycle

5.1 Introduction

In this chapter we consider quantum walks on cycles. The probability distribution of a classical random walker on a cycle with an odd number of sites becomes uniform in the limit of time step $n \to \infty$, moreover the time average of the probability distribution on a cycle with an odd or even number of sites converges the uniform distribution. However, the probability distribution of quantum walk does not converge to any stationary state even for odd case. On the other hand, its time average converges to uniform distribution for an odd number of sites and does not converge to uniform one for an even number of sites (see Aharonov et al. (2001), Bednarska et al. (2003)). For that reason the time-averaged distribution of quantum walk was introduced. It should be kept in mind that the probability of being at position x fluctuates around the time-averaged density. In the case of the Hadmard walk, the time-averaged distribution becomes uniform independently on the ini tial state if the number of site is odd, and it agrees with the classical random walk. The fluctuation of the distribution is not only mathematical object, but related to measurement. The time-averaged distribution is obtained by measuring the state at a random time chosen in a certain interval. If the fluctuation of the density function is small, we can expect to obtain a good time-averaged distribution by a few number of measurements.

Although details of the time-averaged distribution of the Hadamard walk on a cycle are known, (see Aharonov et al. (2001), Bednarska et al. (2003), for examples), little is known about the fluctuation of the quantum walks. In this chapter we introduce a temporal standard deviation to characterize the fluctuation of quantum walk and show that the temporal standard deviation corresponding to the Hadamard walk depends on the location of sites even if time-averaged density function is uniform. This result has a striking difference between quantum and classical cases, since temporal standard deviation of the classical case is zero for any site. Furthermore we consider the dependence of the standard deviation on the initial state. Results in this chapter are based on Inui, Konishi, Konno, and Soshi (2005).

5.2 Definition

The Hadamard walk on a cycle with N sites is given by the following unitary matrix with $2N \times 2N$ elements,

$$\overline{U}_N = \begin{bmatrix} 0 & P & 0 & \cdots & \cdots & 0 & Q \\ Q & 0 & P & 0 & \cdots & \cdots & 0 \\ 0 & Q & 0 & P & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & Q & 0 & P & 0 \\ 0 & \cdots & \cdots & 0 & Q & 0 & P \\ P & 0 & \cdots & \cdots & 0 & Q & 0 \end{bmatrix}, \tag{5.2.1}$$

where

$$P = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}, \quad Q = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 \\ 1 & -1 \end{bmatrix}, \quad 0 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}. \tag{5.2.2}$$

Thus the total state after n step, Ψ_n, is given by $\overline{U}_N^n \Psi_0$ for the initial state Ψ_0.

To express the total state as a function of position x and time n, we use known results on eigenvalues (Lemma 5.1) and eigenvectors (Lemma 5.2) of $\overline{U}_N$ obtained by Aharonov et al. (2001) and Bednarska et al. (2003).

Lemma 5.1. *For $j = 0, 1, \ldots, N-1$ and $k = 0, 1$, the $(2j+k+1)$-th eigenvalue corresponding to $\overline{U}_N$ is given by*

$$c_{jk} = \frac{1}{\sqrt{2}} \left\{ (-1)^k \sqrt{1 + \cos^2\left(\frac{2\,j\,\pi}{N}\right)} + i \sin\left(\frac{2\,j\,\pi}{N}\right) \right\}. \tag{5.2.3}$$

We here define $v^o_{j,k,l}$ and $v^e_{j,k,l}$ to express eigenvectors by

$$v^o_{j,k,l} = a_{jk}\, b_{jk}\, \omega_N^{jl}, \tag{5.2.4}$$

$$v^e_{j,k,l} = a_{jk}\, \omega_N^{jl}, \tag{5.2.5}$$

where

$$\omega_N = e^{\frac{2\,i\,\pi}{N}}, \tag{5.2.6}$$

$$a_{jk} = \frac{1}{\sqrt{N\left(1+|b_{jk}|^2\right)}}, \tag{5.2.7}$$

$$b_{jk} = \omega_N^j \left\{(-1)^k \sqrt{1+\cos^2\xi_j} + \cos\xi_j\right\}, \tag{5.2.8}$$

$$\xi_j = \frac{2j\pi}{N}. \tag{5.2.9}$$

Lemma 5.2. *For $l = 1, 2, \ldots, 2N$, the l-th element of the eigenvectors corresponding to c_{jk} is given by*

$$v_{j,k,l} = \begin{cases} v^o_{j,k,(l+1)/2} & (l = odd), \\ v^e_{j,k,l/2} & (l = even). \end{cases} \tag{5.2.10}$$

For the convenience of readers, from now on here we check directly that eigenvectors $v_{j,k} = {}^T[v_{j,k,1}, \cdots, v_{j,k,2N}]$ satisfy the next equation:

$$\overline{U}_N v_{j,k} = c_{jk} v_{j,k}. \tag{5.2.11}$$

(a) Suppose l is odd, then the $(2m-1)$-th element of the left-hand side of the (5.2.11) for $m = 1, 2, \cdots, N$ is given by

$$\begin{aligned} &(2m-1)\text{-th element of LHS} \\ &= \frac{1}{\sqrt{2}}\left(v^o_{j,k,m+1 \bmod N} + v^e_{j,k,m+1 \bmod N}\right) \\ &= \frac{a_{jk}}{\sqrt{2}}\left[e^{\frac{2j(m+1)i\pi}{N}}\left\{1 + e^{\frac{2ji\pi}{N}}\left((-1)^k\sqrt{1+\cos^2\xi_j} + \cos\xi_j\right)\right\}\right], \end{aligned} \tag{5.2.12}$$

where $\xi_j = 2\pi j/N$. On the other hand, the right-hand side of (5.2.11) is given by

$$\begin{aligned} &(2m-1)\text{-th element of RHS} \\ &= c_{jk} a_{jk} b_{jk} \omega_N^{jm} \\ &= \frac{a_{jk}}{\sqrt{2}}\left[e^{\frac{2j(m+1)i\pi}{N}}\left((-1)^k\sqrt{1+\cos^2\xi_j} + \cos\xi_j\right)\right. \\ &\qquad \left.\times\left((-1)^k\sqrt{1+\cos^2\xi_j} + i\sin\xi_j\right)\right]. \end{aligned} \tag{5.2.13}$$

(b) Similarly suppose l is even, then the $2m$-th element of the left-hand side of the (5.2.11) for $m = 1, 2, \cdots, N$ is given by

$$
\begin{aligned}
&2m\text{-th element of LHS} \\
&= \frac{1}{\sqrt{2}} \left(v^{o}_{j,k,m-1 \bmod N} - v^{e}_{j,k,m-1 \bmod N} \right) \\
&= \frac{a_{jk}}{\sqrt{2}} \left[e^{\frac{2j(m-1)i\pi}{N}} \left\{ -1 + e^{\frac{2ji\pi}{N}} \left((-1)^k \sqrt{1+\cos^2 \xi_j} + \cos \xi_j \right) \right\} \right]. \qquad (5.2.14)
\end{aligned}
$$

On the other hand, the right-hand side of the (5.2.11) is given by

$$
\begin{aligned}
&2m\text{-th element of RHS} \\
&= c_{jk} a_{jk} \omega_N^{jm} \\
&= \frac{a_{jk}}{\sqrt{2}} \left[e^{\frac{2jmi\pi}{N}} \left((-1)^k \sqrt{1+\cos^2 \xi_j} + i \sin \xi_j \right) \right]. \qquad (5.2.15)
\end{aligned}
$$

Using the Euler's formula, we can check that both sides of (5.2.11) coincide for each case.

5.3 Temporal Standard Deviation

Since we obtained the eigenvalues and eigenvectors, matrix $\overline{U}_N$ is transformed into a diagonal matrix and the wave function after n steps is generally expressed by a liner combination of c_{jk}^n. In real system we can not observe the wave function but probability of being at position x at time n, $P_{n,N}(x)$. In contrast to classical random walks, the probability $P_{n,N}(x)$ dose not converge in the limit of $n \to \infty$. Thus we consider a time-averaged distribution defined by

$$
\bar{P}_N(x) = \lim_{T \to \infty} \frac{1}{T} \sum_{n=0}^{T-1} P_{n,N}(x), \qquad (5.3.16)
$$

if the right-hand side of (5.3.16) exists. Aharonov et al. (2001) showed that $\bar{P}_N(x)$ exists, and it is independent of both an initial state and x if all eigenvalues of $\overline{U}_N$ are distinct. If the number of site is odd, then all eigenvalues of $\overline{U}_N$ are distinct, so we immediately have $\bar{P}_N(x) = 1/N$ for any $x = 0, 1, \ldots, N-1$. On the other hand, if N is even, then there exist degenerate eigenvalues of $\overline{U}_N$ and it is possible to derive non-uniform distributions. In the case of the classical random walk, the time-averaged distribution of a walker becomes uniform independently on the parity of the system size. Thus we can not distinguish the classical random walk and the Hadamard walk on a cycle with odd sites only by the time-averaged distribution.

As we mentioned above, the $P_{n,N}(x)$ does not converge in the limit $n \to \infty$. It means that the probability always fluctuates to the upper and lower sides of $P_N(x)$. For this reason, we define the following temporal standard deviation $\sigma_N(x)$:

$$\sigma_N(x) = \sqrt{\lim_{T\to\infty} \frac{1}{T} \sum_{n=0}^{T-1} \left(P_{n,N}(x) - \bar{P}_N(x)\right)^2}, \tag{5.3.17}$$

if the right-hand side of (5.3.17) exists.

Here we consider the classical case. In the case of classical a random walk starting from a site for an odd number of sites (i.e., aperiodic case), there exist $a \in (0,1)$ and $C > 0$ (are independent of x and n) such that

$$|P_{n,N}(x) - \bar{P}_N(x)| \le Ca^n,$$

where $\bar{P}_N(x) = 1/N$ for any $x = 0, 1, \ldots, N-1$, (see page 63 of Schinazi (1999), for example). Therefore we obtain

$$\frac{1}{T} \sum_{n=0}^{T-1} \left(P_{n,N}(x) - \bar{P}_N(x)\right)^2 \le \frac{C^2}{T} \frac{1-a^{2T}}{1-a^2}.$$

The above inequality implies that for any $x = 0, 1, \ldots, N-1$,

$$\sigma_N(x) = 0.$$

in the classical case. As for $N =$ even (i.e., periodic) case, we have the same conclusion $\sigma_N(x) = 0$ for any x by using a little modified argument.

In this situation, we first ask the natural question whether the $\sigma_N(x)$ is always zero or not in the quantum case. Moreover if $\sigma_N(x)$ is not always zero, then we next ask the question whether $\sigma_N(x)$ is uniform or not.

From now on we concentrate our attention to the system with odd sites. Furthermore we assume that the initial state is a fixed $\Psi_0 = {}^T[1, 0, 0, \cdots, 0]$. Let us express the standard deviation $\sigma_N(x)$ starting $\Psi_0 = {}^T[1, 0, 0, \cdots, 0]$ by wave functions. To do so, we have

$$\sigma_N^2(x) = \lim_{T\to\infty} \frac{1}{T} \sum_{n=0}^{T-1} \left(|\Psi_n^L(x)|^2 + |\Psi_n^R(x)|^2 - \frac{1}{N} \right)^2, \tag{5.3.18}$$

where we used the result $\bar{P}(x) = 1/N$ for odd N. Since the matrix $\overline{U}_N$ was already diagonalized in the previous section, the wave functions $\Psi_n^L(x)$ and $\Psi_n^R(x)$ are easily obtained as

$$\Psi_n^L(x) = \sum_{j=0}^{N-1} \left(\alpha_{j0} c_{j0}^n + \alpha_{j1} c_{j1}^n \right), \tag{5.3.19}$$

$$\Psi_n^R(x) = \sum_{j=0}^{N-1} \left(\beta_{j0} c_{j0}^n + \beta_{j1} c_{j1}^n \right), \tag{5.3.20}$$

where

$$\alpha_{jk} = \frac{e^{\frac{2nj\pi i}{N}}}{2N}\left(1+(-1)^k \frac{\cos(\frac{2j\pi}{N})}{\sqrt{1+\cos^2(\frac{2j\pi}{N})}}\right), \tag{5.3.21}$$

$$\beta_{jk} = \frac{(-1)^k e^{\frac{2(n-1)j\pi i}{N}}}{2N\sqrt{1+\cos^2(\frac{2j\pi}{N})}}. \tag{5.3.22}$$

Since the matrix $\overline{U}_N$ is unitary matrix, the eigenvalue c_{jk} is written as $e^{i\theta_{jk}}$ where θ_{jk} is the argument of c_{jk}. Thus the probability $|\Psi_n^L(x)|^2$ is expressed by

$$|\Psi_n^L(x)|^2 = \sum_{j=0}^{N-1}(|\alpha_{j0}|^2+|\alpha_{j1}|^2) + \sum_{j_0,j_1=0}^{N-1}\sum_{k_0,k_1=0}^{1} \delta_{j_0j_1,k_0k_1}\alpha_{j_0k_0}\alpha^*_{j_1k_1}e^{i(\theta_{j_0k_0}-\theta_{j_1k_1})n}, \tag{5.3.23}$$

where

$$\delta_{j_0j_1,k_0k_1} = \begin{cases} 0 & j_0=j_1 \quad \text{and} \quad k_0=k_1, \\ 1 & \text{otherwise.} \end{cases} \tag{5.3.24}$$

The first term of (5.3.23) is constant and the second term vanishes by applying an operation $\lim_{T\to\infty}\frac{1}{T}\sum_{n=0}^{T-1}$. Similarly we can divide $|\Psi_n^R(x)|^2$ into a constant term and a vanishing term:

$$|\Psi_n^R(x)|^2 = \sum_{j=0}^{N-1}(|\beta_{j0}|^2+|\beta_{j1}|^2) + \sum_{j_0,j_1=0}^{N-1}\sum_{k_0,k_1=0}^{1} \delta_{j_0j_1,k_0k_1}\beta_{j_0k_0}\beta^*_{j_1k_1}e^{i(\theta_{j_0k_0}-\theta_{j_1k_1})n}. \tag{5.3.25}$$

As a result we have

$$\bar{P}_N(x) = \sum_{j=0}^{N-1}(|\alpha_{j0}|^2+|\alpha_{j1}|^2+|\beta_{j0}|^2+|\beta_{j1}|^2). \tag{5.3.26}$$

Plugging (5.3.21)-(5.3.22) into (5.3.26) gives confirm $\bar{P}_N(x) = 1/N$ for any $x = 0, 1, \ldots, N-1$.

Let express $\sigma_N^2(x)$ as a function of eigenvalues. By using (5.3.18), (5.3.23) and (5.3.25), we get

$$\sigma_N^2(x) = \lim_{T\to\infty} \frac{1}{T} \sum_{n=0}^{T-1} \sum_{j_0,j_1,j_2,j_3=0}^{N-1} \sum_{k_0,k_1,k_2,k_3=0}^{1} \delta_{j_0 j_1, k_0 k_1} \delta_{j_2 j_3, k_2 k_3}$$
$$\times (\alpha_{j_0k_0}\alpha^*_{j_1k_1} + \beta_{j_0k_0}\beta^*_{j_1k_1})(\alpha_{j_2k_2}\alpha^*_{j_3k_3} + \beta_{j_2k_2}\beta^*_{j_3k_3})e^{i\Delta\theta n}, \quad (5.3.27)$$

where

$$\Delta\theta \equiv \Delta\theta(j_0,k_0,j_1,k_1,j_2,k_2,j_3,k_3)$$
$$= \theta_{j_0k_0} - \theta_{j_1k_1} + \theta_{j_2k_2} - \theta_{j_3k_3}. \quad (5.3.28)$$

If $\Delta\theta \neq 0 \pmod{2\pi}$, then $\lim_{T\to\infty} \sum_{n=0}^{T-1} e^{i\Delta\theta n}/T$ converges to 0. Thus the variance $\sigma_N^2(x)$ is obtained by taking the sum of

$$(\alpha_{j_0k_0}\alpha^*_{j_1k_1} + \beta_{j_0k_0}\beta^*_{j_1k_1})\,(\alpha_{j_2k_2}\alpha^*_{j_3k_3} + \beta_{j_2k_2}\beta^*_{j_3k_3})$$

over combinations $j_0, k_0, \ldots, j_3, k_3$ satisfying $\Delta\theta = 0 \pmod{2\pi}$. For this reason, we consider the combinations which satisfy $\Delta\theta = 0 \pmod{2\pi}$ for a given combination (j_0, k_0, j_1, k_1). We define the following four conditions:

$$\begin{array}{lllll} (a) & \Re(c_{j_0k_0}) = \Re(c_{j_1k_1}) & \text{and} & \Im(c_{j_0k_0}) = -\Im(c_{j_1k_1}), \\ (b) & \Re(c_{j_0k_0}) = -\Re(c_{j_1k_1}) & \text{and} & \Im(c_{j_0k_0}) = \Im(c_{j_1k_1}), \\ (c) & \Re(c_{j_0k_0}) = -\Re(c_{j_1k_1}) & \text{and} & \Im(c_{j_0k_0}) = -\Im(c_{j_1k_1}), \\ (d) & \Re(c_{j_0k_0}) = \Re(c_{j_1k_1}) & \text{and} & \Im(c_{j_0k_0}) = \Im(c_{j_1k_1}), \end{array} \quad (5.3.29)$$

where $\Re(z)$ (resp. $\Im(z)$) is the real (resp. imaginary) part of $z \in \mathbb{C}$. If each condition from (a) to (d) is not satisfied, there are four different combinations which satisfy $\Delta\theta = 0 \pmod{2\pi}$ for a given combination (j_0, k_0, j_1, k_1):

$$\begin{array}{ll} (a) & j_2 = N - j_0 \mod N,\ \ k_2 = k_0,\ \ j_3 = N - j_1 \mod N,\ \ k_3 = k_1, \\ (b) & j_2 = j_0,\ \ k_2 = 1 - k_0,\ \ j_3 = j_1,\ \ k_3 = 1 - k_1, \\ (c) & j_2 = N - j_1 \mod N,\ \ k_2 = 1 - k_1,\ \ j_3 = N - j_0 \mod N,\ \ k_3 = 1 - k_0, \\ (d) & j_2 = j_1,\ \ k_2 = k_1,\ \ j_3 = j_0,\ \ k_3 = k_0. \end{array} \quad (5.3.30)$$

If one of conditions in (5.3.29) is satisfied, we find the same values in (5.3.30).

We can introduce a geometrical picture into these combinations. All eigenvalues lie on the unit cycle in the complex plane and there is a symmetry in these points. For example, when we find $c_{j_0k_0}$ at the point A, we can find always another eigenvalue on a point which is obtained by reflecting point A in the x-axis and its eigenvalue is expressed by $c_{N-j_0 \bmod N, k_0}$. We also find always an eigenvalue on a point which is obtained by reflecting point A in the y-axis and its eigenvalues is expressed by $c_{j_0,1-k_0}$. Additionally, we note that if the relation between $c_{j_0k_0}$ and $c_{j_1k_1}$ is symmetrical with respect to the origin and the relation between $c_{j_2k_2}$ and $c_{j_3k_3}$ is also symmetrical with respect to the origin, then $\Delta\theta = 0 \pmod{2\pi}$.

From the relation (5.3.30) we express j_2,k_2,j_3 and k_3 as a function of j_0, k_0, j_1 and k_1. Thus $\sigma_N^2(x)$ is obtained by summation over j_0, k_0, j_1 and k_1. Taking the degeneracy into account correctly we obtain $\sigma_N^2(x)$ by some computations. Before showing the result we define next functions

$$S_0 = \sum_{j=0}^{N-1} \frac{1}{3+\cos\theta_j}, \tag{5.3.31}$$

$$S_1 = \sum_{j=0}^{N-1} \frac{\cos\theta_j}{3+\cos\theta_j}, \tag{5.3.32}$$

$$S_+(x) = \sum_{j=0}^{N-1} \frac{\cos((x-1)\theta_j) + \cos(x\theta_j)}{3+\cos\theta_j}, \tag{5.3.33}$$

$$S_-(x) = \sum_{j=0}^{N-1} \frac{\cos((x-1)\theta_j) - \cos(x\theta_j)}{3+\cos\theta_j}, \tag{5.3.34}$$

$$S_2(x) = \sum_{j=1}^{N-1} \frac{7+\cos 2\theta_j + 8\cos\theta_j \cos^2\left[\left(x-\frac{1}{2}\right)\theta_j\right]}{(3+\cos\theta_j)^2}, \tag{5.3.35}$$

where $\theta_j \equiv 4\pi j/N$. Now we show $\sigma_N^2(x)$ as main result in this chapter:

Theorem 5.3. *When N is odd, we have*

$$\sigma_N^2(x) = \frac{1}{N^4}\left[2\left\{S_+^2(x)+S_-^2(x)\right\} + 11S_0^2 + 10S_0S_1 + 3S_1^2 - S_2(x)\right] - \frac{2}{N^3}, \tag{5.3.36}$$

for any $x = 0, 1, \dots, N-1$.

5.4 Dependence of $\sigma_N(x)$ on the Position and System Size

The formula obtained for $\sigma_N(x)$ is written in the form of a single summation, therefore, it is calculated very easily in comparison with (5.3.27). We consider $\sigma_N(x)$ for $N = 3, 5, \cdots, 11$.

First we find that $\sigma_N(x)$ depends on the position and it has the maximum value at $x = 0$ and 1. The dependence of $\sigma_N(n)$ on the position from 2 to $N-1$ is not clear, however we find that $\sigma_N(x)= \sigma_N(N+1-x) \pmod N$ for any x and all values are distinct except a pair x and $N+1-x \pmod N$.

Next we consider asymptotic behavior of $\sigma_N(0)$ for large N to observe the dependence on the system size. Setting $x = 0$ in (5.3.36) gives

$$\sigma_N^2(0) = \frac{1}{N^3}\left[\sum_{j=0}^{N-1}\frac{7\cos\theta_j}{3+\cos\theta_j} - 2\right]$$
$$+\frac{1}{N^4}\left[\left(\sum_{j=0}^{N-1}\frac{1}{3+\cos\theta_j}\right)\left(\sum_{j=0}^{N-1}\frac{15-11\cos\theta_j}{3+\cos\theta_j}\right)\right.$$
$$\left.-\sum_{j=1}^{N-1}\frac{9+4\cos\theta_j+3\cos 2\theta_j}{(3+\cos\theta_j)^2}\right]. \qquad (5.4.37)$$

On the other hand, we have

$$\lim_{N\to\infty}\frac{1}{N}\sum_{j=0}^{N-1}\frac{1}{3+\cos\theta_j} = \frac{1}{4\pi}\int_0^{4\pi}\frac{1}{3+\cos x}dx = \frac{1}{2\sqrt{2}},$$
$$\lim_{N\to\infty}\frac{1}{N}\sum_{j=0}^{N-1}\frac{\cos\theta_j}{3+\cos\theta_j} = \frac{1}{4\pi}\int_0^{4\pi}\frac{\cos x}{3+\cos x}dx = 1-\frac{3}{2\sqrt{2}},$$
$$\lim_{N\to\infty}\frac{1}{N}\sum_{j=0}^{N-1}\frac{1}{(3+\cos\theta_j)^2} = \frac{1}{4\pi}\int_0^{4\pi}\frac{1}{(3+\cos x)^2}dx = \frac{3}{16\sqrt{2}},$$
$$\lim_{N\to\infty}\frac{1}{N}\sum_{j=0}^{N-1}\frac{\cos\theta_j}{(3+\cos\theta_j)^2} = \frac{1}{4\pi}\int_0^{4\pi}\frac{\cos x}{(3+\cos x)^2}dx = -\frac{1}{16\sqrt{2}},$$
$$\lim_{N\to\infty}\frac{1}{N}\sum_{j=0}^{N-1}\frac{\cos(2\theta_j)}{(3+\cos\theta_j)^2} = \frac{1}{4\pi}\int_0^{4\pi}\frac{\cos 2x}{(3+\cos x)^2}dx = 2-\frac{45}{16\sqrt{2}}.$$

Using the above results, we obtain the asymptotic behavior of the variance $\sigma_N^2(0)$ for sufficiently large N as follows:

Proposition 5.4. *For $N \to \infty$, we have*

$$\sigma_N^2(0) = \frac{13-8\sqrt{2}}{N^2} + \frac{7\sqrt{2}-16}{2N^3} + o\left(\frac{1}{N^3}\right). \qquad (5.4.38)$$

The above result implies that the fluctuation $\sigma_N(0)$ decays in the form $1/N$ as N increases.

5.5 Dependence of $\sigma_N(x)$ on Initial States and Parity of System Size

Dependence of $\sigma_N(x)$ on Initial States

In the previous sections, we have shown only results covering the case where the system size is odd and the initial state is $\Psi_0^L(0) = 1$. The time averaged distribution on a cycle including odd sites is independent of the initial state. Is also the temporal standard deviation independent of the initial state? We consider here whether the temporal standard deviation depends on the initial state even if the initial probability distribution is the same.

In order to observe the dependence of the temporal standard deviation on initial state without changing the initial probability distribution, we set $\Psi_0^L(0)=\alpha$ and $\Psi_0^R(0)=\sqrt{1-\alpha^2}\, i$ where $\alpha \in [0,1]$. As a particular case, we have a symmetrical initial state by setting $\alpha = 1/\sqrt{2}$. Thus we can observe the dependence of $\sigma_N(x,\alpha)$ on symmetry break down by changing α. We first present the result for $N = 3$. The standard deviation $\sigma_3(x,\alpha)$ for the above initial state is obtained as follows:

$$\sigma_3(0,\alpha) = \frac{2\sqrt{46}}{45}, \tag{5.5.39}$$

$$\sigma_3(1,\alpha) = \frac{2}{45}\sqrt{96\,\alpha^4 - 75\,\alpha^2 + 25}, \tag{5.5.40}$$

$$\sigma_3(2,\alpha) = \frac{2}{45}\sqrt{96\,\alpha^4 - 117\,\alpha^2 + 46}. \tag{5.5.41}$$

One clearly finds that $\sigma_3(0,\alpha)$ is independent of the initial and both $\sigma_3(1,\alpha)$ and $\sigma_3(2,\alpha)$ depend on α. We further find that $\sigma_3(1,\alpha)$ is equal to $\sigma_3(2,\alpha)$ at the symmetrical case $\alpha = 1/\sqrt{2}$ and the minimum values are located near $\alpha = 1/\sqrt{2}$.

Next we consider $N = 5$ and $N = 7$. As in the case of $N = 3$, the temporal standard deviation at the position $x = 0$ is independent of the parameter α and the minimum values are located near $\alpha = 1/\sqrt{2}$. The dependence of $\sigma_N(x,\alpha)$ on the position is weak between 2 and $N-2$, and they seem to be in close on a single line.

Temporal Standard Deviation on a Cycle with Even Sites

We have concentrated our attention on the case where the number of the system size is odd. The main reason why we avoid even cases is that the eigenvalues of matrix $\overline{U}_N$ are highly degenerate, and the time averaged distribution itself depends on the position of site and the initial state. While the eigenvalues for even cases is exactly obtained by (5.2.3), there are many possible combinations of eigenvalues which satisfy $\Delta\theta = 0 \pmod{2\pi}$ for the even case. Thus we can not calculate $\sigma_N(x)$ in the same way with odd cases. Therefore, we here try to carry out approximate calculations instead of seeking analytic results for $N = 4, 6, \cdots, 12$ under the same initial condition $\Psi_0^L(0) = 1$ and $T = 10^4$.

First we find that the values of the temporal standard deviation for odd N are almost the same except $x = 0, 1$, while the values for even N are strongly dependent on the location. Second we find that the maximum values of $\sigma_N(x)$

for odd N exist only at $x = 0$ and $x = 1$, while the four same peaks are found for $N = 4, 8, 12$. We confirm numerically that this behavior is always observed up to $N = 22$ when N is a multiple of 4.

5.6 Summary

We expressed the temporal standard deviation of the Hadamard walk on a cycle with odd sites for a pure initial state $\Psi_0^L(0) = 1$ in an analytical form. The formula is obtained by calculating four Fourier coefficients which come from "L" and "R" states. Unlike the time-averaged distribution, the temporal standard deviation depends on the location of the site. The fluctuations decrease in inverse proportion to the system size for large N and its coefficient was calculated rigorously.

When we set the initial state in the form $\Psi_0^L(0)=\alpha$ and $\Psi_0^R(0)=\sqrt{1-\alpha^2}\,i$, the analytical result for $N = 3$ and numerical simulations indicated that the temporal standard deviation depends on the initial state except $x = 0$. We would speculate that the temporal standard deviation takes the maximum value at $x = 0$ and its value is independent of α. The values of the temporal standard deviation at neighbor sites of the origin is somewhat larger than other at sites and the remains are almost the same. The dependence of the temporal standard deviation on the position for even system size is more complex than that for odd system size due to degeneration of eigenvalues. Several peaks are observed when the system size is a multiple of 4.

From the viewpoint of technology, it seen to be of value to consider whether the temporal standard deviation is controlled or not. It is shown that the time-averaged distribution can not be controlled for odd system size, however, for even system size, it is controlled thanks to the degeneracy of eigenvalues. Our results show that the standard deviation can be controlled. First the dependence of temporal standard deviation on location is used. Second the dependence on the initial state is also used. However we note here that $\sigma_N(0)$ for $N = 3$ is independent of the initial state. In this sense, its control is limited.

6 Absorption Problems

6.1 Introduction

In this chapter we consider absorption problems for quantum walks given by $U \in \mathrm{U}(2)$ located on the sets $\{0, 1, \ldots, N\}$ or $\{0, 1, \ldots\}$. Results in this chapter appeared in Konno, Namiki, Soshi, and Sudbury (2003). Before we move to the quantum case, we first describe the classical random walk on a finite set $\{0, 1, \ldots, N\}$ with two absorbing barriers at locations 0 and N (see Grimmett and Stirzaker (1992), Durrett (1999), for examples). The particle moves at each step either one unit to the left with probability p or one unit to the right with probability $q = 1-p$ until it hits one of the absorbing barriers. The directions of different steps are independent of each other. The classical random walk starting from $m \in \{0, 1, \ldots, N\}$ at time n is denoted by S_n^m here. Let

$$T_\ell = \min\{n \geq 0 : S_n^m = \ell\}$$

be the time of the first visit to $\ell \in \{0, 1, \ldots, N\}$. Using the subscript m to indicate $S_0^m = m$, we let

$$P^{(N,m)} = P(T_0 < T_N)$$

be the probability that the particle hits 0 starting from m before it arrives at N. The absorption problem is well known as the Gambler's ruin problem.

6.2 Definition

An extension of the Hadamard walk considered here is:

$$\widehat{H}(\rho) = \begin{bmatrix} \sqrt{\rho} & \sqrt{1-\rho} \\ \sqrt{1-\rho} & -\sqrt{\rho} \end{bmatrix},$$

where $0 \leq \rho \leq 1$. Note that $\rho = 1/2$ is the Hadamard walk, that is, $H = \widehat{H}(1/2)$.

We should remark that P, Q, R, and S form an orthonormal basis of the vector space of complex 2×2 matrices $M_2(\mathbb{C})$ with respect to the trace inner product $\langle A|B \rangle = \text{ tr } (A^* B)$. Therefore we can express any 2×2 matrix A conveniently in the form,

$$A = \text{tr}(P^* A)P + \text{tr}(Q^* A)Q + \text{tr}(R^* A)R + \text{tr}(S^* A)S. \qquad (6.2.1)$$

The $n \times n$ unit and zero matrices are written I_n and O_n respectively. For instance, if $A = I_2$, then

$$I_2 = \overline{a}P + \overline{d}Q + \overline{c}R + \overline{b}S. \qquad (6.2.2)$$

Now we describe the evolution and measurement of quantum walks starting from location m on $\{0, 1, \ldots, N\}$ with absorbing boundaries (see Ambainis et al. (2001), Bach et al. (2002), and Kempe (2002) for more detailed information, for examples).

First we consider $N = \infty$ case. In this case, an absorbing boundary is present at location 0. The evolution mechanism is described as follows:

Step 1. Initialize the system $\varphi \in \Phi$ at location m.

Step 2. (a) Perform one step time evolution. (b) Measure the system to see where it is or is not at location 0.

Step 3. If the result of measurement revealed that the system was at location 0, then terminate the process, otherwise repeat step 2.

In this setting, let $\Xi_n^{(\infty,m)}$ be the sum over possible paths for which the particle first hits 0 at time n starting from m. For example,

$$\Xi_5^{(\infty,1)} = P^2QPQ + P^3Q^2 = (ab^2c + a^2bd)R. \tag{6.2.3}$$

The probability that the particle first hits 0 at time n starting from m is

$$P_n^{(\infty,m)}(\varphi) = ||\Xi_n^{(\infty,m)}\varphi||^2. \tag{6.2.4}$$

So the probability that the particle hits 0 starting from m is

$$P^{(\infty,m)}(\varphi) = \sum_{n=0}^{\infty} P_n^{(\infty,m)}(\varphi).$$

Next we consider $N < \infty$ case. This case is similar to the $N = \infty$ case, except that two absorbing boundaries are present at locations 0 and N as follows:

Step 1. Initialize the system $\varphi \in \Phi$ at location m.

Step 2. (a) Perform one step time evolution. (b) Measure the system to see where it is or is not at location 0. (c) Measure the system to see where it is or is not at location N.

Step 3. If the result of either measurement revealed that the system was either at location 0 or location N, then terminate the process, otherwise repeat step 2.

Let $\Xi_n^{(N,m)}$ be the sum over possible paths for which the particle first hits 0 at time n starting from m before it arrives at N. For example,

$$\Xi_5^{(3,1)} = P^2QPQ = ab^2cR.$$

In a similar way, we can define $P_n^{(N,m)}(\varphi)$ and $P^{(N,m)}(\varphi)$.

6.3 Facts for the Classical and Quantum Cases

In this section we review some results and conjectures on absorption problems related to this chapter for both classical and quantum walks in one dimension.

First we review the classical case. As we described in Section 6.1, $P^{(N,m)} = P(T_0 < T_N)$ denotes the probability that the particle hits 0 starting from m

before it arrives at N. We may use conditional probabilities to see that $P^{(N,m)}$ satisfies the following difference equation:

$$P^{(N,m)} = pP^{(N,m-1)} + qP^{(N,m+1)} \qquad (1 \le m \le N-1), \tag{6.3.5}$$

with boundary conditions:

$$P^{(N,0)} = 1, \quad P^{(N,N)} = 0. \tag{6.3.6}$$

The solution of such a difference equation is given by

$$P^{(N,m)} = 1 - \frac{m}{N} \qquad if \quad p = 1/2, \tag{6.3.7}$$

$$P^{(N,m)} = \frac{(p/q)^m - (p/q)^N}{1-(p/q)^N} \qquad if \quad p \neq 1/2, \tag{6.3.8}$$

for any $0 \le m \le N$. Therefore, when $N = \infty$, we see that

$$P^{(\infty,m)} = 1 \qquad if \quad 1/2 \le p \le 1, \tag{6.3.9}$$

$$P^{(\infty,m)} = (p/q)^m \qquad if \quad 0 \le p < 1/2. \tag{6.3.10}$$

Furthermore,

$$\lim_{m\to\infty} P^{(\infty,m)} = 1 \qquad if \quad 1/2 \le p \le 1, \tag{6.3.11}$$

$$\lim_{m\to\infty} P^{(\infty,m)} = 0 \qquad if \quad 0 \le p < 1/2. \tag{6.3.12}$$

Let T_0 be the first hitting time to 0. We consider the conditional expectation of T_0 starting from $m = 1$ given the event $\{T_0 < \infty\}$, that is, $E^{(\infty,1)}(T_0|T_0 < \infty) = E^{(\infty,1)}(T_0; T_0 < \infty)/P^{(\infty,1)}(T_0 < \infty) = E^{(\infty,1)}(T_0; T_0 < \infty)/P^{(\infty,1)}$. Then

$$E^{(\infty,1)}(T_0|T_0 < \infty) = \frac{2p}{\sqrt{1-4pq}} - 1 \qquad if \quad 1/2 < p \le 1,$$

$$E^{(\infty,1)}(T_0|T_0 < \infty) = \infty \qquad if \quad p = 1/2,$$

$$E^{(\infty,1)}(T_0|T_0 < \infty) = \frac{2q}{\sqrt{1-4pq}} - 1 \qquad if \quad 0 \le p < 1/2.$$

Next we review the quantum case. In the case of $U = H$ (the Hadamard walk), when $N = \infty$, that is, when the state space is $\{0, 1, \ldots, \}$ case, Ambainis et al. (2001) proved

$$P^{(\infty,1)}({}^T[0,1]) = P^{(\infty,1)}({}^T[1,0]) = \frac{2}{\pi}, \tag{6.3.13}$$

and Bach et al. (2002) showed

$$\lim_{m\to\infty} P^{(\infty,m)}(\varphi) = \left(\frac{1}{2}\right)|\alpha|^2 + \left(\frac{2}{\pi} - \frac{1}{2}\right)|\beta|^2 + 2\left(\frac{1}{\pi} - \frac{1}{2}\right)\Re(\overline{\alpha}\beta).$$

for any initial qubit state $\varphi = {}^T[\alpha,\beta] \in \Phi$. Furthermore, in the case of $U = \widehat{H}(\rho)$, Bach et al. (2002) gave

$$\lim_{m\to\infty} P^{(\infty,m)}({}^T[0,1]) = \frac{\rho}{1-\rho}\left(\frac{\cos^{-1}(1-2\rho)}{\pi} - 1\right) + \frac{2}{\pi\sqrt{1/\rho - 1}},$$
$$\lim_{m\to\infty} P^{(\infty,m)}({}^T[1,0]) = \frac{\cos^{-1}(1-2\rho)}{\pi}.$$

The second result was conjectured by Yamasaki, Kobayashi, and Imai (2002).

When N is finite, the following conjecture by Ambainis et al. (2001) is still open for the $U = H$ case:

$$P^{(N+1,1)}({}^T[0,1]) = \frac{2P^{(N,1)}({}^T[0,1]) + 1}{2P^{(N,1)}({}^T[0,1]) + 2} \quad (N \geq 1), \qquad P^{(1,1)}({}^T[0,1]) = 0.$$

Solving the above recurrence gives

$$P^{(N,1)}({}^T[0,1]) = \frac{1}{\sqrt{2}} \times \frac{(3+2\sqrt{2})^{N-1} - 1}{(3+2\sqrt{2})^{N-1} + 1} \quad (N \geq 1). \tag{6.3.14}$$

However in contrast with $P^{(\infty,1)}({}^T[0,1]) = 2/\pi$, Ambainis et al. (2001) proved

$$\lim_{N\to\infty} P^{(N,1)}({}^T[0,1]) = 1/\sqrt{2}.$$

It should be noted that $P^{(\infty,m)} = \lim_{N\to\infty} P^{(N,m)}$ for any $0 \leq m \leq N$ in the classical case (see (6.3.7) - (6.3.10)).

We are not aware of results concerning $E^{(\infty,1)}(T_0|T_0 < \infty)$ having been published, however we will give such a result in the next section.

6.4 Results

In the first half of this section, we consider the general setting including a hitting time to N before it arrives at 0 or a hitting time to 0 before it arrives at N, when N is finite. In the case of $N = \infty$, a similar argument holds, so we will omit it here.

Noting that $\{P, Q, R, S\}$ is a basis of $M_2(\mathbb{C})$, $\Xi_n^{(N,m)}$ can be written as

$$\Xi_n^{(N,m)} = p_n^{(N,m)} P + q_n^{(N,m)} Q + r_n^{(N,m)} R + s_n^{(N,m)} S.$$

Therefore (6.2.4) implies

$$P_n^{(N,m)}(\varphi) = ||\Xi_n^{(N,m)}\varphi||^2 = C_1(n)|\alpha|^2 + C_2(n)|\beta|^2 + 2\Re(C_3(n)\overline{\alpha}\beta),$$

where $\Re(z)$ is the real part of $z \in \mathbb{C}$, $\varphi = {}^T[\alpha, \beta] \in \Phi$ and

$$\begin{aligned} C_1(n) &= |ap_n^{(N,m)} + cr_n^{(N,m)}|^2 + |as_n^{(N,m)} + cq_n^{(N,m)}|^2, \\ C_2(n) &= |bp_n^{(N,m)} + dr_n^{(N,m)}|^2 + |bs_n^{(N,m)} + dq_n^{(N,m)}|^2, \\ C_3(n) &= \overline{(ap_n^{(N,m)} + cr_n^{(N,m)})}(bp_n^{(N,m)} + dr_n^{(N,m)}) \\ &\qquad + \overline{(as_n^{(N,m)} + cq_n^{(N,m)})}(bs_n^{(N,m)} + dq_n^{(N,m)}). \end{aligned}$$

From now on we assume $N \geq 3$. Noting the definition of $\Xi_n^{(N,m)}$, we see that for $1 \leq m \leq N-1$,

$$\Xi_n^{(N,m)} = \Xi_{n-1}^{(N,m-1)} P + \Xi_{n-1}^{(N,m+1)} Q.$$

The above equation is a quantum version of the difference equation, i.e., (6.3.5) for the classical random walk. Then we have

$$\begin{aligned} p_n^{(N,m)} &= ap_{n-1}^{(N,m-1)} + cr_{n-1}^{(N,m-1)}, \\ q_n^{(N,m)} &= dq_{n-1}^{(N,m+1)} + bs_{n-1}^{(N,m+1)}, \\ r_n^{(N,m)} &= bp_{n-1}^{(N,m+1)} + dr_{n-1}^{(N,m+1)}, \\ s_n^{(N,m)} &= cq_{n-1}^{(N,m-1)} + as_{n-1}^{(N,m-1)}. \end{aligned}$$

Next we consider boundary condition related to (6.3.6) in the classical case. When $m = N$,

$$P_0^{(N,N)}(\varphi) = ||\Xi_0^{(N,N)} \varphi||^2 = 0,$$

for any $\varphi \in \Phi$. So we take $\Xi_0^{(N,N)} = O_2$, i.e.,

$$p_0^{(N,N)} = q_0^{(N,N)} = r_0^{(N,N)} = s_0^{(N,N)} = 0.$$

If $m = 0$, then

$$P_0^{(N,0)}(\varphi) = ||\Xi_0^{(N,0)} \varphi||^2 = 1,$$

for any $\varphi \in \Phi$. So we choose $\Xi_0^{(N,0)} = I_2$. From (6.2.2), we have

$$p_0^{(N,0)} = \overline{a}, \ \ q_0^{(N,0)} = \overline{d}, \ \ r_0^{(N,0)} = \overline{c}, \ \ s_0^{(N,0)} = \overline{b}.$$

Let

$$v_n^{(N,m)} = \begin{bmatrix} p_n^{(N,m)} \\ r_n^{(N,m)} \end{bmatrix}, \quad w_n^{(N,m)} = \begin{bmatrix} q_n^{(N,m)} \\ s_n^{(N,m)} \end{bmatrix}.$$

Then we see that for $n \geq 1$ and $1 \leq m \leq N-1$,

$$v_n^{(N,m)} = \begin{bmatrix} a & c \\ 0 & 0 \end{bmatrix} v_{n-1}^{(N,m-1)} + \begin{bmatrix} 0 & 0 \\ b & d \end{bmatrix} v_{n-1}^{(N,m+1)}, \qquad (6.4.15)$$

$$w_n^{(N,m)} = \begin{bmatrix} 0 & 0 \\ c & a \end{bmatrix} w_{n-1}^{(N,m-1)} + \begin{bmatrix} d & b \\ 0 & 0 \end{bmatrix} w_{n-1}^{(N,m+1)}, \qquad (6.4.16)$$

and for $1 \le m \le N$,

$$v_0^{(N,0)} = \begin{bmatrix} \overline{a} \\ \overline{c} \end{bmatrix}, \quad v_0^{(N,m)} = \begin{bmatrix} 0 \\ 0 \end{bmatrix},$$
$$w_0^{(N,0)} = \begin{bmatrix} \overline{d} \\ \overline{b} \end{bmatrix}, \quad w_0^{(N,m)} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

Moreover,

$$v_n^{(N,0)} = v_n^{(N,N)} = w_n^{(N,0)} = w_n^{(N,N)} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (n \ge 1).$$

From now on we focus on $1 \le m \le N-1$ case. So we consider only $n \ge 1$. Moreover from the definition of $\Xi_n^{(N,m)}$, it is easily shown that there exist only two types of paths, that is, $P \dots P$ and $P \dots Q$. Therefore we see that $q_n^{(N,m)} = s_n^{(N,m)} = 0$ $(n \ge 1)$. So we have

Lemma 6.1.

$$P^{(N,m)}(\varphi) = \sum_{n=1}^{\infty} P_n^{(N,m)}(\varphi),$$
$$P_n^{(N,m)}(\varphi) = C_1(n)|\alpha|^2 + C_2(n)|\beta|^2 + 2\Re(C_3(n)\overline{\alpha}\beta),$$

where $\varphi = {}^T[\alpha, \beta] \in \Phi$ *and*

$$C_1(n) = |ap_n^{(N,m)} + cr_n^{(N,m)}|^2,$$
$$C_2(n) = |bp_n^{(N,m)} + dr_n^{(N,m)}|^2,$$
$$C_3(n) = \overline{(ap_n^{(N,m)} + cr_n^{(N,m)})}(bp_n^{(N,m)} + dr_n^{(N,m)}).$$

To solve $P^{(N,m)}(\varphi)$, we introduce generating functions of $p_n^{(N,m)}$ and $r_n^{(N,m)}$ as follows:

$$p^{(N,m)}(z) = \sum_{n=1}^{\infty} p_n^{(N,m)} z^n,$$
$$r^{(N,m)}(z) = \sum_{n=1}^{\infty} r_n^{(N,m)} z^n.$$

By (6.4.15), we have

$$p^{(N,m)}(z) = azp^{(N,m-1)}(z) + czr^{(N,m-1)}(z),$$
$$r^{(N,m)}(z) = bzp^{(N,m+1)}(z) + dzr^{(N,m+1)}(z).$$

Solving these, we see that both $p^{(N,m)}(z)$ and $r^{(N,m)}(z)$ satisfy the same recurrence:

$$dp^{(N,m+2)}(z) - \left(\triangle z + \frac{1}{z}\right) p^{(N,m+1)}(z) + ap^{(N,m)}(z) = 0,$$
$$dr^{(N,m+2)}(z) - \left(\triangle z + \frac{1}{z}\right) r^{(N,m+1)}(z) + ar^{(N,m)}(z) = 0.$$

From the characteristic equations with respect to the above recurrences, we have the same roots: if $a \neq 0$, then

$$\lambda_{\pm} = \frac{\triangle z^2 + 1 \mp \sqrt{\triangle^2 z^4 + 2\triangle(1-2|a|^2)z^2 + 1}}{2\triangle \overline{a} z},$$

where $\triangle = \det U = ad - bc$.

From now on we consider mainly $U = H$ (the Hadamard walk) with $N = \infty$. Remark that the definition of $\Xi_n^{(\infty,1)}$ gives $p_n^{(\infty,1)} = 0 (n \geq 2)$ and $p_1^{(\infty,1)} = 1$. So we have $p^{(\infty,1)}(z) = z$. Moreover noting $\lim_{m\to\infty} p^{(\infty,m)}(z) < \infty$, the following explicit form is obtained:

$$p^{(\infty,m)}(z) = z\lambda_+^{m-1},$$
$$r^{(\infty,m)}(z) = \frac{-1+\sqrt{z^4+1}}{z}\lambda_+^{m-1},$$

where

$$\lambda_{\pm} = \frac{z^2 - 1 \pm \sqrt{z^4+1}}{\sqrt{2}z}.$$

Therefore for $m = 1$,

$$r^{(\infty,1)}(z) = \frac{-1+\sqrt{z^4+1}}{z}.$$

From the above equation and the definition of the hypergeometric series ${}_2F_1(a,b;c;z)$, we have

$$\sum_{n=1}^{\infty} (r_n^{(\infty,1)})^2 z^n = \sum_{n=1}^{\infty} \binom{1/2}{n}^2 z^{4n-1} = \frac{{}_2F_1(-1/2,-1/2;1;z^4) - 1}{z}.$$

On the other hand, it should be noted that

$${}_2F_1(a,b;c;1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} \qquad (\Re(a+b-c) < 0),$$

where $\Gamma(z)$ is the gamma function defined by

$$\Gamma(z) = \int_0^\infty e^{-t} t^{z-1}\, dt \qquad (\Re(z) > 0).$$

Therefore

$$\sum_{n=1}^{\infty} (r_n^{(\infty,1)})^2 = \frac{\Gamma(1)\Gamma(2)}{\Gamma(3/2)^2} - 1 = \frac{4}{\pi} - 1,$$

since $\Gamma(1) = \Gamma(2) = 1$ and $\Gamma(3/2) = \sqrt{\pi}/2$. By Lemma 6.1,

$$P^{(\infty,1)}(\varphi) = \sum_{n=1}^{\infty} \left[\frac{1}{2} \left\{ (p_n^{(\infty,1)})^2 + (r_n^{(\infty,1)})^2 \right\} \right.$$
$$\left. + p_n^{(\infty,1)} r_n^{(\infty,1)} (|\alpha|^2 - |\beta|^2) + \frac{1}{2} \left\{ (p_n^{(\infty,1)})^2 - (r_n^{(\infty,1)})^2 \right\} (\alpha\bar{\beta} + \bar{\alpha}\beta) \right].$$

Note that $p_n^{(\infty,1)} r_n^{(\infty,1)} = 0$ $(n \geq 1)$, since $p_n^{(\infty,1)} = 0\, (n \geq 2)$, $p_1^{(\infty,1)} = 1$ and $r_1^{(\infty,1)} = 0$. So we have

$$P^{(\infty,1)}(\varphi) = \frac{2}{\pi} + 2\left(1 - \frac{2}{\pi}\right) \Re(\overline{\alpha}\beta), \tag{6.4.17}$$

for any initial qubit state $\varphi = {}^T[\alpha, \beta] \in \Phi$. This result is a generalization of (6.3.13) given by Ambainis et al. (2001). From (6.4.17), we get the range of $P^{(\infty,1)}(\varphi)$:

$$\frac{4-\pi}{\pi} \leq P^{(\infty,1)}(\varphi) \leq 1.$$

The equality holds in the following cases:

$$P^{(\infty,1)}(\varphi) = 1 \text{ iff } \varphi = \frac{e^{i\theta}}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \text{ and } P^{(\infty,1)}(\varphi) = \frac{4-\pi}{\pi} \text{ iff } \varphi = \frac{e^{i\theta}}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix},$$

where $0 \leq \theta < 2\pi$.

Moreover we consider the conditional expectation of the first hitting time to 0 starting from $m = 1$ given an event $\{T_0 < \infty\}$, that is, $E^{(\infty,1)}(T_0 | T_0 < \infty) = E^{(\infty,1)}(T_0; T_0 < \infty)/P^{(\infty,1)}(T_0 < \infty)$. Let

$$f(z) = \sum_{n=1}^{\infty} (r_n^{(\infty,1)})^2 z^n \left(= \frac{{}_2F_1(-1/2, -1/2; 1; z^4) - 1}{z} \right).$$

In this case we have to know the value of $f'(1)$. It should be noted that

$$\frac{d}{dz} \left({}_2F_1(a, b; c; g(z)) \right) = \left(\frac{ab}{c} \right) {}_2F_1(a+1, b+1; c+1; g(z)) g'(z).$$

The above formula gives

$$f'(z) = \frac{z^4 {}_2F_1(1/2, 1/2; 2; z^4) - {}_2F_1(-1/2, -1/2; 1; z^4) + 1}{z^2}.$$

Moreover noting

$${}_2F_1(-1/2, -1/2; 1; 1) = {}_2F_1(1/2, 1/2; 2; 1) = \frac{4}{\pi},$$

we have $f'(1) = 1$. Therefore the desired conclusion is obtained:

$$E^{(\infty,1)}(T_0 | T_0 < \infty) = \frac{\sum_{n=1}^{\infty} n P^{(\infty,1)}(T_0 = n)}{\sum_{n=1}^{\infty} P^{(\infty,1)}(T_0 = n)} = \frac{1}{P^{(\infty,1)}(\varphi)},$$

since

$$\begin{aligned}
&\sum_{n=1}^{\infty} n P^{(\infty,1)}(T_0 = n) \\
&= \sum_{n=1}^{\infty} n \left[\frac{1}{2} \left\{ (p_n^{(\infty,1)})^2 + (r_n^{(\infty,1)})^2 \right\} + \frac{1}{2} \left\{ (p_n^{(\infty,1)})^2 - (r_n^{(\infty,1)})^2 \right\} (\alpha\bar{\beta} + \bar{\alpha}\beta) \right] \\
&= \frac{1}{2}\{1 + f'(1)\} + \frac{1}{2}\{1 - f'(1)\}(\alpha\bar{\beta} + \bar{\alpha}\beta) = 1.
\end{aligned}$$

In a similar way we see that $f''(1) = \infty$ implies

$$E^{(\infty,1)}((T_0)^2 | T_0 < \infty) = \infty,$$

so the ℓ-th moment $E^{(\infty,1)}((T_0)^\ell | T_0 < \infty)$ diverges for $\ell \geq 2$.

Next we consider the finite N case. Then $p^{(N,m)}(z)$ and $r^{(N,m)}(z)$ satisfy

$$\begin{aligned}
p^{(N,m)}(z) &= A_z \lambda_+^{m-1} + B_z \lambda_-^{m-1}, \\
r^{(N,m)}(z) &= C_z \lambda_+^{m-N+1} + D_z \lambda_-^{m-N+1},
\end{aligned}$$

since $\lambda_+ \lambda_- = -1$.

All we have to do is to determine the coefficients A_z, B_z, C_z, D_z by using the boundary conditions: $p^{(N,1)}(z) = z$ and $r^{(N,N-1)}(z) = 0$ come from the definition of $\Xi_n^{(N,m)}$. The boundary conditions imply $C_z + D_z = 0$ and $A_z + B_z = z$, so we see

$$p^{(N,m)}(z) = \left(\frac{z}{2} + E_z\right) \lambda_+^{m-1} + \left(\frac{z}{2} - E_z\right) \lambda_-^{m-1}, \tag{6.4.18}$$

$$r^{(N,m)}(z) = C_z (\lambda_+^{m-N+1} - \lambda_-^{m-N+1}), \tag{6.4.19}$$

where $E_z = A_z - z/2 = z/2 - B_z$.

To obtain E_z and C_z, we use $r^{(N,1)}(z) = (p^{(N,2)}(z) - r^{(N,2)}(z))z/\sqrt{2}$ and $r^{(N,N-2)}(z) = (p^{(N,N-1)}(z) - r^{(N,N-1)}(z))z/\sqrt{2} = p^{(N,N-1)}(z)z/\sqrt{2}$. Therefore

$$C_z(\lambda_+ - \lambda_-) = \frac{z}{\sqrt{2}}\left\{\left(\frac{z}{2} + E_z\right)\lambda_+^{N-2} + \left(\frac{z}{2} - E_z\right)\lambda_-^{N-2}\right\},$$

$$C_z(\lambda_+^{N-2} - \lambda_-^{N-2}) = \frac{z}{\sqrt{2}}\Bigg\{\left(\frac{z}{2} + E_z\right)(-1)^{N-1}\lambda_+ + \left(\frac{z}{2} - E_z\right)(-1)^{N-1}\lambda_- + C_z(\lambda_+^{N-3} - \lambda_-^{N-3})\Bigg\}.$$

Solving the above equations gives

$$C_z = \frac{z^2}{\sqrt{2}}(-1)^{N-2}(\lambda_+^{N-3} - \lambda_-^{N-3}) \times\Bigg\{(\lambda_+^{N-2} - \lambda_-^{N-2})^2 - \frac{z}{\sqrt{2}}(\lambda_+^{N-2} - \lambda_-^{N-2})(\lambda_+^{N-3} - \lambda_-^{N-3}) -(-1)^{N-3}(\lambda_+ - \lambda_-)^2\Bigg\}^{-1}, \qquad (6.4.20)$$

$$E_z = -\frac{z}{2(\lambda_+^{N-2} - \lambda_-^{N-2})}\Bigg[2(-1)^{N-3}(\lambda_+ - \lambda_-)(\lambda_+^{N-3} - \lambda_-^{N-3}) \times\Bigg\{(\lambda_+^{N-2} - \lambda_-^{N-2})^2 - \frac{z}{\sqrt{2}}(\lambda_+^{N-2} - \lambda_-^{N-2})(\lambda_+^{N-3} - \lambda_-^{N-3}) -(-1)^{N-3}(\lambda_+ - \lambda_-)^2\Bigg\}^{-1} + (\lambda_+^{N-2} + \lambda_-^{N-2})\Bigg]. \qquad (6.4.21)$$

By Lemma 6.1, we obtain

Theorem 6.2.

$$P^{(N,m)}(\varphi) = C_1|\alpha|^2 + C_2|\beta|^2 + 2\Re(C_3\overline{\alpha}\beta),$$

where $\varphi = {}^T[\alpha, \beta] \in \Phi$ *and*

$$C_1 = \frac{1}{2\pi}\int_0^{2\pi} |ap^{(N,m)}(e^{i\theta}) + cr^{(N,m)}(e^{i\theta})|^2 d\theta,$$
$$C_2 = \frac{1}{2\pi}\int_0^{2\pi} |bp^{(N,m)}(e^{i\theta}) + dr^{(N,m)}(e^{i\theta})|^2 d\theta,$$
$$C_3 = \frac{1}{2\pi}\int_0^{2\pi} \overline{(ap^{(N,m)}(e^{i\theta}) + cr^{(N,m)}(e^{i\theta}))}(bp^{(N,m)}(e^{i\theta}) + dr^{(N,m)}(e^{i\theta}))d\theta,$$

with $a = b = c = -d = 1/\sqrt{2}$, *here* $p^{(N,m)}(z)$ *and* $r^{(N,m)}(z)$ *satisfy (6.4.18) and (6.4.19), and* C_z *and* E_z *satisfy (6.4.20) and (6.4.21).*

Therefore to compute $P^{(N,m)}(\varphi)$, we need to obtain both $p^{(N,m)}(z)$ and $r^{(N,m)}(z)$, and calculate the above $C_i (i = 1, 2, 3)$ explicitely.

Here we consider $U = H$ (the Hadamard walk), $\varphi = {}^T[\alpha, \beta]$ and $m = 1$. From Theorem 6.2, noting that $p^{(N,1)}(z) = z$ for any $N \geq 2$, we have

Corollary 6.3. *For $N \geq 2$,*

$$P^{(N,1)}(\varphi) = \frac{1}{2}\left(1 + \frac{1}{2\pi}\int_0^{2\pi} |r^{(N,1)}(e^{i\theta})|^2 d\theta\right)(1 + 2\Re(\overline{\alpha}\beta)),$$

where $r^{(2,1)}(z) = 0$, $r^{(3,1)}(z) = z^3/(2 - z^2)$,

$$r^{(4,1)}(z) = \frac{z^3(1-z^2)}{2 - 2z^2 + z^4},$$
$$r^{(5,1)}(z) = \frac{z^3(2 - 3z^2 + 2z^4)}{4 - 6z^2 + 5z^4 - 2z^6},$$
$$r^{(6,1)}(z) = \frac{2z^3(1-z^2)(1-z^2+z^4)}{4 - 8z^2 + 9z^4 - 6z^6 + 2z^8},$$

and in general for $N \geq 4$

$$r^{(N,1)}(z) = -\frac{z^2 J_{N-3}(z) J_{N-4}(z)}{\sqrt{2}(J_{N-3}(z))^2 - zJ_{N-3}(z)J_{N-4}(z) - \sqrt{2}(-1)^{N-3}},$$

with

$$J_n(z) = \sum_{\ell=0}^{n} \lambda_+^{\ell} \lambda_-^{n-\ell}, \quad \lambda_+ + \lambda_- = \sqrt{2}\left(z - \frac{1}{z}\right), \quad \lambda_+\lambda_- = -1.$$

In particular, when $\varphi = {}^T[0,1] = |R\rangle$, $m = 1$ and $N = 2, \ldots, 6$, Corollary 6.3 gives

$$P^{(2,1)}({}^T[0,1]) = \frac{1}{2}, \quad P^{(3,1)}({}^T[0,1]) = \frac{2}{3}, \quad P^{(4,1)}({}^T[0,1]) = \frac{7}{10},$$
$$P^{(5,1)}({}^T[0,1]) = \frac{12}{17}, \quad P^{(6,1)}({}^T[0,1]) = \frac{41}{58}.$$

It is easily checked that the above values $P^{(N,1)}({}^T[0,1])\,(N = 2, \ldots, 6)$ satisfy the conjecture given by (6.3.14).

6.5 Summary

In this chapter we consider absorption problems for quantum walks on $\{0, 1, \ldots, N\}$ for both $N < \infty$ and $N = \infty$ cases. Here we summarize the results.

First we describe $N = \infty$ case. In this case, we have

$$P^{(\infty,1)}(\varphi) = \frac{2}{\pi} + 2\left(1 - \frac{2}{\pi}\right)\Re(\overline{\alpha}\beta),$$

and

$$E^{(\infty,1)}(T_0 | T_0 < \infty) = \frac{1}{P^{(\infty,1)}(\varphi)},$$
$$E^{(\infty,1)}((T_0)^\ell | T_0 < \infty) = \infty \quad (\ell \geq 2),$$

for any initial qubit state $\varphi = {}^T[\alpha, \beta] \in \varPhi$, where $P^{(\infty,1)}(\varphi)$ is the probability that the particle first hits location 0 starting from location 1 and $E^{(\infty,1)}((T_0)^\ell | T_0 < \infty)$ is the conditional ℓ-th moment of T_0 starting from location 1 given $\{T_0 < \infty\}$ where T_0 is the first hitting time to location 0.

Next we describe $N < \infty$ case. In this case, we obtain the following explicit expression of $P^{(N,1)}(\varphi)$:

$$P^{(N,1)}(\varphi) = \frac{1}{2}\left(1 + \frac{1}{2\pi}\int_0^{2\pi} |r^{(N,1)}(e^{i\theta})|^2 d\theta\right)(1 + 2\Re(\overline{\alpha}\beta)),$$

for any initial qubit state $\varphi = {}^T[\alpha, \beta] \in \varPhi$, where $P^{(N,1)}(\varphi)$ is the probability that the particle first hits location 0 starting from location 1 before it arrives at location N, and $r^{(N,1)}(z)$ is given by Corollary 6.3 in the previous section.

The above result guarantees that the conjecture presented by Ambainis et al. (see (6.3.14)) is true for $N = 2, \ldots, 6$. However, their conjecture is still open for arbitrary N. So one of the future interesting problems is to find and prove an explicit formula like (6.3.14) for any $N(\leq \infty)$, $m \in \{1, \ldots, N-1\}$, and $\varphi \in \varPhi$.

Part II: Continuous-Time Quantum Walks

7 One-Dimensional Lattice

7.1 Introduction

The quantum walk can be considered as a quantum analog of the classical random walk. However there are some differences between them. For the discrete-time symmetric *classical* random walk Y_t^o starting from the origin, the central limit theorem shows that $Y_t^o/\sqrt{t} \to e^{-x^2/2}dx/\sqrt{2\pi}$ as $t \to \infty$. The same weak limit theorem holds for the continuous-time classical symmetric random walk. On the other hand, concerning a *discrete-time* quantum walk $X_t^{(d)}$ with a symmetric distribution on the line, whose evolution is described by the Hadamard transformation, it was shown by the author (Konno (2002a, 2005a)) that the following weak limit theorem holds: $X_t^{(d)}/t \to dx/\pi(1-x^2)\sqrt{1-2x^2}$ as $t \to \infty$. This chapter presents a similar type of weak limit theorem for a *continuous-time* quantum walk $X_t^{(c)}$ on the line, $X_t^{(c)}/t \to dx/\pi\sqrt{1-x^2}$ as $t \to \infty$. Both limit density f unctions for quantum walks have two peaks at the two end points of the supports. This chapter deals also with the issue of the relationship between discrete and continuous-time quantum walks. This topic, subject of a long debate in the previous literature, is treated within the formalism of matrix representation and the limit distributions are exhaustively compared in the two cases.

As a corollary, we have the following result. Let $\sigma^c_{(d)}(t)$ (resp. $\sigma^c_{(c)}(t)$) be the standard deviation of the probability distribution for a discrete-time (resp. continuous-time) classical random walk on the line starting from the origin at time t. Similarly, $\sigma^q_{(d)}(t)$ (resp. $\sigma^q_{(c)}(t)$) denotes the standard deviation for a discrete-time (resp. continuous-time) quantum walk. Then, it is well known that $\sigma^c_{(d)}(t), \sigma^c_{(c)}(t) \asymp \sqrt{t}$, where $f(t) \asymp g(t)$ indicates that $f(t)/g(t) \to c_*(\neq 0)$ as $t \to \infty$. In contrast, $\sigma^q_{(d)}(t), \sigma^q_{(c)}(t) \asymp t$ holds. That is,

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the quantum walks spread over the line faster than the classical walks in the both discrete- and continuous-time cases. Results in this chapter appeared in Konno (2005c).

7.2 Model and Results

To define the continuous-time quantum walk on $\mathbb{Z}$, we introduce an $\infty \times \infty$ adjacency matrix of $\mathbb{Z}$ denoted by A as follows:

$$A = \begin{array}{c} \\ \vdots \\ -3 \\ -2 \\ -1 \\ 0 \\ +1 \\ +2 \\ \vdots \end{array} \begin{array}{c} \begin{array}{cccccccc} \dots & -3 & -2 & -1 & 0 & +1 & +2 & \dots \end{array} \\ \left(\begin{array}{cccccccc} \ddots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \dots & 0 & 1 & 0 & 0 & 0 & 0 & \dots \\ \dots & 1 & 0 & 1 & 0 & 0 & 0 & \dots \\ \dots & 0 & 1 & 0 & 1 & 0 & 0 & \dots \\ \dots & 0 & 0 & 1 & 0 & 1 & 0 & \dots \\ \dots & 0 & 0 & 0 & 1 & 0 & 1 & \dots \\ \dots & 0 & 0 & 0 & 0 & 1 & 0 & \dots \\ \dots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \ddots \end{array} \right) \end{array}.$$

The amplitude wave function of the walk at time t, Ψ_t, is defined by

$$\Psi_t = U_t \Psi_0,$$

where

$$U_t = e^{itA/2}.$$

Note that U_t is a unitary matrix. As initial state, we take

$$\Psi_0 = {}^T[\dots, 0, 0, 0, 1, 0, 0, 0, \dots].$$

Let $\Psi_t(x)$ be the amplitude wave function at location x at time t. The probability that the particle is at location x at time t, $P_t(x)$, is given by

$$P_t(x) = |\Psi_t(x)|^2.$$

There are various results for a walk on a cycle C_N, where $C_N = \{0, 1, \dots, N-1\}$ (see Adamczak et al. (2003), Ahmadi et al. (2003), Inui, Kasahara, Konishi, and Konno (2005)).

We will obtain an explicit form of U_t first. Our approach is based on a direct computation of the $\infty \times \infty$ matrix A without using its eigenvalues and eigenvectors in order to clarify between the continuous-time and discrete-time quantum walks, (another approach and the same explicit form can be found in Section III C of Childs et al. (2003)). Let $J_k(x)$ denote the Bessel function of the first kind of order k. As for the Bessel function, see Watson (1944) and Chapter 4 in Andrews, Askey, and Roy (1999).

Proposition 7.1. *In our setting, we have*

$$U_t = \begin{array}{c} \\ \vdots \\ -3 \\ -2 \\ -1 \\ 0 \\ +1 \\ +2 \\ \vdots \end{array} \begin{array}{c} \begin{array}{cccccccc} \ldots & -3 & -2 & -1 & 0 & +1 & +2 & \ldots \end{array} \\ \left(\begin{array}{cccccccc} \ddots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \ldots \\ \ldots & J_0(t) & iJ_1(t) & i^2J_2(t) & i^3J_3(t) & i^4J_4(t) & i^5J_5(t) & \ldots \\ \ldots & iJ_1(t) & J_0(t) & iJ_1(t) & i^2J_2(t) & i^3J_3(t) & i^4J_4(t) & \ldots \\ \ldots & i^2J_2(t) & iJ_1(t) & J_0(t) & iJ_1(t) & i^2J_2(t) & i^3J_3(t) & \ldots \\ \ldots & i^3J_3(t) & i^2J_2(t) & iJ_1(t) & J_0(t) & iJ_1(t) & i^2J_2(t) & \ldots \\ \ldots & i^4J_4(t) & i^3J_3(t) & i^2J_2(t) & iJ_1(t) & J_0(t) & iJ_1(t) & \ldots \\ \ldots & i^5J_5(t) & i^4J_4(t) & i^3J_3(t) & i^2J_2(t) & iJ_1(t) & J_0(t) & \ldots \\ \ldots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \ddots \end{array} \right) \end{array}.$$

That is, the (l,m) component of U_t is given by $i^{|l-m|}J_{|l-m|}(t)$.

From Proposition 7.1, looking at a column of U_t, we have immediately

Corollary 7.2. *The amplitude wave function of our model is given by*

$$\Psi_t = {}^T[\ldots, i^3J_3(t), i^2J_2(t), iJ_1(t), J_0(t), iJ_1(t), i^2J_2(t), i^3J_3(t), \ldots],$$

that is, $\Psi_t(x) = i^{|x|}J_{|x|}(t)$ for any location $x \in \mathbb{Z}$ and time $t \geq 0$.

Moreover, noting that $J_{-x}(t) = (-1)^x J_x(t)$ ((4.5.4) in Andrews, Askey, and Roy (1999)), we have

Corollary 7.3. *The probability distribution is*

$$P_t(x) = J^2_{|x|}(t) = J^2_x(t),$$

for any location $x \in \mathbb{Z}$ and time $t \geq 0$.

In fact, the following result (see (4.9.5) in Andrews, Askey, and Roy (1999)):

$$J_0^2(t) + 2\sum_{x=1}^{\infty} J_x^2(t) = 1$$

ensures that $\sum_{x=-\infty}^{\infty} P_t(x) = 1$ for any $t \geq 0$. Remark that the distribution is symmetric for any time, i.e., $P_t(x) = P_t(-x)$.

One of the interesting points of the result is as follows. Fix a positive integer r. We suppose that the unitary matrix $U^{(r)}$ has the following form:

$$
U^{(r)} = \begin{array}{c} \\ \vdots \\ -3 \\ -2 \\ -1 \\ 0 \\ +1 \\ +2 \\ \vdots \end{array}
\begin{array}{c} \begin{array}{cccccccc} \dots & -3 & -2 & -1 & 0 & +1 & +2 & \dots \end{array} \\
\left(\begin{array}{cccccccc}
\ddots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\
\dots & w_0 & w_1 & w_2 & w_3 & w_4 & w_5 & \dots \\
\dots & w_{-1} & w_0 & w_1 & w_2 & w_3 & w_4 & \dots \\
\dots & w_{-2} & w_{-1} & w_0 & w_1 & w_2 & w_3 & \dots \\
\dots & w_{-3} & w_{-2} & w_{-1} & w_0 & w_1 & w_2 & \dots \\
\dots & w_{-4} & w_{-3} & w_{-2} & w_{-1} & w_0 & w_1 & \dots \\
\dots & w_{-5} & w_{-4} & w_{-3} & w_{-2} & w_{-1} & w_0 & \dots \\
\dots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \ddots
\end{array}\right) \end{array},
$$

with $w_x \in \mathbb{C}$ $(x \in \mathbb{Z})$ and $w_s = 0$ for $|s| > r$. Then the *No-Go lemma* (see Meyer (1996)) shows that the only non-zero w_* have $|w_*| = 1$; that is, there exists no non-trivial, homogeneous finite-range model governed by the $U^{(r)}$. For example, when $r = 1$, we have "$|w_{-1}| = 1, w_0 = w_1 = 0$", "$|w_0| = 1, w_{-1} = w_1 = 0$", or "$|w_1| = 1, w_0 = w_{-1} = 0$". Thus, the model has a trivial probability distribution. However, our homogeneous, but *infinite-range* model has a non-trivial probability distribution given by squared Bessel functions (Corollary 7.3).

One of the open problems of quantum walks is to clarify a relation between discrete-time and continuous-time quantum walks (see Ambainis (2003), for example). To explain the reason, we introduce the following matrices as in Chapter 4 (see also Hamada, Konno, and Segawa (2005)):

$$
P_A = \begin{bmatrix} a & b \\ 0 & 0 \end{bmatrix}, \quad Q_A = \begin{bmatrix} 0 & 0 \\ c & d \end{bmatrix} \quad \text{and} \quad P_B = \begin{bmatrix} a & 0 \\ c & 0 \end{bmatrix}, \quad Q_B = \begin{bmatrix} 0 & b \\ 0 & d \end{bmatrix},
$$

where we assume that $U = P_j + Q_j$ $(j = A, B)$ is a 2×2 unitary matrix. Here we consider two types of the discrete-time case; one is A-type, the other is B-type. The precise definition is given in Chapter 4. Then the unitary matrix of the discrete-time quantum walk on the line is described as

$$
U^{(d)} = \begin{bmatrix}
\ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\dots & O & P_j & O & O & O & \dots \\
\dots & Q_j & O & P_j & O & O & \dots \\
\dots & O & Q_j & O & P_j & O & \dots \\
\dots & O & O & Q_j & O & P_j & \dots \\
\dots & O & O & O & Q_j & O & \dots \\
\dots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{bmatrix} \qquad \text{with} \qquad O = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix},
$$

for $j = A$ and B. The unitary matrix $U^{(d)}$ for the discrete-time case corresponds to U_t for our continuous-time case at time $t = 1$. More generally, $(U^{(d)})^n$ corresponds to U_n for $n = 0, 1, \ldots$. Once an explicit formula of U_t is obtained, the difference between continuous and discrete walks becomes clear. As we stated before, U_t has an infinite-range form. On the other hand, $U^{(d)}$

has a finite-range form. Moreover, we see that $U^{(d)}$ is not homogeneous. It is believed that the difference seems to be derived from the fact that discrete quantum walk has a coin but continuous quantum walk does not. However, the situation is not so simple, since the discrete-time case also does not necessarily need the coin (see Chapter 4 for more detailed discussion).

We define a continuous-time quantum walk on $\mathbb{Z}$ by X_t whose probability distribution is defined by $P(X_t = x) = P_t(x)$ for any location $x \in \mathbb{Z}$ and time $t \geq 0$. Note that it follows from Corollary 7.3 that $P_t(x) = J_x^2(t)$. Then we obtain a weak limit theorem for a continuous-time quantum walk on the line:

Theorem 7.4. *If* $t \to \infty$, *then*

$$\frac{X_t}{t} \quad \Rightarrow \quad Z^{(c)},$$

where $Z^{(c)}$ *has the following density:*

$$\frac{1}{\pi\sqrt{1-x^2}}\, I_{(-1,1)}(x) \qquad (x \in \mathbb{R}).$$

For a more general setting, Gottlieb (2005) obtained weak limit theorems for continuous-time quantum walks on $\mathbb{Z}$ by a different method. Note that

$$\int_{-1}^{1} \frac{x^{2m}}{\pi\sqrt{1-x^2}}\, dx = \frac{2}{\pi}\int_0^{\pi/2} \sin^{2m}\varphi\, d\varphi = \frac{(2m-1)!!}{(2m)!!}, \tag{7.2.1}$$

for $m = 1, 2, \ldots$, where $n!! = n(n-2)\cdot\cdots\cdot 5\cdot 3\cdot 1$, if n is odd, $= n(n-2)\cdot\cdots\cdot 6\cdot 4\cdot 2$, if n is even. From Proposition 7.1 and (7.2.1), we have

Corollary 7.5. *For* $m = 1, 2, \ldots,$

$$E((X_t/t)^{2m}) \quad \to \quad (2m-1)!!/(2m)!! \qquad (t \to \infty).$$

By this corollary, for the standard deviation of our walk, $\sigma^q_{(c)}(t)$, we see that

$$\sigma^q_{(c)}(t)/t \quad \to \quad 1/\sqrt{2} = 0.70710\ldots \qquad (t \to \infty).$$

We consider a *discrete-time* quantum walk $X_n^{(d)}$ with a symmetric distribution on the line, whose evolution is described by the Hadamard transformation, that is,

$$U = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

The walk is often called the Hadamard walk. In contrast with the continuous-time case, for the Hadamard walk, the following weak limit theorem holds (see Theorem 1.6 or Konno (2002a, 2005a)): If $n \to \infty$, then

$$\frac{X_n^{(d)}}{n} \quad \Rightarrow \quad Z^{(d)},$$

where $Z^{(d)}$ has the following density:

$$\frac{1}{\pi(1-x^2)\sqrt{1-2x^2}}\, I_{(-1/\sqrt{2},1/\sqrt{2})}(x) \qquad (x \in \mathbb{R}).$$

As a corollary, we have

$$\sigma^q_{(d)}(n)/n \quad \to \quad \sqrt{(2-\sqrt{2})/2} = 0.54119\ldots \qquad (n \to \infty).$$

Comparing with the discrete-time case, the scaling in our continuous-time case is same, but the limit density function is different. However, both density functions have some similar properties, for example, they have two peaks at the end points of the support.

7.3 Proof of Proposition 7.1

To begin with, A is rewritten as

$$A = \begin{array}{r} \\ \vdots \\ -1 \\ 0 \\ +1 \\ +2 \\ \vdots \end{array} \begin{array}{c} \begin{array}{cccccc} \ldots & -1 & 0 & +1 & +2 & \ldots \end{array} \\ \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \ldots & T & P & O & O & \ldots \\ \ldots & Q & T & P & O & \ldots \\ \ldots & O & Q & T & P & \ldots \\ \ldots & O & O & Q & T & \ldots \\ \ldots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \end{array}, \tag{7.3.2}$$

where

$$P = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \quad T = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad Q = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}.$$

The following algebraic relations are useful for some computations:

$$P^2 = Q^2 = O, \quad PT + TP = QT + TQ = I, \quad PQ + QP = T, \tag{7.3.3}$$

where O is 2×2 zero matrix and I is 2×2 unit matrix. From now on, for simplicity, (7.3.2) is written as

$$A = [\ldots, O, O, O, O, Q, T, P, O, O, O, O, O, \ldots].$$

A direct computation gives

$$\begin{aligned} A^2 &= [\ldots, O, O, O, O, I, 2I, I, O, O, O, O, \ldots], \\ A^4 &= [\ldots, O, O, O, I, 4I, 6I, 4I, I, O, O, O, \ldots], \\ A^6 &= [\ldots, O, O, I, 6I, 15I, 20I, 15I, 6I, I, O, O, \ldots]. \end{aligned}$$

It follows by induction that

$$A^{2n} = [\ldots, O, O, A_{-n}^{(2n)}, \ldots, A_{-1}^{(2n)}, A_0^{(2n)}, A_1^{(2n)}, \ldots, A_n^{(2n)}, O, O, \ldots],$$

where $A_k^{(2n)} = A_{-k}^{(2n)} = a_k^{(2n)} I$ and

$$a_k^{(2n)} = \binom{2n}{n-k},$$

for any $k = 0, 1, \ldots, n$. On the other hand, by using $A^{2n+1} = A^{2n} \times A$ and (7.3.3), we have

$$A^{2n+1} = [\ldots, O, A_{-(n+1)}^{(2n+1)}, \ldots, A_{-1}^{(2n+1)}, A_0^{(2n+1)}, A_1^{(2n+1)}, \ldots, A_{n+1}^{(2n+1)}, O, \ldots],$$

where

$$\begin{aligned}
&A_{-(n+1)}^{(2n+1)} = a_n^{(2n)} Q, \quad A_{-n}^{(2n+1)} = a_n^{(2n)} T + a_{n-1}^{(2n)} Q, \\
&A_{-(n-1)}^{(2n+1)} = (a_{n-1}^{(2n)} + a_n^{(2n)}) T + (a_{n-2}^{(2n)} - a_n^{(2n)}) Q, \ldots, \\
&A_{-1}^{(2n+1)} = (a_1^{(2n)} + a_2^{(2n)}) T + (a_0^{(2n)} - a_2^{(2n)}) Q, \quad A_0^{(2n+1)} = (a_0^{(2n)} + a_1^{(2n)}) T, \\
&A_1^{(2n+1)} = (a_1^{(2n)} + a_2^{(2n)}) T + (a_0^{(2n)} - a_2^{(2n)}) P, \ldots, \\
&A_n^{(2n+1)} = a_n^{(2n)} T + a_{n-1}^{(2n)} P, \quad A_{(n+1)}^{(2n+1)} = a_n^{(2n)} P.
\end{aligned}$$

The definition of U_t gives

$$\begin{aligned}
U_t = e^{itA/2} &= \sum_{n=0}^{\infty} \frac{\left(\frac{it}{2}\right)^n}{n!} A^n \\
&= \sum_{n=0}^{\infty} (-1)^n \frac{\left(\frac{t}{2}\right)^{2n}}{(2n)!} A^{2n} + i \sum_{n=0}^{\infty} (-1)^n \frac{\left(\frac{t}{2}\right)^{2n+1}}{(2n+1)!} A^{2n+1}.
\end{aligned}$$

Therefore we obtain $U_t = B(t) + iC(t)$, where

$$\begin{aligned}
B(t) &= [\ldots, B_{-k}, \ldots, B_{-1}, B_0, B_1, \ldots, B_k, \ldots], \\
C(t) &= [\ldots, C_{-k}, \ldots, C_{-1}, C_0, C_1, \ldots, C_k, \ldots],
\end{aligned}$$

with

$$B_k = B_{-k} = b_k I, \qquad b_k = \sum_{n=0}^{\infty} (-1)^n \frac{\left(\frac{t}{2}\right)^{2n}}{(2n)!} \binom{2n}{n-k} \quad (k = 0, 1, \ldots),$$

and

$$
\begin{aligned}
&C_{-k} = c_k I + d_k Q, \qquad C_k = c_k I + d_k P \quad (k = 0, 1, \ldots), \\
&c_k = \sum_{n=0}^{\infty} (-1)^n \frac{\left(\frac{t}{2}\right)^{2n+1}}{(2n+1)!} \left\{ \binom{2n}{n-k} + \binom{2n}{n-(k+1)} \right\} \quad (k = 0, 1, \ldots), \\
&d_0 = 0, \\
&d_k = \sum_{n=0}^{\infty} (-1)^n \frac{\left(\frac{t}{2}\right)^{2n+1}}{(2n+1)!} \left\{ \binom{2n}{n-(k-1)} + \binom{2n}{n-(k+1)} \right\} \quad (k = 1, 2, \ldots).
\end{aligned}
$$

Remark that

$$
J_k(x) = \left(\frac{x}{2}\right)^k \sum_{m=0}^{\infty} \frac{\left(\frac{ix}{2}\right)^{2m}}{(k+2m)!} \binom{k+2m}{m}, \tag{7.3.4}
$$

(see (4.9.5) in Andrews, Askey, and Roy (1999)). Finally, by using (7.3.4) and the following relation:

$$
\binom{2n}{k} + \binom{2n}{k-1} = \binom{2n+1}{k},
$$

we have the desired conclusion.

7.4 Proof of Theorem 7.4

We begin by stating the following result (see page 214 in Andrews, Askey, and Roy (1999)): suppose that a, b, and c are lengths of sides of a triangle and $c^2 = a^2 + b^2 - 2ab\cos\xi$. Then

$$
J_0(c) = \sum_{k=-\infty}^{\infty} J_k(a) J_k(b) e^{ik\xi}. \tag{7.4.5}
$$

If we set $t = a = b$ in (7.4.5), then

$$
J_0(t\sqrt{2(1-\cos\xi)}) = \sum_{k=-\infty}^{\infty} J_k^2(t) e^{ik\xi}. \tag{7.4.6}
$$

From (7.4.6), we see that the characteristic function of a continuous-time quantum walk on the line is given by

$$
E(e^{i\xi X_t}) = \sum_{k=-\infty}^{\infty} e^{ik\xi} J_k^2(t) = J_0(t\sqrt{2(1-\cos\xi)}). \tag{7.4.7}
$$

First we consider that t is a positive integer case, that is, $n(=t)=1,2,\ldots$. By using (7.4.7), we have

$$E(e^{i\xi X_n/n}) = J_0(n\,\sqrt{2(1-\cos(\xi/n))}) \to J_0(\xi),$$

as $n\to\infty$. To know the limit density function, we use the following expression of $J_0(x)$ (see (4.9.11) in Andrews, Askey, and Roy (1999));

$$J_0(\xi) = \frac{1}{\pi}\int_0^{\pi} \cos(\xi\sin\varphi)\,d\varphi = \frac{2}{\pi}\int_0^{\pi/2} \cos(\xi\sin\varphi)\,d\varphi. \qquad (7.4.8)$$

Taking $x=\sin\varphi$, we have

$$J_0(\xi) = \int_{-1}^{1} \cos(\xi x)\frac{1}{\pi\sqrt{1-x^2}}\,dx = \int_{-1}^{1} e^{i\xi x}\frac{1}{\pi\sqrt{1-x^2}}\,dx. \qquad (7.4.9)$$

By using (7.4.8), we get

$$|J_0(\xi)-J_0(0)| \le \frac{2}{\pi}\int_0^{\pi/2} |\cos(\xi\sin\varphi)-1|\,d\varphi.$$

From the bounded convergence theorem, we see that the limit $J_0(\xi)$ is continuous at $\xi=0$, since $\cos(\xi\sin\varphi)\to 1$ as $\xi\to 0$. Therefore, by the continuity theorem and (7.4.9), we conclude that if $n\to\infty$, then X_n/n converges weakly to a random variable whose density function is given by $1/\pi\sqrt{1-x^2}$ for $x\in(-1,1)$. That is, if $-1\le a<b\le 1$, then

$$P(a\le X_n/n\le b) \quad\to\quad \int_a^b \frac{1}{\pi\sqrt{1-x^2}}\,dx,$$

as $n\to\infty$. Next, to deal with values of t that are not integers, we want to show

$$\left|P(a\le X_t/t\le b) - P(a\le X_{[t]}/[t]\le b)\right| \quad\to\quad 0 \qquad (t\to\infty),$$

where $[x]$ denotes the integer part of x. However the rest of the proof is complicated, so we omit it (see Konno (2005c) for the detail).

7.5 Conclusion and Discussion

In contrast with the classical random walk for which the central limit theorem holds, we have shown a weak limit theorem $X_t^{(c)}/t \to dx/\pi\sqrt{1-x^2}\,(t\to\infty)$ for the continuous-time quantum walk on the line (Theorem 7.4). Interestingly, although the definition of the walk is very different from that of discrete-time one, the limit theorem resembles that of the discrete-time case, for example, the symmetric Hadamard walk: $X_n^{(d)}/n \to dx/\pi(1-x^2)\sqrt{1-2x^2}\ (n \to \infty)$.

Romanelli et al. (2004) investigated the continuum time limit for a discrete-time quantum walk on $\mathbb{Z}$ and obtained the position probability distribution. When the initial condition is given by $\tilde{a}_l(0) = \delta_{l,0}, \tilde{b}_l(0) \equiv 0$ in their notation for the Hadamard walk, the distribution becomes the following in our notation: $P_t^{(R)}(x) = J_x^2(t/\sqrt{2})$. More generally, we consider the time evolution given by the following unitary matrix:

$$U(\theta) = \begin{bmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{bmatrix},$$

where $\theta \in (0, \pi/2)$. Note that $\theta = \pi/4$ case is equivalent to the Hadamard walk. Then we have $P_t^{(R,\theta)}(x) = J_x^2(t\,\cos\theta)$. In this case, a similar argument in the proof of Theorem 7.4 implies that if $t \to \infty$, then

$$\frac{X_t^{(R,\theta)}}{t} \quad \Rightarrow \quad Z^{(R,\theta)},$$

where $Z^{(R,\theta)}$ has the following density function:

$$\frac{1}{\pi\sqrt{\cos^2\theta - x^2}}\, I_{(-\cos\theta,\cos\theta)}(x) \qquad (x \in \mathbb{R}).$$

Here $X_t^{(R,\theta)}$ denotes a continuous-time quantum walk whose probability distribution is given by $P_t^{(R,\theta)}(x)$. As a consequence, we obtain

$$E((X_t^{(R,\theta)}/t)^{2m}) \quad \to \quad \cos^{2m}\theta \times (2m-1)!!/(2m)!! \qquad (t \to \infty).$$

In particular, when $m = 1$, the limit $\cos^2\theta/2$ is consistent with (30) in Romanelli et al. (2004).

8 Tree

8.1 Introduction

In this chapter we consider a continuous-time quantum walk on a homogeneous tree in quantum probability theory. Results here appeared in Konno (2006a). The walk is defined by identifying the Hamiltonian of the system with a matrix related to the adjacency matrix of the tree.

Let $\mathbb{T}_M^{(p)}$ denote a homogeneous tree of degree p with M-generation. After we fix a root $o \in \mathbb{T}_M^{(p)}$, a stratification (distance partition) is introduced by the natural distance function in the following way:

$$\mathbb{T}_M^{(p)} = \bigcup_{k=0}^{M} V_k^{(p)}, \quad V_k^{(p)} = \{x \in \mathbb{T}_M^{(p)} : \partial(o,x) = k\}.$$

Here $\partial(x,y)$ stands for the length of the shortest path connecting x and y. Then

$$|V_0^{(p)}| = 1,\ |V_1^{(p)}| = p,\ |V_2^{(p)}| = p(p-1), \ldots, |V_k^{(p)}| = p(p-1)^{k-1}, \ldots,$$

where $|A|$ is the number of elements in a set A. The total number of points in M-generation, $|\mathbb{T}_M^{(p)}|$, is $p(p-1)^M - (p-1)$.

Let $H_M^{(p)}$ be a $|\mathbb{T}_M^{(p)}| \times |\mathbb{T}_M^{(p)}|$ symmetric matrix given by the adjacency matrix of the tree $\mathbb{T}_M^{(p)}$. The matrix is treated as the Hamiltonian of the quantum system. The (i,j) component of $H_M^{(p)}$ denotes $H_M^{(p)}(i,j)$ for $i,j \in \{0,1,\ldots,|\mathbb{T}_M^{(p)}|-1\}$. In our case, the diagonal component of $H_M^{(p)}$ is always zero, i.e., $H_M^{(p)}(i,i) = 0$ for any i. On the other hand, the diagonal component of corresponding matrix $H_{M,MB}^{(p)}$ investigated in Mülken, Bierbaum, and Blumen (2006) for $p=3$ is not zero. For example, $H_{1,MB}^{(3)}(0,0) = -3$, $H_{1,MB}^{(3)}(1,1) = H_{1,MB}^{(3)}(2,2) = H_{1,MB}^{(3)}(3,3) = -1$.

The evolution of the continuous-time quantum walk on the tree of M-generation, $\mathbb{T}_M^{(p)}$, is governed by the following unitary matrix:

$$U_M^{(p)}(t) = e^{itH_M^{(p)}}.$$

The amplitude wave function at time t, $\Psi_M^{(p)}(t)$, is defined by

$$\Psi_M^{(p)}(t) = U_M^{(p)}(t)\Psi_M^{(p)}(0).$$

In this chapter we take $\Psi_M^{(p)}(0) = {}^T[1,0,0,\ldots,0]$ as initial state.

The $(n+1)$-th coordinate of $\Psi_M^{(p)}(t)$ is denoted by $\Psi_M^{(p)}(n,t)$ which is the amplitude wave function at site n at time t for $n = 0,1,\ldots,p(p-1)^M - p$. The probability finding the walker at site n at time t on $\mathbb{T}_M^{(p)}$ is given by

$$P_M^{(p)}(n,t) = |\Psi_M^{(p)}(n,t)|^2.$$

Then we define the continuous-time quantum walk $X_M^{(p)}(t)$ at time t on $\mathbb{T}_M^{(p)}$ by

$$P(X_M^{(p)}(t) = n) = P_M^{(p)}(n,t).$$

In a similar way, let $X_{M,MB}^{(p)}(t)$ be a quantum walk given by $H_{M,MB}^{(p)}$. As we stated before, $H_{M,MB}^{(p)}(i,i)$ depends on i for any finite M. However in $M \to \infty$

limit, the (i,i) component of the matrix becomes $-p$ for any i. Remark that the probability distribution of the continuous-time walk does not depend on the value of the diagonal component of the scalar matrix. Therefore the definitions of the walks imply that both quantum walks coincide in $M \to \infty$ limit, i.e.,

$$\lim_{M\to\infty} P(X_M^{(p)}(t) = n) = \lim_{M\to\infty} P(X_{M,MB}^{(p)}(t) = n),$$

for any t and n.

8.2 Quantum Probabilistic Approach

Finite M case

Let $\mu_M^{(p)}$ denote the spectral distribution of our adjacency matrix $H_M^{(p)}$. From the general theory of an interacting Fock space (see Jafarizadeh and Salimi (2007), Accardi and Bożejko (1998), Hashimoto (2001), Obata (2004), for examples), the orthogonal polynomials $\{Q_n^{(p)}\}$ and $\{Q_n^{(p,*)}\}$ associated with $\mu_M^{(p)}$ satisfy the following three-term recurrence relations with a Szegö-Jacobi parameter $(\{\omega_n\},\{\alpha_n\})$ respectively:

$$Q_0^{(p)}(x) = 1, \;\; Q_1^{(p)}(x) = x - \alpha_1,$$
$$xQ_n^{(p)}(x) = Q_{n+1}^{(p)}(x) + \alpha_{n+1}Q_n^{(p)}(x) + \omega_n Q_{n-1}^{(p)}(x) \;\; (n \geq 1),$$

and

$$Q_0^{(p,*)}(x) = 1, \;\; Q_1^{(p,*)}(x) = x - \alpha_2,$$
$$xQ_n^{(p,*)}(x) = Q_{n+1}^{(p,*)}(x) + \alpha_{n+2}Q_n^{(p,*)}(x) + \omega_{n+1} Q_{n-1}^{(p,*)}(x) \;\; (n \geq 1).$$

In our tree case,

$$\omega_1 = p, \; \omega_2 = \omega_3 = \cdots = \omega_M = p-1, \; \omega_{M+1} = \omega_{M+2} = \cdots = 0,$$
$$\alpha_1 = \alpha_2 = \cdots = 0.$$

Then the Stieltjes transform $G_{\mu_M^{(p)}}$ of $\mu_M^{(p)}$ is given by

$$G_{\mu_M^{(p)}}(x) = \frac{Q_{n-1}^{(p,*)}(x)}{Q_n^{(p)}(x)},$$

where $n = |\mathbb{T}_M^{(p)}| = p(p-1)^M - (p-1)$.

The following result was shown in Jafarizadeh and Salimi (2007):

$$\Psi_M^{(p)}(V_k^{(p)},t) = \sum_{n\in V_k^{(p)}} \Psi_M^{(p)}(n,t) = \frac{1}{\sqrt{|V_k^{(p)}|}} \int_{\mathbb{R}} \exp(itx)\, Q_k^{(p)}(x)\, \mu_M^{(p)}(x)\, dx,$$

for $k = 0,1,2,\ldots$. Remark that $|V_k^{(p)}| = \omega_1\omega_2\cdots\omega_k = p(p-1)^{k-1}$ $(1 \le k \le M)$ and $|V_0^{(p)}| = 1$. It is important to note that

$$\Psi_M^{(p)}(n,t) = \frac{1}{|V_k^{(p)}|} \int_{\mathbb{R}} \exp(itx)\, Q_k^{(p)}(x)\mu_M^{(p)}(x)\, dx,$$

if $n \in V_k^{(p)}$ $(k = 0,1,\ldots,M)$. The proof appeared in Appendix A in Jafarizadeh and Salimi (2007).

$p = 3$ and $M = 2$ case

Here we consider $p = 3$ and $M = 2$ case. Then we have $n = 10$, $\omega_1 = 3$, $\omega_2 = 2, \omega_3 = \omega_4 = \cdots = 0$, $\alpha_1 = \alpha_2 = \cdots = 0$. The definitions of $Q_n^{(3)}(x)$ and $Q_n^{(3,*)}(x)$ imply

$$Q_0^{(3)}(x) = 1,\ Q_1^{(3)}(x) = x,\ Q_2^{(3)}(x) = x^2 - 3,\ Q_k^{(3)}(x) = x^{k-2}(x^2 - 5)\ (k \ge 3),$$

and

$$Q_0^{(3,*)}(x) = 1,\ Q_1^{(3,*)}(x) = x,\ Q_k^{(3,*)}(x) = x^{k-2}(x^2 - 2)\ (k \ge 2).$$

Therefore we obtain the Stieltjes transform:

$$G_{\mu_2^{(3)}}(x) = \frac{Q_9^{(3,*)}(x)}{Q_{10}^{(3)}(x)} = \frac{2}{5}\cdot\frac{1}{x} + \frac{3}{10}\cdot\frac{1}{x+\sqrt{5}} + \frac{3}{10}\cdot\frac{1}{x-\sqrt{5}}.$$

From this, we see that

$$\mu_2^{(3)} = \frac{2}{5}\,\delta_0(x) + \frac{3}{10}\,\delta_{-\sqrt{5}}(x) + \frac{3}{10}\,\delta_{\sqrt{5}}(x).$$

Then

$$\Psi_2^{(3)}(V_0^{(3)},t) = \int_{\mathbb{R}} \exp(itx)\,\mu_2^{(3)}(dx) = \frac{1}{5}\,(2 + 3\cos(\sqrt{5}t)),$$

$$\Psi_2^{(3)}(V_1^{(3)},t) = \frac{1}{\sqrt{\omega_1}} \int_{\mathbb{R}} \exp(itx) Q_1^{(3)}(x)\,\mu_2^{(3)}(dx) = \frac{i\sqrt{3}}{\sqrt{5}}\,\sin(\sqrt{5}t),$$

$$\Psi_2^{(3)}(V_2^{(3)},t) = \frac{1}{\sqrt{\omega_1\omega_2}} \int_{\mathbb{R}} \exp(itx) Q_2^{(3)}(x)\,\mu_2^{(3)}(dx) = \frac{\sqrt{6}}{5}\left(-1 + \cos(\sqrt{5}t)\right).$$

Noting that $\Psi_2^{(3)}(n,t) = \Psi_2^{(3)}(V_k^{(3)},t)/\sqrt{|V_k^{(3)}|}$ for any $k = 0,1,2$, we obtain the same conclusion as the result given by the eigenvalues and the eigenvectors of $H_2^{(3)}$.

$M \to \infty$ case

The quantum probabilistic approach implies that

$$\Psi_\infty^{(p)}(V_k^{(p)},t) = \lim_{M\to\infty} \Psi_M^{(p)}(V_k^{(p)},t) = \frac{1}{\sqrt{|V_k^{(p)}|}} \int_{\mathbb{R}} \exp(itx)\, Q_k^{(p)}(x)\mu_M^{(p)}(x)\, dx,$$

for $k = 0,1,2,\ldots$, where the limit spectral distribution $\mu_M^{(p)}(x)$ is given by

$$\frac{p\sqrt{4(p-1)-x^2}}{2\pi(p^2-x^2)}\, I_{(-2\sqrt{p-1},2\sqrt{p-1})}(x) \qquad (x \in \mathbb{R}).$$

This type of measure was first obtained by Kesten (1959) in a classical random walk with a different method. An immediate consequence is

$$P_\infty^{(p)}(V_k^{(p)},t) = \frac{1}{|V_k^{(p)}|} \left[\left\{ \int_{\mathbb{R}} \cos(tx)\, Q_k^{(p)}(x)\mu_M^{(p)}(x)\, dx \right\}^2 + \left\{ \int_{\mathbb{R}} \sin(tx)\, Q_k^{(p)}(x)\mu_M^{(p)}(x)\, dx \right\}^2 \right],$$

for $k = 0,1,2,\ldots$ Furthermore, as in the case of finite M, we see that

$$\Psi_\infty^{(p)}(n,t) = \frac{1}{|V_k^{(p)}|} \int_{\mathbb{R}} \exp(itx)\, Q_k^{(p)}(x)\mu_M^{(p)}(x)\, dx, \tag{8.2.1}$$

if $n \in V_k^{(p)}$ $(k = 0,1,2,\ldots)$. From (8.2.1) and the Riemann-Lebesgue lemma, we have $\lim_{t\to\infty} \Psi_\infty^{(p)}(n,t) = 0$, for any n, since $Q_k^{(p)}(x)\mu_\infty^{(p)}(x) \in L^1(\mathbb{R})$. Therefore we see that $\lim_{t\to\infty} P_\infty^{(p)}(n,t) = 0$. So we conclude that $\bar{P}_\infty^{(p)}(n) = 0$, where $\bar{P}_\infty^{(p)}(n)$ is the time-averaged distribution of $P_\infty^{(p)}(n,t)$.

$p = 2$ and $M \to \infty$ case

In this subsection, we consider $p = 2$ and $M \to \infty$, i.e., $\mathbb{Z}^1$ case. Then we have

Proposition 8.1.

$$\Psi_\infty^{(2)}(V_0^{(2)},t) = J_0(2t), \qquad \Psi_\infty^{(2)}(V_k^{(2)},t) = \sqrt{2}\, i^k\, J_k(2t) \quad (k = 1,2,\ldots),$$

where $J_n(x)$ is the Bessel function of the first kind of order n.

Proof. Induction on k. For $k = 0$ case, we use the following result (see (4) in page 48 in Watson (1944)):

$$\int_{-1}^{1} \exp(isx)\ (1-x^2)^{\nu-1/2}\, dx = \frac{\Gamma(1/2)\Gamma(\nu+1/2)}{(s/2)^{\nu}}\, J_{\nu}(s), \qquad (8.2.2)$$

where $\Gamma(x)$ is the Gamma function. Combining $\Gamma(3/2) = \sqrt{\pi}/2$, $\Gamma(1/2) = \sqrt{\pi}$ with $Q_0^{(2)}(x) = 1$ and $\nu = 0$ gives

$$\Psi_{\infty}^{(2)}(V_0^{(2)}, t) = \int_{-2}^{2} \exp(itx)\ \frac{dx}{\pi\sqrt{4-x^2}}\ =\ J_0(2t).$$

In a similar fashion, we verify that the result holds for $k = 1, 2$.

Next we suppose that the result is true for all values up to k, where $k \geq 2$. Then we see that

$$\begin{aligned}
\Psi_{\infty}^{(2)}(V_{k+1}^{(2)}, t) &= \frac{1}{\sqrt{2}} \int_{-2}^{2} \exp(itx)\ Q_{k+1}^{(2)}(x)\, \frac{dx}{\pi\sqrt{4-x^2}} \\
&= \frac{1}{\sqrt{2}} \int_{-2}^{2} \exp(itx)\ \left\{ xQ_k^{(2)}(x) - Q_{k-1}^{(2)}(x) \right\}\ \frac{dx}{\pi\sqrt{4-x^2}} \\
&= \frac{1}{i}\,\frac{d}{dt}\left(\frac{1}{\sqrt{2}} \int_{-2}^{2} \exp(itx)\ Q_k^{(2)}(x)\, \frac{dx}{\pi\sqrt{4-x^2}} \right) \\
&\qquad\qquad - \frac{1}{\sqrt{2}} \int_{-2}^{2} \exp(itx)\ Q_{k-1}^{(2)}(x)\, \frac{dx}{\pi\sqrt{4-x^2}} \\
&= \frac{1}{i}\,\frac{d}{dt}(\sqrt{2}\, i^k\ J_k(2t)) - \sqrt{2}\, i^{k-1}\ J_{k-1}(2t) \\
&= \sqrt{2}\, i^{k+1}\ J_{k+1}(2t).
\end{aligned}$$

The second equality follows from the definition of $Q_k^{(2)}(x)$. By induction, we have the fourth equality. For the last equality, we use a recurrence formula for the Bessel coefficients: $2J_k'(2t) = J_{k-1}(2t) - J_{k+1}(2t)$ (see (2) in page 17 of Watson (1944)).

As a consequence, we have

Corollary 8.2.

$$P_{\infty}^{(2)}(V_0^{(2)}, t) = J_0^2(2t), \qquad P_{\infty}^{(2)}(V_k^{(2)}, t) = 2J_k^2(2t) \quad (k = 1, 2, \ldots).$$

We confirm that

$$\sum_{k=0}^{\infty} P_{\infty}^{(2)}(V_k^{(2)}, t) = 1,$$

since it follows from $J_0^2(2t)+2\sum_{k=1}^{\infty} J_k^2(2t) = 1$ (see (3) in page 31 in Watson (1944)). Noting that $V_k^{(2)} = \{-k, k\}$ for any $k \geq 0$, we have an equivalent result given by Corollary 7.3:

$$P_{\infty}^{(2)}(n,t) = J_n^2(2t),$$

for any $n \in \mathbb{Z}$ and $t \geq 0$.

8.3 Quantum Central Limit Theorem

To state a quantum central limit theorem in our case, it is convenient to rewrite as

$$\left\langle \Phi_k^{(p)} \left| \exp\left(itH_{\infty}^{(p)} \right) \right| \Phi_0^{(p)} \right\rangle = \Psi_{\infty}^{(p)}(V_k^{(p)}, t),$$

where

$$\Phi_k^{(p)} = \frac{1}{\sqrt{|V_k^{(p)}|}} \sum_{n \in V_k^{(p)}} I_{\{n\}},$$

and $I_{\{n\}}$ denotes the indicator function of the singleton $\{n\}$. It is easily obtained that

$$\lim_{p\to\infty} \left\langle \Phi_k^{(p)} \left| \exp\left(itH_{\infty}^{(p)} \right) \right| \Phi_0^{(p)} \right\rangle = 0,$$

for any $k \geq 0$. Then we have the following quantum central limit theorem:

Theorem 8.3.

$$\lim_{p\to\infty} \left\langle \Phi_k^{(p)} \left| \exp\left(it\frac{H_{\infty}^{(p)}}{\sqrt{p}} \right) \right| \Phi_0^{(p)} \right\rangle = (k+1)\, i^k \, \frac{J_{k+1}(2t)}{t},$$

for $k = 0, 1, 2, \ldots.$

Proof. Induction on k. First we consider $k = 0$ case. We see that

$$\begin{aligned}
&\lim_{p\to\infty} \left\langle \Phi_0^{(p)} \left| \exp\left(it\frac{H_{\infty}^{(p)}}{\sqrt{p}} \right) \right| \Phi_0^{(p)} \right\rangle \\
&= \lim_{p\to\infty} \int_{\mathbb{R}} \exp\left(it\frac{x}{\sqrt{p}} \right) \mu_M^{(p)}(x)\, dx \\
&= \lim_{p\to\infty} \int_{-2\sqrt{(p-1)/p}}^{2\sqrt{(p-1)/p}} \exp(itx) \, \frac{\sqrt{(2(p-1)/p)^2 - x^2}}{2\pi(1 - x^2/p)} \, dx \\
&= \int_{-1}^{1} \exp(2itx) \, \frac{2\sqrt{1-x^2}}{\pi} \, dx.
\end{aligned}$$

Then (8.2.2) with $\nu = 1$ yields

$$\lim_{p\to\infty}\left\langle \Phi_0^{(p)} \middle| \exp\left(it\frac{H_\infty^{(p)}}{\sqrt{p}}\right) \middle| \Phi_0^{(p)} \right\rangle = \frac{J_1(2t)}{t}.$$

So the result holds for $k = 0$. Similarly we obtain

$$\lim_{p\to\infty}\left\langle \Phi_1^{(p)} \middle| \exp\left(it\frac{H_\infty^{(p)}}{\sqrt{p}}\right) \middle| \Phi_0^{(p)} \right\rangle = \frac{2iJ_2(2t)}{t},$$
$$\lim_{p\to\infty}\left\langle \Phi_2^{(p)} \middle| \exp\left(it\frac{H_\infty^{(p)}}{\sqrt{p}}\right) \middle| \Phi_0^{(p)} \right\rangle = -\frac{3J_3(2t)}{t}.$$

Next we suppose that the result holds for all values up to k, where $k \geq 2$. Then we have

$$\begin{aligned}
&\lim_{p\to\infty}\left\langle \Phi_{k+1}^{(p)} \middle| \exp\left(it\frac{H_\infty^{(p)}}{\sqrt{p}}\right) \middle| \Phi_0^{(p)} \right\rangle \\
&= \lim_{p\to\infty}\frac{1}{\sqrt{|V_{k+1}^{(p)}|}}\int_{\mathbb{R}} \exp\left(it\frac{x}{\sqrt{p}}\right) Q_{k+1}^{(p)}(x)\, \mu_M^{(p)}(x)\, dx \\
&= \lim_{p\to\infty}\frac{1}{\sqrt{p(p-1)^k}}\int_{-2\sqrt{(p-1)/p}}^{2\sqrt{(p-1)/p}} \exp(itx)\, Q_{k+1}^{(p)}(\sqrt{p}x)\frac{\sqrt{(2(p-1)/p)^2 - x^2}}{2\pi(1-x^2/p)}\, dx \\
&= \int_{-2}^{2} \exp(itx)\; Q_{k+1}^{(\infty)}(x)\; \frac{\sqrt{2^2 - x^2}}{2\pi}\, dx \\
&= \int_{-2}^{2} \exp(itx)\; \left\{xQ_k^{(\infty)}(x) - Q_{k-1}^{(\infty)}(x)\right\}\; \frac{\sqrt{2^2 - x^2}}{2\pi}\, dx \\
&= \frac{1}{i}\frac{d}{dt}\left(\int_{-1}^{1} \exp(2itx)\; Q_k^{(\infty)}(2x)\; \frac{2\sqrt{1-x^2}}{\pi}\, dx\right) \\
&\qquad\qquad - \int_{-1}^{1} \exp(2itx)\; Q_{k-1}^{(\infty)}(2x)\; \frac{2\sqrt{1-x^2}}{\pi}\, dx \\
&= i^{k-1}\left\{(k+1)\frac{d}{dt}\left(\frac{J_{k+1}(2t)}{t}\right) - k\frac{J_k(2t)}{t}\right\},
\end{aligned}$$

where the last equality is given by the induction and

$$Q_k^{(\infty)}(x) = \lim_{p\to\infty} Q_k^{(p)}(\sqrt{p}x)/\sqrt{p(p-1)^{k-1}},$$

if the right-hand side exists. We confirm that the limit exists for any $k \geq 1$. For example, we compute $Q_1^{(\infty)}(x) = x$, $Q_2^{(\infty)}(x) = x^2 - 1$, $Q_3^{(\infty)}(x) = x^3 - 2x$,

$Q_4^{(\infty)}(x) = x^4 - 3x^2 + 1, \ldots$ In order to prove the result, it suffices to check the following relation:

$$(k+1)\frac{d}{dt}\left(\frac{J_{k+1}(2t)}{t}\right) - k\frac{J_k(2t)}{t} = -(k+2)\frac{J_{k+2}(2t)}{t}.$$

The left-hand side of this equation becomes

$$\begin{aligned} &(k+1)\frac{2J_{k+1}(2t)}{t} - (k+1)\frac{J_{k+1}(2t)}{t^2} - k\frac{J_k(2t)}{t} \\ &= \frac{J_k(2t)}{t} - (k+1)\frac{J_{k+1}(2t)}{t^2} - (k+1)\frac{J_k(2t)}{t} \\ &= -(k+2)\frac{J_{k+2}(2t)}{t}, \end{aligned}$$

since the first and second equalities are obtained from recurrence formulas for the Bessel coefficients: $2J'_{k+1}(2t) = J_k(2t) - J_{k+2}(2t)$ and $J_k(2t) + J_{k+2}(2t) = (k+1)J_{k+1}(2t)/t$ (see (1) in page 17 of Watson (1944)), respectively. This finishes the proof of the theorem.

Remark that an extension of this theorem for a wider family of graphs and another proof by using Gegenbauer's integral formula for the Bessel function can be found in Obata (2006).

8.4 A New Type of Limit Theorems

We can now state the main result of this chapter. To do so, let define

$$\tilde{\Psi}_\infty^{(\infty)}(V_k^{(\infty)}, t) = \lim_{p\to\infty}\left\langle \Phi_k^{(p)} \middle| \exp\left(it\frac{H_\infty^{(p)}}{\sqrt{p}}\right) \middle| \Phi_0^{(p)} \right\rangle,$$

and

$$\tilde{P}_\infty^{(\infty)}(V_k^{(\infty)}, t) = |\tilde{\Psi}_\infty^{(\infty)}(V_k^{(\infty)}, t)|^2.$$

By Theorem 8.3 and the definition of $\tilde{\Psi}_\infty^{(\infty)}(V_k^{(\infty)}, t)$, we see that

$$\sum_{k=0}^{\infty} \tilde{P}_\infty^{(\infty)}(V_k^{(\infty)}, t) = \sum_{k=1}^{\infty} k^2\,\frac{J_k^2(2t)}{t^2} = 1. \tag{8.4.3}$$

The second equality comes from an expansion of z^2 as a series of squares of Bessel coefficients (see page 37 in Watson (1944)):

$$z^2 = 4\sum_{k=1}^{\infty} k^2\, J_k^2(z).$$

Noting the result (8.4.3), here we define another continuous-time quantum walk $Y(t)$ starting from the root defined by

$$P(Y(t) = k) = \tilde{P}_{\infty}^{(\infty)}(V_k^{(\infty)}, t) = (k+1)^2 \, \frac{J_{k+1}^2(2t)}{t^2}.$$

Then we obtain

Theorem 8.4. *As $t \to \infty$,*

$$\frac{Y(t)}{t} \;\Rightarrow\; Z_*,$$

where Z_* has the following density function:

$$\frac{x^2}{\pi\sqrt{4-x^2}} \, I_{(0,2)}(x) \qquad (x \in \mathbb{R}).$$

Proof. From Theorem 8.3, we begin with computing

$$E\left(\exp\left(i\xi \frac{Y(t)}{t}\right)\right) = \frac{\exp(-i\xi/t)}{t^2} \sum_{k=1}^{\infty} \exp\left(i\xi\frac{k}{t}\right) k^2 J_{k+1}^2(2t),$$

for $\xi \in \mathbb{R}$. By Neumann's addition theorem (see p.358 in Watson (1944)), we have

$$J_0(\sqrt{a^2+b^2-2ab\cos(\xi)}) = \sum_{k=-\infty}^{\infty} J_k(a)J_k(b)\exp(ik\xi).$$

Taking $t = a = b$ in this equation gives

$$J_0(4t\sqrt{\sin(\xi/2)}) = \sum_{k=-\infty}^{\infty} J_k^2(t)\exp(ik\xi).$$

By differentiating both sides of the equation twice with respect to t, we see

$$\sum_{k=1}^{\infty} k^2 J_k^2(t)\exp(ik\xi) = \frac{1}{2}\sum_{k=-\infty}^{\infty} k^2 J_k^2(t)\exp(ik\xi)$$
$$= \frac{t}{4}\sin\left(\frac{\xi}{2}\right) J_0'\left(2t\sin\left(\frac{\xi}{2}\right)\right) - \frac{t^2}{2}\cos^2\left(\frac{\xi}{2}\right) J_0''\left(2t\sin\left(\frac{\xi}{2}\right)\right).$$

Therefore we obtain

$$E\left(\exp\left(i\xi\frac{Y(t)}{t}\right)\right) = \exp\left(-\frac{i\xi}{t}\right)\left\{\frac{1}{2t}\sin\left(\frac{\xi}{2t}\right) J_0'\left(4t\sin\left(\frac{\xi}{2t}\right)\right)\right.$$
$$\left. -2\cos^2\left(\frac{\xi}{2t}\right) J_0''\left(4t\sin\left(\frac{\xi}{2t}\right)\right)\right\}.$$

Then a similar argument as in Konno (2005c) yields

$$\lim_{t\to\infty} E\left(\exp\left(i\xi\frac{Y(t)}{t}\right)\right) = -2J_0''(2\xi).$$

On the other hand, (8.2.2) with $\nu = 0$ gives

$$J_0''(2\xi) = -\int_{-1}^{1} \exp(2i\xi x)\ \frac{x^2}{\pi\sqrt{1-x^2}}\,dx.$$

From the last two equations, we conclude that

$$\lim_{t\to\infty} E\left(\exp\left(i\xi\frac{Y(t)}{t}\right)\right) = \int_{0}^{2} \exp(i\xi x)\ \frac{x^2}{\pi\sqrt{4-x^2}}\,dx.$$

It is interesting to remark that when $p = 2$ case, i.e., $\mathbb{Z}^1$, a similar type of density function can be derived from Theorem 7.4:

$$\frac{2}{\pi\sqrt{1-x^2}}\, I_{(0,1)}(x) \qquad (x \in \mathbb{R}).$$

9 Ultrametric Space

9.1 Introduction

Continuous-time classical random walks on ultrametric spaces have been investigated by some groups to describe the relaxation processes in complex systems, such as glasses, clusters and proteins. On the other hand, a continuous-time quantum walk has been widely studied by various researchers for some important graphs, such as cycle graph, line, hypercube and complete graph, with the hope of finding a new quantum algorithmic technique. However no result is known for a quantum walk on the ultrametric space. Results here appeared in Konno (2006b).

Let X be a set and let ρ be a metric on X. The pair (X,ρ) is called a metric space. Moreover if ρ satisfies the strong triangle inequality:

$$\rho(x,z) \le \max(\rho(x,y), \rho(y,z)),$$

for any $x,y,z \in X$, then ρ is said to be an ultrametric. A set endowed with an ultrametric is called an ultrametric space. Let p be a prime number and $\mathbb{Q}_p$ be the field of p-adic numbers. $\mathbb{Z}_p$ denotes the set of p-adic integers. Then $\mathbb{Z}_p$ is a subring of $\mathbb{Q}_p$ and $\mathbb{Z}_p = \{x \in \mathbb{Q}_p : |x|_p \le 1\}$, where $|\cdot|_p$ is the p-adic absolute value. Remark that the metric $\rho_p(x,y) = |x-y|_p$ is an ultrametric. Every $x \in \mathbb{Z}_p$ can be expanded in the following way:

$$x = y_0 + y_1 p + y_2 p^2 + \cdots + y_n p^n + \cdots,$$

where $y_n \in \{0, 1, \ldots, p-1\}$ for any n. See Khrennikov and Nilsson (2004) for more details. It is important that $\mathbb{Z}_p$ can be represented by the bottom infinite regular Cayley tree of degree p, T_p, in which every branch at each level splits into p other branches. So we consider a continuous-time quantum walk on the bottom of T_p at level (or depth) M, denoted by $T_M^{(p)}$.

We calculate the probability distribution of the quantum walk on $T_M^{(p)}$. From this, we obtain the time-averaged probability distribution on $T_M^{(p)}$ and then take a limit as $M \to \infty$. On the other hand, we can first take the limit as $M \to \infty$ and then derive the time-averaged probability distribution. It is shown that the first limit result coincides with the second one, that is, time-averaged operation and M-limit one are commutative. By using these results, we clarify a difference between classical and quantum cases. A striking difference is that localization occurs at any site for a wide class of quantum walks. Furthermore we compare the results of ultrametric space with those of other graphs, such as cyclic graph, line, hypercube and complete graph in the quantum case. Some applications of p-adic analysis in physics and biology were reported in Khrennikov and Nilsson (2004). Social network models based on the ultrametric distance were present ed and studied (see Watts, Dodds, and Newman (2002), Dodds, Watts, and Sabel (2003)) The disease spreading on a hierarchical metapopulation model was investigated in Watts et al. (2005). Our quantum walk on the ultrametric space may be useful for designing a new quantum search algorithm on graphs with a hierarchical structure.

9.2 Definition

For $M \geq 0$ and $x \in \mathbb{Z}_p$, the closed p-adic ball $B_M^{(p)}(x)$ of radius p^{-M} with center x is defined by

$$B_M^{(p)}(x) = \{y \in \mathbb{Z}_p : \rho_p(x, y) \leq p^{-M}\}.$$

Each ball $B_M^{(p)}(x)$ of radius p^{-M} can be represented as a finite union of disjoint balls $B_{M+1}^{(p)}(x_m)$ of radius $p^{-(M+1)}$:

$$B_M^{(p)}(x) = \bigcup_{m=0}^{p-1} B_{M+1}^{(p)}(x_m),$$

for suitable $x_0, x_1, \ldots, x_{p-1} \in \mathbb{Z}_p$, so we have

$$\mathbb{Z}_p = \bigcup_{m=0}^{p^M-1} B_M^{(p)}(m).$$

When $p = 3$,

$$\mathbb{Z}_p = \bigcup_{m=0}^{3^1-1} B_1^{(3)}(m) = \bigcup_{k=0}^{3^2-1} B_2^{(3)}(k),$$

and

$$\begin{aligned} B_1^{(3)}(0) &= B_2^{(3)}(0) \cup B_2^{(3)}(3) \cup B_2^{(3)}(6), \\ B_1^{(3)}(1) &= B_2^{(3)}(1) \cup B_2^{(3)}(4) \cup B_2^{(3)}(7), \\ B_1^{(3)}(2) &= B_2^{(3)}(2) \cup B_2^{(3)}(5) \cup B_2^{(3)}(8). \end{aligned}$$

We define the distance between two balls B_1 and B_2 as

$$\rho_p(B_1, B_2) = \inf\{\rho_p(x, y) : x \in B_1, y \in B_2\}.$$

We observe that end points of a regular Cayley tree with p degree at level M may be represented as a set of disconnected balls

$$\{B_M^{(p)}(0), B_M^{(p)}(1), \ldots, B_M^{(p)}(p^M - 1)\}$$

with radius p^{-M} covering $\mathbb{Z}_p$. So we can consider p^M balls

$$\{B_M^{(p)}(0), B_M^{(p)}(1), \ldots, B_M^{(p)}(p^M - 1)\}$$

as p^M points $\{0, 1, \ldots, p^M - 1\}$, denoted by $T_M^{(p)}$.

As in the case of classical random walk, let $\psi_M^{(p)}(i, j)$ be the amplitude of a jump from the ball $B_M^{(p)}(i)$ to the ball $B_M^{(p)}(j)$ separated by p-adic distance $p^{-(M-k)}$. Here we put $\epsilon_k = \epsilon_M^{(p)}(k) = \psi_M^{(p)}(i, j)$. Remark that $\psi_M^{(p)}(i, j) = \psi_M^{(p)}(j, i)$.

We consider $p = 3$ and $M = 2$. In this case, ϵ_k is given by

$$\begin{aligned} \epsilon_1 &= \psi_2^{(3)}(0,3) = \psi_2^{(3)}(0,6) = \psi_2^{(3)}(3,0) = \psi_2^{(3)}(3,6) \\ &= \psi_2^{(3)}(6,0) = \psi_2^{(3)}(6,3) = \psi_2^{(3)}(1,4) = \psi_2^{(3)}(1,7) = \cdots, \\ \epsilon_2 &= \psi_2^{(3)}(0,1) = \psi_2^{(3)}(0,4) = \cdots = \psi_2^{(3)}(0,8) \\ &= \psi_2^{(3)}(3,1) = \psi_2^{(3)}(3,4) = \cdots = \psi_2^{(3)}(3,8) = \cdots, \\ &\cdots\cdots. \end{aligned}$$

Let I_n and J_n denote the $n \times n$ identity matrix and the all-one $n \times n$ matrix. We define a $p^M \times p^M$ symmetric matrix $H_M^{(p)}$ on $T_M^{(p)}$ which is treated as the Hamiltonian of the quantum system as follows: for any $M = 1, 2, \ldots,$

$$H_{M+1}^{(p)} = I_p \otimes H_M^{(p)} + (J_p - I_p) \otimes \epsilon_{M+1} I_{p^M},$$
$$H_1^{(p)} = \epsilon_0 I_p + \epsilon_1 (J_p - I_p),$$

where $\epsilon_j \in \mathbb{R}$ $(j = 0, 1, 2, \ldots)$ and $\mathbb{R}$ is the set of real numbers.

The evolution of the continuous-time quantum walk on $T_M^{(p)}$ is governed by the following unitary matrix:

$$U_M^{(p)}(t) = e^{itH_M^{(p)}}.$$

The amplitude wave function at time t, $\Psi_M^{(p)}(t)$, is defined by

$$\Psi_M^{(p)}(t) = U_M^{(p)}(t) \Psi_M^{(p)}(0).$$

In this chapter we take $\Psi_M^{(p)}(0) = {}^T[1, 0, 0, \ldots, 0]$ as initial state.

The $(n+1)$-th coordinate of $\Psi_M^{(p)}(t)$ is denoted by $\Psi_M^{(p)}(n, t)$ which is the amplitude wave function at site n at time t for $n = 0, 1, \ldots, p^M - 1$. The probability finding the walker is at site n at time t on $T_M^{(p)}$ is given by

$$P_M^{(p)}(n, t) = |\Psi_M^{(p)}(n, t)|^2.$$

9.3 Results

Let $\{\eta_m : m = 0, 1, \ldots, M\}$ be defined by

$$\eta_m = \begin{cases} \epsilon_0 - \epsilon_1 & if \;\; m = 0, \\ \epsilon_0 + (p-1) \sum_{k=1}^{m} p^{k-1} \epsilon_k - p^m \epsilon_{m+1} & if \;\; m = 1, 2, \ldots, M-1, \\ 0 & if \;\; m = M. \end{cases}$$

Direct computation yields that $\{\eta_m : m = 0, 1, \ldots, M\}$ is the set of eigenvalues of $H_M^{(p)}$ and eigenvectors for η_m are given in the following way, see Ogielski and Stein (1985) for $p = 2$ case. Let $\omega = \omega_p = \exp(2\pi i/p)$. Put

$$0_n = [\overbrace{0, 0, \ldots, 0}^{n}], \quad 1_n = [\overbrace{1, 1, \ldots, 1}^{n}].$$

The $p^{M-1}(p-1)$ eigenvectors for η_0 are

$$\begin{aligned} u_0(1) &= [1, \omega, \omega^2, \ldots, \omega^{p-1}, 0_{p^M - p}]^T, \\ u_0(2) &= [1, \omega^2, \omega^4, \ldots, \omega^{2(p-1)}, 0_{p^M - p}]^T, \\ &\cdots \\ u_0(p-1) &= [1, \omega^{(p-1)}, \omega^{2(p-1)}, \ldots, \omega^{(p-1)^2}, 0_{p^M - p}]^T, \\ u_0(p) &= [0_p, 1, \omega, \omega^2, \ldots, \omega^{p-1}, 0_{p^M - 2p}]^T, \end{aligned}$$

$$\begin{aligned} u_0(p+1) &= [0_p, 1, \omega^2, \omega^4, \dots, \omega^{2(p-1)}, 0_{p^M-2p}]^T, \\ &\cdots \\ u_0(2(p-1)) &= [0_p, 1, \omega^{(p-1)}, \omega^{2(p-1)}, \dots, \omega^{(p-1)^2}, 0_{p^M-2p}]^T, \\ &\cdots \\ u_0(p^{M-1}(p-1)) &= [0_{p^M-p}, 1, \omega^{(p-1)}, \omega^{2(p-1)}, \dots, \omega^{(p-1)^2}]^T. \end{aligned}$$

The $p^{M-2}(p-1)$ eigenvectors for η_1 are

$$\begin{aligned} u_1(1) &= [1_p, \omega 1_p, \omega^2 1_p, \dots, \omega^{p-1} 1_p, 0_{p^M-p^2}]^T, \\ u_1(2) &= [1_p, \omega^2 1_p, \omega^4 1_p, \dots, \omega^{2(p-1)} 1_p, 0_{p^M-p^2}]^T, \\ &\cdots \\ u_1(p-1) &= [1_p, \omega^{(p-1)} 1_p, \omega^{2(p-1)} 1_p, \dots, \omega^{(p-1)^2} 1_p, 0_{p^M-p^2}]^T, \\ u_1(p) &= [0_{p^2}, 1_p, \omega 1_p, \omega^2 1_p, \dots, \omega^{p-1} 1_p, 0_{p^M-2p^2}]^T, \\ u_1(p+1) &= [0_{p^2}, 1_p, \omega^2 1_p, \omega^4 1_p, \dots, \omega^{2(p-1)} 1_p, 0_{p^M-2p^2}]^T, \\ &\cdots \\ u_1(2(p-1)) &= [0_{p^2}, 1_p, \omega^{(p-1)} 1_p, \omega^{2(p-1)} 1_p, \dots, \omega^{(p-1)^2} 1_p, 0_{p^M-p^2}]^T, \\ &\cdots \\ u_1(p^{M-2}(p-1)) &= [0_{p^M-p^2}, 1_p, \omega^{(p-1)} 1_p, \omega^{2(p-1)} 1_p, \dots, \omega^{(p-1)^2} 1_p]^T. \end{aligned}$$

We have $p^{M-(k+1)}(p-1)$ eigenvectors for η_k ($k = 2, 3, \dots, M-1$) similarly. So the $p-1$ eigenvectors for η_{M-1} are

$$\begin{aligned} u_{M-1}(1) &= [1_{p^{M-1}}, \omega 1_{p^{M-1}}, \omega^2 1_{p^{M-1}}, \dots, \omega^{p-1} 1_{p^{M-1}}]^T, \\ u_{M-1}(2) &= [1_{p^{M-1}}, \omega^2 1_{p^{M-1}}, \omega^4 1_{p^{M-1}}, \dots, \omega^{2(p-1)} 1_{p^{M-1}}]^T, \\ &\cdots \\ u_{M-1}(p-1) &= [1_{p^{M-1}}, \omega^{(p-1)} 1_{p^{M-1}}, \omega^{2(p-1)} 1_{p^{M-1}}, \dots, \omega^{(p-1)^2} 1_{p^{M-1}}]^T. \end{aligned}$$

Finally the only eigenvector for η_M is $[1_{p^M}]^T$.

Throughout this chapter, we assume that

$$0 < \epsilon_M < \epsilon_{M-1} < \cdots < \epsilon_2 < \epsilon_1.$$

This assumption implies that our class of quantum walks does not belong to the class of continuous-time quantum walks given by the adjacency matrix of the graph on which the walk is defined, see Jafarizadeh and Salimi (2007).

Remark that the diagonal component ϵ_0 is an irrelevant phase factor in the wave evolution. So the probability distribution at time t, $\{P_M^{(p)}(n,t) : n = 0, 1, \dots, p^M - 1\}$, does not depend on ϵ_0 and we put

$$\epsilon_0 = -(p-1) \sum_{k=1}^{M} p^{k-1} \epsilon_k < 0,$$

as in the classical case. We should note that $\epsilon_0 < 0 < \epsilon_M < \epsilon_{M-1} < \cdots < \epsilon_2 < \epsilon_1$ is equivalent to $\eta_0 < \eta_1 < \cdots < \eta_{M-1} < \eta_M = 0$.

Let $V_k^{(p)} = \{p^{k-1}, p^{k-1}+1, \ldots, p^k - 1\}$ $(k = 1, 2, \ldots, M)$ and $V_0^{(p)} = \{0\}$. Remark that $\bigcup_{k=0}^{M} V_k^{(p)} = \{0, 1, \ldots, p^M - 1\}$ and $|V_k^{(p)}| = (p-1)p^{k-1}$ for $k = 1, 2, \ldots, M$, where $|A|$ is the number of elements in a set A. By using the eigenvectors, we obtain the amplitude of the quantum walk on $T_M^{(p)}$:

Lemma 9.1.

$$\Psi_M^{(p)}(n,t) = \begin{cases} (p-1)\displaystyle\sum_{m=0}^{M-1} p^{-(m+1)} e^{it\eta_m} + p^{-M} \\ \qquad if\ \ n \in V_0^{(p)}, \\ -p^{-k} e^{it\eta_{k-1}} + (p-1)\displaystyle\sum_{m=k}^{M-1} p^{-(m+1)} e^{it\eta_m} + p^{-M} \\ \qquad if\ \ n \in V_k^{(p)}\ \ (k = 1, 2, \ldots, M-1), \\ p^{-M}(-e^{it\eta_{M-1}} + 1) \\ \qquad if\ \ n \in V_M^{(p)}. \end{cases}$$

The definition of $P_M^{(p)}(n,t)$ implies

Proposition 9.2.

$$P_M^{(p)}(n,t) = \begin{cases} \left\{(p-1)\displaystyle\sum_{m=0}^{M-1} p^{-(m+1)}\cos(t\eta_m) + p^{-M}\right\}^2 \\ \qquad\qquad + (p-1)^2\left\{\displaystyle\sum_{m=0}^{M-1} p^{-(m+1)}\sin(t\eta_m)\right\}^2 \\ \qquad if\ \ n \in V_0^{(p)}, \\ \left\{-p^{-k}\cos(t\eta_{k-1}) + (p-1)\displaystyle\sum_{m=k}^{M-1} p^{-(m+1)}\cos(t\eta_m) + p^{-M}\right\}^2 \\ \qquad + \left\{-p^{-k}\sin(t\eta_{k-1}) + (p-1)\displaystyle\sum_{m=k}^{M-1} p^{-(m+1)}\sin(t\eta_m)\right\}^2 \\ \qquad if\ \ n \in V_k^{(p)}\ \ (k = 1, 2, \ldots, M-1), \\ 2p^{-2M}(1 - \cos(t\eta_{M-1})) \\ \qquad if\ \ n \in V_M^{(p)}. \end{cases}$$

If $n = 0$, then $P_M^{(p)}(0,t)$ is the return probability of the walk on $T_M^{(p)}$. For $p = 3$ and $M = 2$ case, we obtain

$$P_2^{(3)}(n,t) = \begin{cases} \{41 + 24\cos(t(\eta_0 - \eta_1)) + 12\cos(t\eta_0) + 4\cos(t\eta_1)\}/3^4 \\ \qquad\qquad if \;\; n = 0, \\ \{14 - 12\cos(t(\eta_0 - \eta_1)) - 6\cos(t\eta_0) + 4\cos(t\eta_1)\}/3^4 \\ \qquad\qquad if \;\; n = 1, 2, \\ 2\{1 - \cos(t\eta_1)\}/3^4 \\ \qquad\qquad if \;\; n = 3, 4, \ldots, 8. \end{cases}$$

In general, $P_M^{(p)}(n,t)$ does not converge as $t \to \infty$ for any fixed n. So we introduce the time-averaged distribution of $P_M^{(p)}(n,t)$ as follows:

$$\bar{P}_M^{(p)}(n) = \lim_{t\to\infty} \frac{1}{t} \int_0^t P_M^{(p)}(n,s)ds, \qquad (9.3.1)$$

if the right-hand side of (9.3.1) exists. Then Proposition 9.2 gives

Theorem 9.3.

$$\bar{P}_M^{(p)}(n) = \begin{cases} \dfrac{p-1}{p+1} + \dfrac{2}{(p+1)p^{2M}} & if \;\; n \in V_0^{(p)}, \\ \dfrac{2}{p+1}\left(\dfrac{1}{p^{2k-1}} + \dfrac{1}{p^{2M}}\right) & if \;\; n \in V_k^{(p)} \;\; (k = 1, 2, \ldots, M-1), \\ \dfrac{2}{p^{2M}} & if \;\; n \in V_M^{(p)}. \end{cases}$$

It is interesting to note that $\bar{P}_M^{(p)}(n)$ does not depend on $\{\epsilon_k : k = 0, 1, \ldots, M\}$. In the case of $p = 3$ and $M = 2$, we have

$$\bar{P}_2^{(3)}(0) = \frac{41}{3^4}, \quad \bar{P}_2^{(3)}(1) = \bar{P}_2^{(3)}(2) = \frac{14}{3^4}, \quad \bar{P}_2^{(3)}(3) = \cdots = \bar{P}_2^{(3)}(8) = \frac{2}{3^4}.$$

The following result is immediate from Theorem 9.3.

Corollary 9.4.

$$\lim_{M\to\infty} \bar{P}_M^{(p)}(n) = \begin{cases} \dfrac{p-1}{p+1} & if \;\; n \in V_0^{(p)}, \\ \dfrac{2}{(p+1)p^{2k-1}} & if \;\; n \in V_k^{(p)} \;\; (k = 1, 2, \ldots). \end{cases}$$

Here we consider the mean distance from 0 at time t defined by

$$d_M^{(p)}(t) = \sum_{k=1}^{M} \sum_{n \in V_k^{(p)}} p^{-(M-k)} P_M^{(p)}(n,t).$$

Then its time-averaged mean distance is given by

$$\bar{d}_M^{(p)} = \sum_{k=1}^{M} \sum_{n \in V_k^{(p)}} p^{-(M-k)} \bar{P}_M^{(p)}(n).$$

From Theorem 9.3, we get

$$\bar{d}_M^{(p)} = \frac{2(p-1)(M-1)}{(p+1)p^M} + \frac{2\left[\left\{(p-1)(p+1)^2+1\right\}p^{2M-2}-1\right]}{(p+1)^2p^{3M-1}}.$$

This gives

$$\lim_{M\to\infty} \frac{p^M}{M}\bar{d}_M^{(p)} = \frac{2(p-1)}{p+1}.$$

Next we take the limit as $M \to \infty$ first. We define $P_\infty^{(p)}(n,t)$ by $P_\infty^{(p)}(n,t) = \lim_{M\to\infty} P_M^{(p)}(n,t)$, if the right-hand side of the equation exists. By Proposition 9.2, we obtain

Proposition 9.5.

$$P_\infty^{(p)}(n,t) = \begin{cases} (p-1)^2\left[\left\{\sum_{m=0}^{\infty} p^{-(m+1)}\cos(t\eta_m)\right\}^2 + \left\{\sum_{m=0}^{\infty} p^{-(m+1)}\sin(t\eta_m)\right\}^2\right] \\ \qquad if \;\; n \in V_0^{(p)}, \\ \left\{-p^{-k}\cos(t\eta_{k-1}) + (p-1)\sum_{m=k}^{\infty} p^{-(m+1)}\cos(t\eta_m)\right\}^2 \\ \quad + \left\{-p^{-k}\sin(t\eta_{k-1}) + (p-1)\sum_{m=k}^{\infty} p^{-(m+1)}\sin(t\eta_m)\right\}^2 \\ \qquad if \;\; n \in V_k^{(p)} \;\; (k = 1,2,\ldots). \end{cases}$$

In a similar way, the time-averaged distribution $P_\infty^{(p)}(n,t)$ is given by

$$\bar{P}_\infty^{(p)}(n) = \lim_{t\to\infty} \frac{1}{t}\int_0^t P_\infty^{(p)}(n,s)ds, \tag{9.3.2}$$

if the right-hand side of (9.3.2) exists. Combining Theorem 9.3 with Proposition 9.5 yields

Corollary 9.6. *For any $n = 0,1,2,\ldots$, we have*

$$\bar{P}_\infty^{(p)}(n) = \lim_{M\to\infty} \bar{P}_M^{(p)}(n) > 0.$$

Furthermore,

$$\lim_{p\to\infty} \bar{P}_\infty^{(p)}(n) = \delta_0(n),$$

where $\delta_m(n) = 1$, if $n = m$, $= 0$, if $n \neq m$.

In general, we say that localization occurs at site n if the time-averaged probability at the site is positive. Therefore the localization occurs at any site for both any finite M and $M \to \infty$ limit cases.

9.4 Classical Case

In this section we review three classical examples and clarify a difference between classical and quantum walks. Let $P_c^{(p)}(n,t)$ be the probability that a classical random walker starting from 0 is located at site n at time t on $\mathbb{Z}_p$.

In the case of a linear landscape, the transition rate on $T_M^{(p)}$ has the form

$$\epsilon_k = w_0\, p^{-(1+\alpha)(k-M)},$$

for $w_0 > 0$ and $\alpha > 0$. Then Avetisov et al. (2002) showed a power decay law in $M \to \infty$ limit:

$$P_c^{(p)}(0,t) \sim \frac{1}{t^{1/\alpha}} \quad (t \to \infty),$$

where $f(t) \sim g(t)$ $(t \to \infty)$ means there exist positive constants C_1 and C_2 such that

$$C_1 \le \liminf_{t\to\infty} \frac{f(t)}{g(t)} \le \limsup_{t\to\infty} \frac{f(t)}{g(t)} \le C_2.$$

For a logarithmic landscape case, the transition rate on $T_M^{(p)}$ is

$$\epsilon_k = w_0\, p^{-(k-M)} \frac{1}{(\log(1+p^{-(k-M)}))^{\alpha}},$$

for $w_0 > 0$ and $\alpha > 1$. The following stretched exponential decay law (the Kohlrausch-Williams-Watts law) was proved by Avetisov, Bikulov, and Osipov (2003) in $M \to \infty$ limit:

$$\log(P_c^{(p)}(0,t)) \sim -t^{1/\alpha} \quad (t \to \infty).$$

In the case of an exponential landscape, the transition rate on $T_M^{(p)}$ has the form

$$\epsilon_k = w_0\, p^{-(k-M)} \exp(-\alpha p^{(k-M)}),$$

for $w_0 > 0$ and $\alpha > 0$. Then Avetisov, Bikulov, and Osipov (2003) obtained a logarithmic decay law taking a limit as $M \to \infty$:

$$P_c^{(p)}(0,t) \sim \frac{1}{\log t} \quad (t \to \infty).$$

The above three facts imply that the localization does not occur at position 0. In contrast to the classical case, the localization occurs at any position for our quantum case.

9.5 Quantum Case for Other Graphs

We consider the time-averaged probability distribution for continuous-time quantum walk starting from a site on other graphs, such as cycle graph, line, hypercube and complete graph. Then the Hamiltonian of the walk is given by the adjacency matrix of the graph.

In the case of a cycle graph C_N with N sites, we have obtained the following result (see Chapter 10 or Inui, Kasahara, Konishi, and Konno (2005)):

$$\bar{P}_N(n) = \frac{1}{N} + \frac{2R_N(n)}{N^2},$$

for any $n = 0, 1, \ldots, N-1$, where

$$R_N(n) = \begin{cases} -1/2 & if \;\; N = \text{odd}, \quad \xi_{2n} \neq 0 \pmod{2\pi}, \\ -1 & if \;\; N = \text{even}, \quad \xi_{2n} \neq 0 \pmod{2\pi}, \\ \bar{N} & if \;\; \xi_{2n} = 0 \pmod{2\pi}. \end{cases}$$

Here $\xi_j = 2\pi j/N$, $\bar{N} = [(N-1)/2]$, and $[x]$ is the smallest integer greater than x. When $N = \text{odd}$ (i.e., $\bar{N} = (N-1)/2$),

$$\bar{P}_N = \Big(\frac{1}{N} + \frac{N-1}{N^2}, \overbrace{\frac{1}{N} - \frac{1}{N^2}, \ldots, \frac{1}{N} - \frac{1}{N^2}}^{N-1}\Big),$$

when $N = \text{even}$ (i.e., $\bar{N} = (N-2)/2$),

$$\bar{P}_N = \Big(\frac{1}{N} + \frac{N-2}{N^2}, \overbrace{\frac{1}{N} - \frac{2}{N^2}, \ldots, \frac{1}{N} - \frac{2}{N^2}}^{(N-2)/2}, \frac{1}{N} + \frac{N-2}{N^2}, \overbrace{\frac{1}{N} - \frac{2}{N^2}, \ldots, \frac{1}{N} - \frac{2}{N^2}}^{(N-2)/2}\Big).$$

Then we have

$$\lim_{N\to\infty} \bar{P}_N(n) = 0,$$

for any n.

In $\mathbb{Z}$ case, the probability distribution $P(n,t)$ of the walk starting from the origin at location n and time t is given by

$$P(n,t) = J_n^2(t),$$

where $J_n(t)$ is the Bessel function of the first kind of order n, see Chapter 7, for example. The asymptotic behavior of $J_n(t)$ at infinity is as follows:

$$J_n(t) = \sqrt{\frac{2}{\pi t}} \left(\cos(t-\theta(n)) - \sin(t-\theta(n)) \frac{4n^2-1}{8t} + O(t^{-2}) \right), \quad t \to \infty,$$

where $\theta(n) = (2n+1)\pi/4$, see page 195 in Watson (1944). From this fact and $|J_n(t)| \le 1$ for any t and n (see page 31 in Watson (1944)), we obtain

$$\bar{P}(n) = \lim_{t\to\infty} \frac{1}{t} \int_0^t J_n^2(s)\, ds = 0,$$

for any $n \in \mathbb{Z}$.

Next we consider the quantum walk starting from a site, denoted by 0, on a hypercube with 2^N sites, W_N. Then the probability finding the walker at site n at time t is

$$P_N(n,t) = \cos(t/N)^{2(N-k)} \sin(t/N)^{2k} \qquad if \;\; n \in V_k \quad (0 \le k \le N),$$

where $V_k = \{x \in W_N : ||x|| = k\}$ and $||x||$ is the path length from 0 to x in W_N. A derivation is shown in Jafarizadeh and Salimi (2007). From the result we see that

$$\bar{P}_N(n) = \frac{1}{2^{2N}} \binom{N}{k}^{-1} \binom{2k}{k} \binom{2(N-k)}{N-k},$$

if $n \in V_k$ $(0 \le k \le N)$. For example, when $N = 4$,

$$\bar{P}_4(n) = \begin{cases} 35/128 & if \;\; n \in V_0 \cup V_4, \\ 5/128 & if \;\; n \in V_1 \cup V_3, \\ 3/128 & if \;\; n \in V_2. \end{cases}$$

For general N, we have

$$\lim_{N\to\infty} \bar{P}_N(n) = 0,$$

for any $n = 0, 1, \ldots$. Moreover if we let

$$\bar{P}_N(V_k) = \sum_{n \in V_k} \bar{P}_N(n),$$

for $k = 0, 1, \ldots, N$, then we get

$$\bar{P}_N(V_k) = \frac{1}{2^{2N}}\binom{2k}{k}\binom{2(N-k)}{N-k},$$

since $|V_k| = N!/(N-k)!k!$. It is interesting to note that this probability corresponds to the well-known arcsine law for the classical random walk.

Therefore, in three cases, C_N (cycle graph) and W_N (N-cube) as $N \to \infty$ and $\mathbb{Z}$, the localization does not occur at any location.

In the case of the complete graph with N sites, K_N, the Hamiltonian H_N is defined by $H_N = I_N - NJ_N$. Then eigenvalues of H_N are $\eta_0 = 0, \eta_1 = \eta_2 = \cdots = \eta_{N-1} = -N$. The eigenvectors are given by the Vandermonde matrix, see Ahmadi et al. (2003). Then direct computation yields

$$P_N(n,t) = \begin{cases} \dfrac{(N-1)^2 + 1 + 2(N-1)\cos(Nt)}{N^2} & if\ \ n = 0, \\ \dfrac{2(1-\cos(Nt))}{N^2} & if\ \ n = 1, 2, \ldots, N-1. \end{cases}$$

Therefore

$$\bar{P}_N(n) = \begin{cases} \dfrac{(N-1)^2 + 1}{N^2} & if\ \ n = 0, \\ \dfrac{2}{N^2} & if\ \ n = 1, 2, \ldots, N-1. \end{cases}$$

So we have

$$\lim_{N\to\infty} \bar{P}_N(n) = \delta_0(n),$$

for any $n = 0, 1, \ldots$. Therefore the localization occurs only at $n = 0$. This corresponds to our case for $p \to \infty$.

9.6 Conclusion

We have derived the expression of the probability distribution of a continuous-time quantum walk on $T_M^{(p)}$ corresponding to $\mathbb{Z}_p$ in the $M \to \infty$ limit. As a result, we obtained

$$\bar{P}_\infty^{(p)}(n) = \lim_{M\to\infty} \bar{P}_M^{(p)}(n) > 0 \quad (n = 0, 1, 2, \ldots),$$

for a class of ϵ_k satisfying

$$\epsilon_0 < 0 < \epsilon_M < \epsilon_{M-1} < \cdots < \epsilon_2 < \epsilon_1.$$

Therefore the localization occurs at any location. For C_N (cycle graph) and W_N (N-cube) as $N \to \infty$ and $\mathbb{Z}$ cases, the localization does not happen at any location. For K_N (complete graph) as $N \to \infty$ case, the localization occurs only at 0. In three typical classical cases, the localization does not occur even at 0 site. We hope that this property of our quantum walk can be useful in search problems on a tree-like hierarchical structure.

10 Cycle

10.1 Introduction

In this chapter we treat the continuous-time quantum walk on C_N which is the cycle with N vertices, i.e., $C_N = \{0, 1, \dots, N-1\}$. Results here appeared in Inui, Kasahara, Konishi, and Konno (2005). Let A be the $N \times N$ adjacency matrix of C_N. The continuous-time quantum walk considered here is given by the following unitary matrix:

$$U(t) = e^{-itA/2}.$$

Following the paper of Ahmadi et al. (2003), we take $-itA/2$ instead of $itA/2$. The amplitude wave function at time t, $\Psi_N(t)$, is defined by

$$\Psi_N(t) = U(t)\Psi_N(0).$$

The $(n+1)$-th coordinate of $\Psi_N(t)$ is denoted by $\Psi_N(n,t)$ which is the amplitude wave function at vertex n at time t for $n = 0, 1, \dots, N-1$. In this chapter we take $\Psi_N(0) = {}^T[1, 0, 0, \dots, 0]$ as initial state. The probability that the particle is at vertex n at time t, $P_N(n,t)$, is given by

$$P_N(n,t) = |\Psi_N(n,t)|^2.$$

Here we give a connection between a continuum time limit model for discrete-time quantum walk on $\mathbb{Z}$ given by Romanelli et al. (2003) and continuous-time quantum walk on circles. Ahmadi et al. (2003) showed

$$\Psi_N(n,t) = \frac{1}{N} \sum_{j=0}^{N-1} e^{-i(t\cos\xi_j - n\xi_j)}, \tag{10.1.1}$$

for any $t \geq 0$ and $n = 0, 1, \dots, N-1$, where $\xi_j = 2\pi j/N$. As Ahmadi et al. (2003) pointed out, $\Psi_N(n,t)$ can be also expressed by using the Bessel function, that is,

$$\Psi_N(n,t) = \sum_{k=n\ (modN)} (-i)^k J_k(t) = \frac{1}{2} \sum_{k=\pm n\ (modN)} (-i)^k J_k(t), \tag{10.1.2}$$

where $J_\nu(z)$ is the Bessel function. In fact, the generating function of the Bessel function:

$$\exp\left[\frac{t}{2}\left(z-\frac{1}{z}\right)\right] = \sum_{\nu\in\mathbb{Z}} z^\nu J_\nu(t),$$

gives

$$e^{-it\cos\xi_j} = \sum_{\nu\in\mathbb{Z}}(-i)^\nu e^{i\nu\xi_j} J_\nu(t).$$

By using (10.1.1), the amplitude wave function is then calculated as

$$\Psi_N(n,t) = \frac{1}{N}\sum_{j=0}^{N-1}\sum_{\nu\in\mathbb{Z}}(-i)^\nu e^{i(n+\nu)\xi_j} J_\nu(t). \tag{10.1.3}$$

In a similar way, we have

$$\Psi_N(n,t) = \frac{1}{N}\sum_{j=0}^{N-1}\sum_{\nu\in\mathbb{Z}}(-i)^\nu e^{i(n-\nu)\xi_j} J_\nu(t). \tag{10.1.4}$$

From (10.1.3) and (10.1.4), we obtain (10.1.2). Moreover, (10.1.2) gives

$$\begin{aligned} P_N(n,t) &= \sum_{j,k\in\mathbb{Z}} \cos\left(\frac{\pi}{2}(j-k)N\right) J_{jN+n}(t) J_{kN+n}(t) \\ &= \sum_{k\in\mathbb{Z}} J_{kN+n}(t)^2 \\ &\quad + \sum_{j\neq k: j,k\in\mathbb{Z}} \cos\left(\frac{\pi}{2}(j-k)N\right) J_{jN+n}(t) J_{kN+n}(t). \end{aligned} \tag{10.1.5}$$

The following formula is well known (see page 213 in Andrews, Askey, and Roy (1999)):

$$\sum_{k\in\mathbb{Z}} J_k(t)^2 = 1, \tag{10.1.6}$$

for $t \geq 0$. That is, $\{J_k(t)^2 : k \in \mathbb{Z}\}$ is a probability distribution on $\mathbb{Z}$ for any time t. Then (10.1.6) can be rewritten as

$$\sum_{n=0}^{N-1}\sum_{k\in\mathbb{Z}} J_{kN+n}(t)^2 = 1, \tag{10.1.7}$$

for $t \geq 0$. Thus (10.1.5) and (10.1.7) give

$$\sum_{n=0}^{N-1} \sum_{j \neq k : j,k \in \mathbb{Z}} \cos\left(\frac{\pi}{2}(j-k)N\right) J_{jN+n}(t) J_{kN+n}(t) = 0.$$

Romanelli et al. (2003) studied a continuum time limit for a discrete-time quantum walk on $\mathbb{Z}$ and obtained the position probability distribution. When the initial condition is given by $\tilde{a}_l(0) = \delta_{l,0}, \tilde{b}_l(0) \equiv 0$ in their notation for the Hadamard walk, the distribution becomes the following in our notation:

$$P(n,t) = J_n(t/\sqrt{2})^2.$$

More generally, we consider a discrete-time quantum walk whose coin flip transformation is given by the following unitary matrix:

$$U = \begin{bmatrix} a & b \\ c & d \end{bmatrix}.$$

Note that $a = b = c = -d = 1/\sqrt{2}$ case is equivalent to the Hadamard walk. In a similar fashion, we have

$$P(n,t) = J_n(at)^2. \qquad (10.1.8)$$

In fact, (10.1.6) guarantees $\sum_{n \in \mathbb{Z}} P(n,t) = 1$ for any $t \geq 0$. From the probability theoretical point of view, it is interesting that a continuum time limit model for a discrete-time quantum walk on $\mathbb{Z}$ gives a simple model having a squared Bessel distribution in the above meaning. For large N, (10.1.5) is similar to (10.1.8) except for the second term of the right-hand side of (10.1.5).

To investigate fluctuations for continuous-time quantum walks, we consider both instantaneous uniform mixing property (see below) and temporal standard deviation (see Section 10.4). The former corresponds to a spatial fluctuation and the latter corresponds a temporal one.

A walk starting from 0 on C_N has the instantaneous uniform mixing property (IUMP) if there exists $t > 0$ such that $P_N(n,t) = 1/N$ for any $n = 0, 1, \ldots, N-1$. To restate this definition, we introduce the total variation distance which is the notion of distance between probability distributions defined as

$$||P - Q|| = \max_{A \subset C_N} |P(A) - Q(A)| = \frac{1}{2} \sum_{n \in C_N} |P(n) - Q(n)|. \qquad (10.1.9)$$

By using this, the IUMP can be rewritten as follows: if there exists $t > 0$ such that $||P_N(\cdot,t) - \pi_N|| = 0$, where π_N is the uniform distribution on C_N. As we will mention in Section 10.3, continuous-time quantum walks on C_N for $N = 3, 4$ have the IUMP. On the other hand, Ahmadi et al. (2003) conjectured that continuous-time quantum walks on C_N for $N \geq 5$ do not have the IUMP. Carlson et al. (2006) showed that the conjecture is true for

$N = 5$. It is easily checked that the conjecture is true for $N = 6$ by a direct computation (see Section 10.3). Remark that the continuous-time classical random walk on C_N does not have the IUMP for any $N \geq 3$.

10.2 Classical Case

First we review the classical case on C_N, (see Schinazi (1999) and references in his book, for example). In the continuous-time classical random walk,

$$P_N(n,t) = \frac{1}{N}\sum_{j=0}^{N-1} \cos(\xi_j n) e^{t(\cos \xi_j - 1)},$$

for any $t \geq 0$ and $n = 0, 1, \ldots, N-1$. In this walk, the distribution for the random time between two jumps is the exponential distribution. As for the discrete-time classical random walk,

$$P_N(n,t) = \frac{1}{N}\sum_{j=0}^{N-1} \cos(\xi_j n)(\cos \xi_j)^t,$$

for any $t = 0, 1, \ldots,$ and $n = 0, 1, \ldots, N-1$. Here a time-averaged distribution in the continuous-time case is given by

$$\bar{P}_N(n) = \lim_{T\to\infty} \frac{1}{T}\int_0^T P_N(n,t)dt, \qquad (10.2.10)$$

if the right-hand side of (10.2.10) exists. As for the discrete-time case,

$$\bar{P}_N(n) = \lim_{T\to\infty} \frac{1}{T}\sum_{t=0}^{T-1} P_N(n,t), \qquad (10.2.11)$$

if the right-hand side of (10.2.11) exists. Concerning the continuous-time classical case, it is easily shown that $P_N(n,t) \to 1/N$ $(t \to \infty)$ for any $n = 0, 1, \ldots, N-1$. Then we have immediately $\bar{P}_N(n) = 1/N$ for any $n = 0, 1, \ldots, N-1$. On the other hand, in the discrete-time classical case, if N is odd, then $P_N(n,t) \to 1/N$ as $t \to \infty$, and, if N is even, then it does not converge in the limit of $t \to \infty$. However, an important property is that $\bar{P}_N$ is a uniform distribution in both the continuous- and discrete-time classical cases.

10.3 Quantum Case

Now we consider continuous-time quantum walks. As we will see later, in contrast to classical case, $\bar{P}_N$ does not become uniform distribution for any $N \geq 3$ in quantum case. From (10.1.1), we have

$$P_N(n,t) = \frac{1}{N} + \frac{2R_N(n,t)}{N^2}, \tag{10.3.12}$$

where

$$R_N(n,t) = \sum_{0 \leq j < k \leq N-1} \cos\{t(\cos\xi_j - \cos\xi_k) - n(\xi_j - \xi_k)\}, \tag{10.3.13}$$

for any $t \geq 0$ and $n = 0, 1, \ldots, N-1$. It is easily checked that

$$R_N(n,t) = R_N(N-n,t),$$

for any $t \geq 0$ and $n = 1, \ldots, \bar{N}$, where $\bar{N} = [(N-1)/2]$ and $[x]$ is the smallest integer greater than x. For example, when $N = 3$,

$$\begin{aligned} R_3(0,t) &= 2\cos(3t/2) + 1, \\ R_3(1,t) &= R_3(2,t) = -\cos(3t/2) - 1/2, \end{aligned}$$

when $N = 4$,

$$\begin{aligned} R_4(0,t) &= \cos(2t) + 4\cos(t) + 1, \\ R_4(1,t) &= R_4(3,t) = -\cos(2t) - 1, \\ R_4(2,t) &= \cos(2t) - 4\cos(t) + 1. \end{aligned}$$

So if $N = 3$, then $R_3(n,t) = 0$ for any $t = \pm 4\pi/9 + 4m\pi/3$ $(m \in \mathbb{Z})$ and $n = 0, 1, 2$, and if $N = 4$, then $R_4(n,t) = 0$ for any $t = \pi/2 + m\pi$ $(m \in \mathbb{Z})$ and $n = 0, 1, 2, 3$. Therefore continuous-time quantum walks on C_3 and C_4 have IUMP. This result was given in Ahmadi et al. (2003). On the other hand, when $N = 6$,

$$\begin{aligned} R_6(0,t) &= \cos(2t) + 4\cos(3t/2) + 4\cos(t) + 4\cos(t/2) + 2, \\ R_6(1,t) &= R_6(5,t) = -\cos(2t) - 2\cos(3t/2) - \cos(t) + 2\cos(t/2) - 1, \\ R_6(2,t) &= R_6(4,t) = \cos(2t) - 2\cos(3t/2) + \cos(t) - 2\cos(t/2) - 1, \\ R_6(3,t) &= -\cos(2t) + 4\cos(3t/2) - 4\cos(t) - 4\cos(t/2) + 2. \end{aligned}$$

Direct computation implies that a continuous-time quantum walk on C_6 does not have IUMP.

Now we consider the time-averaged distribution for continuous-time case. By using (10.3.12), we have

Theorem 10.1.

$$\bar{P}_N(n) = \frac{1}{N} + \frac{2R_N(n)}{N^2}, \tag{10.3.14}$$

for any $n = 0, 1, \ldots, N-1$, *where*

$$R_N(n) = \begin{cases} -1/2 & \text{if } N = \text{odd}, \quad \xi_{2n} \neq 0 \pmod{2\pi}, \\ -1 & \text{if } N = \text{even}, \quad \xi_{2n} \neq 0 \pmod{2\pi}, \\ \bar{N} & \text{if } \xi_{2n} = 0 \pmod{2\pi}. \end{cases}$$

This result gives

$$\bar{P}_N(0) = \frac{1}{N} + \frac{2\bar{N}}{N^2}. \tag{10.3.15}$$

As for discrete-time quantum case given by the Hadamard transformation, Aharonov et al. (2001) and Bednarska et al. (2003) showed that $\bar{P}_N(n) \equiv 1/N$ if N is odd or $N = 4$, and $\bar{P}_N(n) \not\equiv 1/N$, otherwise. So in contrast to classical continuous- and discrete-time and quantum discrete-time cases, $\bar{P}_N$ in quantum continuous-time case is not uniform distribution on C_N for any $N \geq 3$. In fact, when $N =$ odd (i.e., $\bar{N} = (N-1)/2$),

$$\bar{P}_N = \Big(\frac{1}{N} + \frac{N-1}{N^2}, \overbrace{\frac{1}{N} - \frac{1}{N^2}, \ldots, \frac{1}{N} - \frac{1}{N^2}}^{N-1}\Big),$$

when $N =$ even (i.e., $\bar{N} = (N-2)/2$),

$$\bar{P}_N = \Big(\frac{1}{N} + \frac{N-2}{N^2}, \overbrace{\frac{1}{N} - \frac{2}{N^2}, \ldots, \frac{1}{N} - \frac{2}{N^2}}^{(N-2)/2}, \\ \frac{1}{N} + \frac{N-2}{N^2}, \overbrace{\frac{1}{N} - \frac{2}{N^2}, \ldots, \frac{1}{N} - \frac{2}{N^2}}^{(N-2)/2}\Big).$$

For examples,

$$\bar{P}_3 = \left(\frac{5}{9}, \frac{2}{9}, \frac{2}{9}\right), \qquad \bar{P}_4 = \left(\frac{3}{8}, \frac{1}{8}, \frac{3}{8}, \frac{1}{8}\right).$$

10.4 Temporal Standard Deviation

We consider the following temporal standard deviation $\sigma_N(n)$ in the continuous-time case as in the discrete-time case:

$$\sigma_N(n) = \lim_{T\to\infty} \sqrt{\frac{1}{T}\int_0^T \left(P_N(n,t) - \bar{P}_N(n)\right)^2 dt}, \qquad (10.4.16)$$

if the right-hand side of (10.4.16) exists. In the discrete-time case,

$$\sigma_N(n) = \lim_{T\to\infty} \sqrt{\frac{1}{T}\sum_{t=0}^{T-1} \left(P_N(n,t) - \bar{P}_N(n)\right)^2}, \qquad (10.4.17)$$

if the right-hand side of (10.4.17) exists. In both continuous- and discrete-time classical cases,

$$\sigma_N(n) = 0,$$

for $N \geq 3$ and $n = 0, 1, \ldots, N-1$. The reason is as follows. In the case of classical random walk starting from a site for $N =$ odd (i.e., aperiodic case), a coupling method implies that there exist $a \in (0,1)$ and $C > 0$ (are independent of n and t) such that

$$|P_N(n,t) - \bar{P}_N(n)| \leq Ca^t,$$

for any n and t (see page 63 of Schinazi (1999), for example). Therefore we obtain

$$\frac{1}{T}\sum_{t=0}^{T-1} \left(P_N(n,t) - \bar{P}_N(n)\right)^2 \leq \frac{C^2}{T}\frac{1-a^{2T}}{1-a^2}.$$

The above inequality implies that $\sigma_N(n) = 0$ $(n = 0, 1, \ldots, N-1)$. As for $N =$ even (i.e., periodic) case, we have the same conclusion $\sigma_N(n) = 0$ for any n by using a little modified argument. The same conclusion can be extended to the continuous-time classical case in a standard fashion.

For the discrete-time quantum case, Theorem 5.3 gives

$$\sigma_N^2(n) = \frac{1}{N^4}\left[2\left\{S_+^2(n) + S_-^2(n)\right\} + 11S_0^2 + 10S_0S_1 + 3S_1^2 - S_2(n)\right] - \frac{2}{N^3}, \qquad (10.4.18)$$

for any $n = 0, 1, \ldots, N-1$, where $N(\geq 3)$ is odd and

$$S_0 = \sum_{j=0}^{N-1} \frac{1}{3+\cos\theta_j}, \qquad S_1 \;=\; \sum_{j=0}^{N-1} \frac{\cos\theta_j}{3+\cos\theta_j},$$
$$S_+(n) = \sum_{j=0}^{N-1} \frac{\cos((n-1)\theta_j) + \cos(n\theta_j)}{3+\cos\theta_j},$$
$$S_-(n) = \sum_{j=0}^{N-1} \frac{\cos((n-1)\theta_j) - \cos(n\theta_j)}{3+\cos\theta_j},$$
$$S_2(n) = \sum_{j=1}^{N-1} \frac{7+\cos(2\theta_j) + 8\cos\theta_j \cos^2((n-1/2)\theta_j)}{(3+\cos\theta_j)^2},$$

with $\theta_j = \xi_{2j} = 4\pi j/N$. For example,

$$\sigma_3(0) = \sigma_3(1) = \frac{2\sqrt{46}}{45}, \quad \sigma_3(2) = \frac{2}{9}. \tag{10.4.19}$$

Furthermore from Proposition 5.4 we have

$$\sigma_N(0) = \frac{\sqrt{13-8\sqrt{2}}}{N} + o\left(\frac{1}{N}\right), \tag{10.4.20}$$

as $N \to \infty$. The above result implies that the temporal standard deviation $\sigma_N(0)$ in the discrete-time case decays in the form $1/N$ as N increases.

Now we consider the continuous-time quantum case. For example, direct computation gives

$$\sigma_3(0) = \frac{2\sqrt{2}}{9}, \quad \sigma_3(1) = \sigma_3(2) = \frac{\sqrt{2}}{9},$$
$$\sigma_4(0) = \sigma_4(2) = \frac{\sqrt{34}}{16}, \quad \sigma_4(1) = \sigma_4(3) = \frac{\sqrt{2}}{16},$$
$$\sigma_5(0) = \frac{4\sqrt{3}}{25}, \quad \sigma_5(1) = \sigma_5(2) = \sigma_5(3) = \sigma_5(4) = \frac{2\sqrt{2}}{25},$$
$$\sigma_6(0) = \sigma_6(3) = \frac{7\sqrt{2}}{36}, \quad \sigma_6(1) = \sigma_6(2) = \sigma_5(4) = \sigma_5(5) = \frac{\sqrt{5}}{18}.$$

From now on we focus on general $N =$ odd case to obtain results corresponding to the discrete-time case (i.e., (10.4.18) and (10.4.20)). The definition of $\sigma_N(n)$ implies

$$\begin{aligned} \sigma_N^2(n) &= \frac{4}{N^4} \times \lim_{T\to\infty} \frac{1}{T} \int_0^T (R_N(n,t) - R_N(n))^2 \, dt \\ &= \frac{4}{N^4} \times \left\{ \lim_{T\to\infty} \frac{1}{T} \int_0^T R_N(n,t)^2 dt - R_N(n)^2 \right\}. \end{aligned}$$

For $N =$ odd case, we have

$$R_N(n) = \begin{cases} (N-1)/2 & n = 0, \\ -1/2 & n = 1, 2, \ldots, N-1. \end{cases}$$

From (10.3.13), we have

$$\begin{aligned}
&\lim_{T\to\infty} \frac{1}{T} \int_0^T R_N^2(n,t)dt \\
&= \lim_{T\to\infty} \frac{1}{T} \int_0^T \left[\sum_{0\le j_1<k_1\le N-1} \cos\{t(\cos\xi_{j_1} - \cos\xi_{k_1}) - n(\xi_{j_1} - \xi_{k_1})\} \right] \\
&\qquad \times \left[\sum_{0\le j_2<k_2\le N-1} \cos\{t(\cos\xi_{j_2} - \cos\xi_{k_2}) - n(\xi_{j_2} - \xi_{k_2})\} \right] dt \\
&= \lim_{T\to\infty} \frac{1}{2T} \int_0^T dt \sum_{0\le j_1<k_1\le N-1} \sum_{0\le j_2<k_2\le N-1} \\
&\Big[\cos\{t((\cos\xi_{j_1} - \cos\xi_{k_1}) - (\cos\xi_{j_2} - \cos\xi_{k_2})) - n((\xi_{j_1} - \xi_{k_1}) - (\xi_{j_2} - \xi_{k_2}))\} \\
&+ \cos\{t((\cos\xi_{j_1} - \cos\xi_{k_1}) + (\cos\xi_{j_2} - \cos\xi_{k_2})) - n((\xi_{j_1} - \xi_{k_1}) + (\xi_{j_2} - \xi_{k_2}))\}\Big].
\end{aligned}$$

Remark that each $(N^2 - N)^2$ term becomes zero except in the following two cases:

$$\cos\xi_{j_1} - \cos\xi_{k_1} - \cos\xi_{j_2} + \cos\xi_{k_2} = 0,$$
$$\cos\xi_{j_1} - \cos\xi_{k_1} + \cos\xi_{j_2} - \cos\xi_{k_2} = 0.$$

Therefore some complicated computations imply

$$\begin{aligned}
\lim_{T\to\infty} \frac{1}{T} \int_0^T R_N^2(0,t)dt &= \frac{5}{8}(N-1)^2 + \frac{1}{8}(N-1)(5N-13) \\
&= \frac{1}{4}(N-1)(5N-9),
\end{aligned}$$

and

$$\begin{aligned}
\lim_{T\to\infty} \frac{1}{T} \int_0^T R_N^2(n,t)dt &= \frac{1}{8}\left(2N^2 - 4N + 6 - \frac{1}{\cos^2 \frac{n\pi}{N}}\right) \\
&\qquad + \frac{1}{8}\left(-6N + 12 + \frac{1}{\cos^2 \frac{n\pi}{N}}\right) \\
&= \frac{1}{4}(N^2 - 5N + 9),
\end{aligned}$$

for any $n = 1, 2, \ldots, N-1$. Then we have the following main result.

Theorem 10.2. *When $N(\geq 3)$ is odd,*

$$\sigma_N(0) = \frac{2\sqrt{N^2 - 3N + 2}}{N^2},$$
$$\sigma_N(n) = \frac{\sqrt{N^2 - 5N + 8}}{N^2} \quad (n = 1, \ldots, N-1). \tag{10.4.21}$$

In particular, $\sigma_N(0) > \sigma_N(n)$ for any $n = 1, \ldots, N-1$.

We should remark that there is a difference between the continuous-time case and the discrete-time one, since, for example, (10.4.19) gives $\sigma_3(0) = \sigma_3(1) > \sigma_3(2)$ in the discrete-time case. Furthermore (10.4.21) implies

Corollary 10.3.

$$\sigma_N(0) = \frac{2}{N} + o\left(\frac{1}{N}\right),$$
$$\sigma_N(n) = \frac{1}{N} + o\left(\frac{1}{N}\right) \quad (n = 1, \ldots, N-1), \tag{10.4.22}$$

as $N \to \infty$.

The above result implies that the temporal fluctuation $\sigma_N(0)$ in the continuous-time case decays in the form $1/N$ as N increases as in the discrete-time case. However, from $\sqrt{13 - 8\sqrt{2}} < 2$ (see (10.4.20) and (10.4.22)), it follows that the temporal standard deviation of the continuous-time case at site 0 is greater than that of the discrete-time case for large N.

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Edited by J.-M. Morel, F. Takens, B. Teissier, P.K. Maini

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