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Editors

Spectral Analysis of Quantum Hamiltonians

Spectral Days 2010

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Preface

Spectral analysis has been thriving for years as a vital part of mathematical physics and analysis. Conferences dealing with various aspects of spectral analysis are frequently organized, but the spectral community is only beginning to build its own organization. The International Spectral Network was formed in 2010 by a number of research groups around the world with the aim of fostering worldwide collaboration in the field. One of the aims of the Network is to establish Spectral Days as the regular conference on spectral analysis where researchers will meet to discuss and record recent progress.

Spectral Days 2010 was the first conference organized by the Spectral Network. It took place in Santiago, Chile, in September 2010. This volume contains expanded versions of many of the research talks and surveys delivered in Santiago. The second Spectral Days conference took place in Munich in April 2012 and we hope that the reader will soon peruse the second of many volumes covering recent progress in Spectral Analysis.

This volume contains surveys as well as research articles in topics ranging from spectral continuity for magnetic and pseudodifferential operators, localization in random media, stability of matter, to properties of Aharonov–Bohm Hamiltonians and spectral properties of Quantum Hall Hamiltonians. Also included are studies of operators associated to waveguides, resonance in time-dependent systems, supersymmetric models with singular potentials, non-linear equations related to bosonic strings, dissipative fermion systems and conjugate operators in connection with time operators and time delay.

We take the opportunity to heartily thank the Chilean *Iniciativa Científica Milenio* whose generous funding of the Scientific Nucleus ICM P07-027-F "Mathematical Theory of Quantum and Classical Magnetic Systems" made the conference possible. We also thank the Mathematics Faculty of the Pontificia Universidad Católica de Chile for hosting and supporting the conference. Our thanks also go to the International Spectral Network for choosing Santiago as the first venue of Spectral Days and for travel support for several participants.

We also wish to warmly thank Liliya Simeonova. Without her help, Spectral Days 2010 could not have taken place and this volume would not have seen the light of day.

Rafael Benguria Eduardo Friedman Marius Mantoiu

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Remarks on Sojourn Time Estimates for Periodic Time-dependent Quantum Systems

J. Asch[1)], O. Bourget[2)], V.H. Cortés[3)] and C. Fernández[4)]

Abstract. We study some solutions of the Schrödinger equation,

$$i\frac{\partial u}{\partial t} = H(t)u$$

where $H(\cdot)$ is a periodic time-dependent Hamiltonian acting on a Hilbert space $\mathcal{H}$. We prove sojourn time estimates, first by means of an extension of the energy-time Uncertainty Principle, and then, for a specific model by explicit computations.

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1. Introduction

The long-time behavior of a time-dependent quantum system is related to the spectral properties of its Floquet Hamiltonian [5], [6] or its Floquet operator in the periodic case [4]. Among the systems considered in the literature, a particular attention has been devoted to time-periodic perturbations of absolutely continuous systems (see for example [1], [2], [14] and references therein).

The long time behavior is also closely connected with the concept of resonance, understood here in a dynamical way. Roughly speaking, a state is resonant if it exhibits slow exponential decay of its autocorrelation function at least for a certain time range [3], [12]. For precise results in the case of perturbation of a Hamiltonian having a simple embedded bound state, see [3] and references therein. In [8], the author shows this behavior for a truncated resonant state, see also [13].

In this paper we will concentrate on the slowness of the decay instead of its precise nature. To this end we will establish lower bounds on the sojourn time,

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2) Fondecyt 1080675, ECOS-Conicyt 2010-022, ICM PROY-P07-027-F,
3) Fondecyt 1080455,
4) Fondecyt 1100304, ECOS-Conicyt 2010-022.

i.e., an integrated version of the autocorrelation function of "resonant" states. As a thumb rule remark that (a hypothetical decay) $t \mapsto \exp(-\Gamma|t|)$ would lead to a sojourn time of order $\mathcal{O}(\Gamma^{-1})$. In the following, we show an energy-time Uncertainty Principle, which provides a lower bound for the sojourn time. We review Lavine's results for the autonomous case and extend them for abstract periodic time-dependent Hamiltonians. As an application we obtain a time-dependent version of the results in [8]. In Section 3, we illustrate the resonant behavior for a specific non-autonomous model by explicit computations.

2. Energy-time Uncertainty Principle

We establish an energy-time Uncertainty Principle for periodic time-dependent Hamiltonians. To this end we will follow the framework of Floquet theory.

2.1. The autonomous case: a review

We begin by recalling the Uncertainty Principle for the autonomous case, following a result of Lavine [7].

We recall that the solution of the autonomous Schrödinger equation

$$i\frac{\partial u}{\partial t} = Hu \quad , \quad u(s) = \varphi \in \mathcal{D}(H)$$

where $s \in \mathbb{R}$ and $\mathcal{D}(H)$ denotes the domain of the self-adjoint operator H, is expressed by $u(t) = e^{-iH(t-s)}\varphi$.

Definition 2.1. *Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$, and A be a bounded self-adjoint operator acting on $\mathcal{H}$. Let us denote by $\mathcal{T}_H(A)$, the operator whose quadratic form is,*

$$\langle \varphi, \mathcal{T}_H(A)\varphi\rangle = \int_{-\infty}^{\infty} \langle e^{-iH\sigma}\varphi, Ae^{-iH\sigma}\varphi\rangle \, d\sigma \ , \tag{2.1}$$

defined for all $\varphi \in \mathcal{H}$ such that the integral converges.

If φ in $\mathcal{H}$ is a normalized state, i.e., $\|\varphi\| = 1$, its sojourn time is defined by $\mathcal{T}(\varphi) = \mathcal{T}_H(|\varphi><\varphi|)$ where $|\varphi><\varphi|$ is the one-rank projector in the direction of φ:

$$\mathcal{T}(\varphi) = \int_{-\infty}^{\infty} |\langle \varphi, e^{-iH\sigma}\varphi\rangle|^2 \, d\sigma \ .$$

Remark: In Definition 2.1, $\mathcal{T}(\varphi)$ represents the total expected amount of time the system spends in its initial state φ.

In the following, unless otherwise stated, we will suppose that the state φ is normalized and belongs to the domains of the operators acting on it.

Lemma 2.1. *Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$ with domain $\mathcal{D}(H)$. Let $\lambda_0 \in I\!R$ and $\varphi \in \mathcal{D}(H)$ such that $\|\varphi\| = 1$ and $\epsilon \equiv \|(H-\lambda_0)\varphi\| > 0$. Then*

$$1 \leq 2\,\epsilon\, \|(H-\lambda_0)\varphi\| \ \|(H-\lambda_0-i\epsilon)^{-1}\varphi\|^2 \ . \tag{2.2}$$

Proof. Let $d\langle\varphi, E_\lambda\varphi\rangle$ denote the spectral measure associated to the self-adjoint operator H. Hence, $1 = \|\varphi\|^2 = |\int d\langle\varphi, E_\lambda\varphi\rangle|^2$. By Hölder's inequality,

$$1 \leq \left(\int_{-\infty}^{\infty} \frac{(\lambda-\lambda_0)^2+\epsilon^2}{\epsilon}\, d\langle\varphi, E_\lambda\varphi\rangle\right)\left(\int_{-\infty}^{\infty} \frac{\epsilon}{(\lambda-\lambda_0)^2+\epsilon^2}\, d\langle\varphi, E_\lambda\varphi\rangle\right) \quad (2.3)$$

for any $\epsilon > 0$. Using the spectral theorem for H we obtain,

$$\int_{-\infty}^{\infty} \frac{(\lambda-\lambda_0)^2+\epsilon^2}{\epsilon}\, d\langle\varphi, E_\lambda\varphi\rangle = \frac{1}{\epsilon}\|(H-\lambda_0)\varphi\|^2 + \epsilon\,.$$

If we choose $\epsilon = \|(H-\lambda_0)\varphi\|$, then

$$\int_{-\infty}^{\infty} \frac{(\lambda-\lambda_0)^2+\epsilon^2}{\epsilon}\, d\langle\varphi, E_\lambda\varphi\rangle = 2\epsilon\,. \quad (2.4)$$

On the other hand, again, applying the spectral theorem we have

$$\int \frac{\epsilon}{(\lambda-\lambda_0)^2+\epsilon^2}\, d\langle\varphi, E_\lambda\varphi\rangle = \epsilon\,\|(H-\lambda_0-i\epsilon)^{-1}\varphi\|^2\,.$$

Clearly the lemma now follows from the above identity together with (2.3) and (2.4). □

Lemma 2.2. *Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$ with domain $\mathcal{D}(H)$. Let $\lambda_0 \in \mathbb{R}$, $\varphi \in \mathcal{D}(H)$ such that $\|\varphi\| = 1$ and $\epsilon > 0$. We have the following lower bounds for the sojourn time $\mathcal{T}(\varphi)$:*

$$\mathcal{T}(\varphi) \geq 2\epsilon\,|\langle\varphi, (H-\lambda_0-i\epsilon)^{-1}\varphi\rangle|^2$$
$$\mathcal{T}(\varphi) \geq 4\epsilon^3\,\|(H-\lambda_0-i\epsilon)^{-1}\varphi\|^4\ .$$

Proof. Take $\epsilon > 0$ and consider the Laplace transform representation of $(H-\lambda_0-i\epsilon)^{-1}$, i.e.,

$$(H-\lambda_0-i\epsilon)^{-1} = i\int_0^\infty e^{-\epsilon\, t}e^{-i(H-\lambda_0)\, t}\, dt\,. \quad (2.5)$$

Let $\varphi \in \mathcal{D}(H)$, $\phi \in \mathcal{H}$, and P be a bounded operator acting on $\mathcal{H}$. Since $\|\varphi\| = 1$,

$$\begin{aligned}|\langle\phi, P(H-\lambda_0-i\epsilon)^{-1}\varphi\rangle|^2 &\leq \left|\int_0^\infty e^{-\epsilon\, t}|\,\langle\phi, Pe^{-iHt}\varphi\rangle|\, dt\right|^2 \\ &\leq \int_0^\infty e^{-2\epsilon\, t}dt\int_0^\infty |\,\langle\phi, Pe^{-iHt}\varphi\rangle|^2\, dt\,.\end{aligned}$$

Taking supremum over $\|\phi\| = 1$ in the above inequality we have

$$\|P(H-\lambda_0-i\epsilon)^{-1}\varphi\|^2 \leq \frac{1}{2\,\epsilon}\int_0^\infty \|Pe^{-iHt}\varphi\|^2\, dt\,.$$

Taking the orthogonal projector $P = |\varphi><\varphi|$ in the direction of φ, we obtain the first inequality. Concerning the second inequality, by Laplace representation:

$$(H-\lambda_0-i\epsilon)^{-1} - (H-\lambda_0+i\epsilon)^{-1} = i\int_{-\infty}^\infty e^{-\epsilon\,|t|}e^{-i(H-\lambda_0)\, t}\, dt\,. \quad (2.6)$$

Using the above representation, we obtain that:

$$\langle\varphi,((H-\lambda_0-i\epsilon)^{-1}-(H-\lambda_0+i\epsilon)^{-1})\varphi\rangle = i\int_{-\infty}^{\infty} e^{-\epsilon\,|t|}e^{i\lambda_0\,t}\langle\varphi,e^{-iH\,t}\varphi\rangle dt\,.$$

Now by the Schwarz's inequality,

$$|\langle\varphi,\left((H-\lambda_0-i\epsilon)^{-1}-(H-\lambda_0+i\epsilon)^{-1}\right)\varphi\rangle| \leq \frac{1}{\sqrt{\epsilon}}\left(\mathcal{T}(\varphi)\right)^{1/2}\,. \tag{2.7}$$

On the other hand,

$$|\langle\varphi,\left((H-\lambda_0-i\epsilon)^{-1}-(H-\lambda_0+i\epsilon)^{-1}\right)\varphi\rangle| = 2\,\epsilon\|(H-\lambda_0-i\epsilon)^{-1}\varphi\|^2$$

The inequality now follows from the above identity and estimate (2.7). □

The next result follows immediately from Lemma 2.1 and 2.2.

Theorem 2.1 (First Uncertainty Principle). *Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$ with domain $\mathcal{D}(H)$. Let $\lambda_0 \in I\!R$, $\varphi \in \mathcal{D}(H)$ such that $\|\varphi\| = 1$ and $(H-\lambda_0)\varphi \neq 0$. Then*

$$1 \leq \|(H-\lambda_0)\varphi\|\,\mathcal{T}(\varphi)\,. \tag{2.8}$$

This result gives a lower bound for the sojourn time and it can be used to construct long living states. But, a much better lower bound can be obtained in terms of the so-called *energy width.*

Definition 2.2. *Given a self-adjoint operator H on $\mathcal{H}$, a real number λ and a state φ, the energy width $\Delta_H(\lambda,\varphi)$ for the Hamiltonian H is defined by:*

$$\Delta_H(\lambda,\varphi) = \inf_{\epsilon>0}\left\{\epsilon^2\|(H-\lambda-i\epsilon)^{-1}\varphi\|^2 \geq \frac{1}{2}\right\}.$$

Remark: The energy width is zero if and only if $H\varphi = \lambda\varphi$.

Theorem 2.2 (Second Uncertainty Principle).

$$\frac{1}{2} \leq \Delta_H(\lambda,\varphi)\,\mathcal{T}(\varphi)\,. \tag{2.9}$$

We refer to [7] for a proof.

Remark: Let us consider a Hamiltonian of the form $H_\beta = H_0 + \beta V$. Assume λ_0 is a simple, embedded eigenvalue of H_0 with associated eigenvector φ: $H_0\varphi = \lambda_0\varphi$. Under suitable hypotheses, [3] shows that when t tends to infinity, up to small errors,

$$\langle\varphi,e^{-iH_\beta t}\varphi\rangle \approx e^{-i(\lambda_\beta - i\Gamma_\beta)t},$$

where β is small, λ_β is close to λ_0, Γ_β is positive and of order β^2 (Fermi Golden Rule). Therefore, the sojourn time of φ is $\mathcal{O}(\beta^{-2})$. Lavine's second Uncertainty Principle gives precisely a lower bound of this order (with no extra hypothesis), while the one involving the variance only gives $\mathcal{O}(\beta^{-1})$.

2.2. The non-autonomous case

In this section, some of the ideas exposed before are adapted to the non-autonomous context.

For simplicity, the Hamiltonian $(H(t))_{t\in\mathbb{R}}$ will stand for a strongly continuous family of self-adjoint operators with common domain $\mathcal{D}$. We assume it satisfies adequate conditions so that the solution of the associated Schrödinger equation

$$i\,\frac{\partial u}{\partial t} = H(t)u \ , \ u(s) = \varphi \in \mathcal{D} \tag{2.10}$$

is given by a strongly continuous unitary propagator $(U(t,s))$ [10], [11].

We start by an adaptation of the concept of the sojourn time into this framework:

Definition 2.3. *Let $(U(t,s))$ be a strongly continuous unitary propagator defined on some Hilbert space $\mathcal{H}$ and φ in $\mathcal{H}$. The sojourn time associated to the evolution of the state φ starting at time s ($s \in \mathbb{R}$) is defined by:*

$$\mathcal{T}_s(\varphi) = \int_{\mathbb{R}} |\langle \varphi, U(s, s-\sigma)\varphi\rangle|^2 \, d\sigma \ .$$

Since we deal in this manuscript with periodic time-dependent Hamiltonian (with period T, $T > 0$), the mean sojourn time associated to the state φ is denoted by:

$$\langle \mathcal{T}\rangle(\varphi) = \frac{1}{T}\int_0^T \mathcal{T}_s(\varphi)\, ds \ .$$

Remark: If the Hamiltonian is time-independent, i.e., $H(t) \equiv H$ for all t in $\mathbb{R}$, then for all (s,σ) in $\mathbb{R}^2$, $U(s, s-\sigma) = e^{-i\sigma H}$ and

$$\mathcal{T}_s(\varphi) = \langle \mathcal{T}\rangle(\varphi) = \mathcal{T}(\varphi) \ .$$

Our main result is an extension of Theorem 2.1 for periodic time-dependent quantum systems. In the following, the period of the system is denoted by T. Following [5], we write: $\mathcal{K} = L^2(\mathbb{R}/T\mathbb{Z}, \mathcal{H})$.

Theorem 2.3. *Let $\lambda_0 \in I\!R$ and $\varphi \in \mathcal{D}$ such that $\|\varphi\| = 1$ and $(H(t) - \lambda_0)\varphi \neq 0$ for some $t \in [0,T)$. Consider the propagator $(U(t,s))$ generated by the evolution equation* (2.10)*. Then,*

$$1 \leq \langle \mathcal{T}\rangle(\varphi) \cdot \sqrt{\frac{1}{T}\int_0^T \|(H(t) - \lambda_0)\varphi\|^2 \, dt} \ . \tag{2.11}$$

Proof. Following [5], we consider on the Hilbert space $\mathcal{K}$, the self-adjoint Floquet Hamiltonian

$$K = -i\,\partial_t + H(t)$$

with periodic boundary conditions. Let f in $\mathcal{K}$ defined by: $f(t) \equiv \varphi$ for all t. In particular, f belongs to the domain of K, $\mathcal{D}(K)$, $\|f\|_{\mathcal{K}} = 1$ and $(K - \lambda_0)f \neq 0$. Applying Theorem 2.1, we have that:

$$1 \leq \|(K - \lambda_0)f\|_{\mathcal{K}} \, \mathcal{T}_K(f) \, .$$

In addition, we have that for all $t \in \mathbb{R}$,

$$\|((K - \lambda_0)f)(t)\| = \|(H(t) - \lambda_0)\varphi\|$$

$$\text{and} \quad \|(K - \lambda_0)f\|_{\mathcal{K}}^2 = \frac{1}{T} \int_0^T \|(H(t) - \lambda_0)\varphi\|^2 \, dt \ .$$

On the other hand, the sojourn time $\mathcal{T}_K(f)$ for the state f in $\mathcal{K}$ is defined by

$$\mathcal{T}_K(f) = \int_{-\infty}^{\infty} |\langle f, e^{-iK\sigma} f \rangle_{\mathcal{K}}|^2 \, d\sigma \, .$$

Since for all t and σ in $\mathbb{R}$, $(e^{-iK\sigma} f)(t) = U(t, t - \sigma) f(t - \sigma)$, we have that:

$$\begin{aligned} \mathcal{T}_K(f) &= \int_{-\infty}^{\infty} \left| \frac{1}{T} \int_0^T \langle \varphi, U(t, t - \sigma)\varphi \rangle \, dt \right|^2 d\sigma \\ &\leq \frac{1}{T} \int_{-\infty}^{\infty} \int_0^T |\langle \varphi, U(t, t - \sigma)\varphi \rangle|^2 \, dt \, d\sigma \\ &\leq \langle \mathcal{T} \rangle(\phi) \ . \end{aligned}$$

Inequality (2.11) follows. □

Corollary 2.1. *Let H_0 be a self-adjoint operator defined on the Hilbert space $\mathcal{H}$ with domain $\mathcal{D}$. Assume that λ_0 is an eigenvalue of H_0 and φ a corresponding normalized eigenvector. Let $(V(t))$ be a strongly continuous periodic time-dependent family of symmetric and bounded operators on $\mathcal{H}$ (with period T, $T > 0$). For $\beta \in \mathbb{R}$, define the Hamiltonian $(H_\beta(t))_{t \in \mathbb{R}}$ by: $H_\beta(t) = H_0 + \beta V(t)$. Then, if $\beta \in \mathbb{R} \setminus \{0\}$ and $H_\beta(t)\varphi \neq 0$ for some $t \in [0, T)$,*

$$|\beta| \sup_{t \in [0,T)} \|V(t)\| \cdot \langle \mathcal{T}_\beta \rangle(\varphi) \geq 1 \, .$$

3. A model

In this paragraph, we consider a variation of the two-states quantum model presented in [9].

In the following $\mathcal{H}$ denotes the Hilbert space $\mathbb{C} \oplus L^2(\mathbb{R})$ with inner product

$$\langle (z_1, f_1), (z_2, f_2) \rangle = \bar{z}_1 z_2 \ + \ \langle f_1, f_2 \rangle \, .$$

M stand for the multiplication operator by x on $L^2(\mathbb{R})$ and E_0 is a fixed real number. Let us define the time-dependent Hamiltonian $(H(t))_{t \in \mathbb{R}}$ on $\mathcal{H}$ by: $H(t) =$

$H_0 + \beta h(t)V$ where $\beta \in \mathbb{R}$, h is a C^1, T-periodic real-valued function ($T > 0$) and

$$H_0 = \begin{pmatrix} E_0 & 0 \\ 0 & M \end{pmatrix} \ . \tag{3.1}$$

The perturbation operator V is defined by:

$$V = \begin{pmatrix} 0 & w^* \\ w & 0 \end{pmatrix} \tag{3.2}$$

with $w : \mathbb{C} \to L^2(\mathbb{R})$ given by $w(z) = z\omega$ where $|\omega(x)|^2 = \pi^{-1}(1+x^2)^{-1}$ and $w^*(f) =< \omega, f >$. The spectrum of the unperturbed operator H_0 may be described as an absolutely continuous component $\mathbb{R}$ with an embedded eigenvalue E_0 of multiplicity one. The associated eigenvector $(1,0)^t$ will be denoted by ψ. For simplicity, we assume that $E_0 = 0$. If the propagator associated to the Hamiltonian $(H(t))$ is denoted by $(U(t,s))$, we write:

$$\begin{pmatrix} z(t,s) \\ f(t,s) \end{pmatrix} \equiv U(t,s) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \ . \tag{3.3}$$

In particular, for all $(t,s) \in \mathbb{R}^2$, $\langle \psi, U(t,s)\psi \rangle = z(t,s)$.

We start our discussion by the following lemma:

Lemma 3.1. *Assume that for all t, $h(t) \neq 0$. Then, given s in $\mathbb{R}$, for all $t \geq s$, the function $z : t \mapsto z(t,s)$ is solution of the following Cauchy problem:*

$$\frac{\partial^2 z}{\partial t^2} + \left(1 - \frac{\partial \ln |h|}{\partial t}\right) \frac{\partial z}{\partial t} + \beta^2 h^2 z = 0 \tag{3.4}$$

with $z(s,s) = 1$, $\partial_t z(s,s) = 0$.

Proof. Following our notations, the Schrödinger equation

$$i\partial_t U(t,s)\psi = H(t)U(t,s)\psi$$

may be rewritten as a system:

$$i\frac{\partial z}{\partial t} = \beta h(t) \langle \omega, f \rangle \tag{3.5}$$

$$i\frac{\partial f}{\partial t} = Mf + \beta h(t) z\omega \tag{3.6}$$

with initial conditions: $z(s,s) = 1$, $f(s,s) = 0$. We deduce that

$$f(t,s) = \left(-i\beta \int_s^t e^{ix(\tau - t)} h(\tau) z(\tau, s)\, d\tau \right) \omega \, .$$

Plugging it into equation (3.5) and using the fact that for $\tau \leq t$,

$$\langle \omega, e^{ix(\tau - t)}\omega \rangle = e^{-(t-\tau)}$$

we obtain that:

$$\frac{\partial z}{\partial t}(t,s) = -\beta^2 h(t) e^{-t} \int_s^t h(\tau) z(\tau, s) e^{\tau}\, d\tau \ .$$

The result follows by derivation. □

Remark: If the function h is constant ($h \equiv h_0$ for some $h_0 \in \mathbb{R}$), which corresponds to the autonomous version of the model, equation (3.4) becomes:

$$\frac{\partial^2 z}{\partial t^2} + \frac{\partial z}{\partial t} + \beta^2 h_0^2 z = 0 \ . \tag{3.7}$$

If $0 < |\beta h_0| < 1/2$, the characteristic values associated to equation (3.7) are negative: $-\gamma_+ < -\gamma_- < 0$ where

$$\gamma_\pm = \frac{1}{2} \pm \frac{\sqrt{1 - 4\beta^2 h_0^2}}{2} \ . \tag{3.8}$$

Rewriting equation (3.7) as a first-order linear system of differential equations,

$$X_t(t,s) = A_0 X(t,s) \ ,$$

$X(s,s) = (1,0)^t$ where $X(t,s) = (z(t,s), \partial_t z(t,s))^t$ and

$$A_0 = \begin{pmatrix} 0 & 1 \\ -\beta^2 h_0^2 & -1 \end{pmatrix} \ , \tag{3.9}$$

we obtain that there exists a positive constant C (independent of s) such that: $\|X(t,s)\| \leq Ce^{-\gamma_-(t-s)}$ for all $t \geq s$. One finds that:

$$\mathcal{T}(\psi) \leq \frac{C}{\gamma_-} \ .$$

Since $\gamma_- \simeq \beta^2$ when $|\beta| \ll 1$, we recover an upper bound of order $\mathcal{O}(\beta^{-2})$ for the corresponding sojourn time. Moreover, contrasting with the original model studied in [9], the state ψ exhibits exponential decay for all $t \geq s$. mind that the spectrum of the Hamiltonian $H + \beta h_0 V$ covers the whole real line [12].

Under some suitable conditions on β and the function h, we show that this decaying behavior is preserved in our periodic setting and give an upper bound on the mean sojourn-time associated to the vector ψ. Let us precise our main result:

Proposition 3.1. *Let $\beta \in \mathbb{R}$ and $h \in C^1(\mathbb{R}, \mathbb{R})$ be a periodic time-dependent function with period T, $T > 0$ such that for all t in $\mathbb{R}$, $h(t) \neq 0$. Its average over one period is denoted by h_0. Assume that: $|\beta h_0| < 1/2$ and that*

$$\gamma \equiv \gamma_- - \sqrt{\beta^4 \sup_t [h(t)^2 - h_0^2]^2 + \sup_t [\partial_t \ln |h(t)|]^2} > 0 \ ,$$

where γ_- has been defined in (3.8)*. Then, there exists a positive constant C, independent of s, such that for all $t \geq s$:*

$$|z(t,s)| \leq Ce^{-\gamma(t-s)} \ .$$

Proof. We rewrite equation (3.4) as the following first-order system

$$X_t(t,s) = A(t) X(t,s) \ , \tag{3.10}$$

$X(s,s) = (1,0)^t$ where $X(t,s) = (z(t,s), \partial_t z(t,s))^t$ and

$$A(t) - A_0 = \begin{pmatrix} 0 & 0 \\ -\beta^2 (h(t)^2 - h_0^2) & \partial_t \ln |h(t)| \end{pmatrix} \ .$$

Following the above remark, we know that there exists $C > 0$ (independent of s) such that for all $t \geq s$,

$$\|e^{A_0(t-s)}\| \leq Ce^{-\gamma_-(t-s)} \ .$$

On the other hand, for any $t \geq s$, the solution of (3.10) satisfies,

$$X(t,s) = e^{A_0(t-s)}X(s,s) + \int_s^t e^{A_0(t-\tau)}(A(\tau) - A_0)X(\tau,s)\,d\tau$$

which, given our initial condition, implies that:

$$\|X(t,s)\| \leq Ce^{-\gamma_-(t-s)} + C\int_s^t e^{-\gamma_-(t-\tau)}\|A(\tau) - A_0\|\|X(\tau,s)\|\,d\tau \ .$$

Since for all t in $\mathbb{R}$,

$$\|A(t) - A_0\| = \sqrt{\beta^4(h(t)^2 - h_0^2)^2 + (\partial_t \ln|h(t)|)^2}$$

we obtain, using Gronwall's inequality,

$$\|X(t,s)\| \leq Ce^{-\gamma_-(t-s)}e^{\int_s^t \|A(\tau)-A_0\|\,d\tau} \leq Ce^{-\gamma(t-s)} \ . \qquad \square$$

Corollary 3.1. *Following Proposition* 3.1*, for any* $s \in [0,T)$*,*

$$\mathcal{T}_s(\psi) \leq \frac{C}{\gamma} \quad \textit{and} \quad \langle\mathcal{T}\rangle(\psi) \leq \frac{C}{\gamma} \ .$$

Proof. Since U denotes a unitary propagator, for $(s,t) \in \mathbb{R}^2$, $U(s,t) = U(t,s)^*$ and

$$\begin{aligned}\mathcal{T}_s(\psi) &= \int_{\mathbb{R}} |\langle\psi, U(s,s-\sigma)\psi\rangle|^2\,d\sigma \\ &= \int_{-\infty}^0 |\langle U(s-\sigma,s)\psi,\psi\rangle|^2\,d\sigma + \int_0^\infty |\langle\psi, U(s,s-\sigma)\psi\rangle|^2\,d\sigma \\ &= \int_{-\infty}^0 |z(s-\sigma,s)|^2\,d\sigma + \int_0^\infty |z(s,s-\sigma)|^2\,d\sigma \ .\end{aligned}$$

Applying Proposition 3.1, the result follows. $\square$

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Continuity of Spectra in Rieffel's Pseudodifferential Calculus

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Abstract. Using the fact that Rieffel's quantization sends covariant continuous fields of C^*-algebras in continuous fields of C^*-algebras, we prove spectral continuity results for families of Rieffel-type pseudodifferential operators.

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Introduction

One naturally expects that topics or tools coming from the standard pseudodifferential theory could make sense and even work in the more general setting of Rieffel's calculus. In [16, 17], some C^*-algebraic techniques of spectral analysis ([3, 4, 10, 15, 18] and references therein) were tuned with Rieffel quantization [24], getting results on spectra and essential spectra of certain self-adjoint operators that seemed to be out of reach by other methods. In the present article we continue the project by studying *spectral continuity*.

Pioneering work on applying C^*-algebraic methods to spectral continuity problems and applications to discrete physical systems may be found in [3, 5, 8]. Results on continuity of spectra for unbounded Schrödinger-like Hamiltonians (especially with magnetic fields) appear in [1, 2, 13, 20] and references therein.

Roughly, the abstract problem can be stated as follows: For each point t of the locally compact space T we are given a self-adjoint element (a classical observable) $f(t)$ of a C^*-algebra $\mathcal{A}(t)$, which is Abelian for most of the applications, and we assume some simple-minded continuity property in the variable t for this family. By quantization, $f(t)$ is turned into a quantum observable $\mathfrak{f}(t)$ belonging to a new, non-commutative C^*-algebra $\mathfrak{A}(t)$ (in spite of the notation, rather often $\mathfrak{f}(t)$ is just $f(t)$ with a new interpretation). We inquire if the family $S(t) := \mathrm{sp}\,[\mathfrak{f}(t)]$

of spectra computed in these new algebras vary continuously with t. Intuitively, outer continuity says that the family cannot suddenly expand: if for some t_0 there is a gap in the spectrum of $f(t_0)$ around a point $\lambda_0 \in \mathbb{R}$, then for t close to t_0 all the spectra $S(t)$ will have gaps around λ_0. On the other hand, inner continuity insures that if $f(t_0)$ has some spectrum in a non-trivial interval of $\mathbb{R}$, this interval will contain spectral points of all the elements $f(t)$ for t close to t_0. Although traditionally $\mathfrak{A}(t)$ is thought to be a C^*-algebra of bounded operators in some Hilbert space, the abstract situation is both natural and fruitful. One can work with abstract C^*-algebras $\mathfrak{A}(t)$ and then, if necessarily, represent them faithfully in Hilbert spaces; the spectrum will be preserved under representation.

It is well known (see Theorem 3.2) that spectral continuity can be obtained from corresponding continuity properties of resolvent families of the elements $\mathfrak{f}(t)$ but this involves both inversion and norm in each complicated C^*-algebra $\mathfrak{A}(t)$. Things are smoothed out if the family $\{\mathfrak{A}(t) \mid t \in T\}$ has a priori continuity properties, that may be connected to the concept of (upper or lower semi)-continuous C^*-bundle, cf. [25, 26] and Definition 1.1. We are going to investigate the case in which $\{\mathfrak{A}(t) \mid t \in T\}$ in obtained from another family $\{\mathcal{A}(t) \mid t \in T\}$ of simpler (classical) C^*-algebras by Rieffel quantization.

Rieffel's calculus [24, 14] is a method that transforms "simpler" C^*-algebras and morphisms into more complicated ones. The ingredients to do this are an action of the vector group $\Xi := \mathbb{R}^d$ by automorphisms of the "simple" algebra as well as a skew symmetric linear operator of Ξ. The initial data are naturally defining a Poisson structure, regarded as a mathematical modelization of the observables of a classical physical system. After applying the machine to this classical data one gets a C^*-algebra seen as the family of observables of the same system, but written in the language of Quantum Mechanics.

In simple situations the multiplication in the initial C^*-algebra is just pointwise multiplication of functions defined on some locally compact topological space Σ, on which Ξ acts by homeomorphisms. The non-commutative product in the quantized algebra can be interpreted as a symbol composition of a pseudodifferential type. Actually the concrete formulae generalize and are motivated by the usual Weyl calculus [9].

The basic technical fact is that *by Rieffel quantization an upper semi-continuous fields of C^*-algebras is turned into an upper semi-continuous fields of C^*-algebras and the same is true if upper semi-continuity is replaced by lower semi-continuity.* This is shown in [6]; a partial result without proof is announced in [11] (see also [12]). For the convenience of the readers, we are going to sketch a new proof in Section 1, relying on results from [7, 23].

As said before the most interesting cases, those which are closer to the initial spirit of Weyl quantization, involve Abelian initial algebras $\mathcal{A}$. In this situation the information is encoded in a topological dynamical system with locally compact space Σ and the upper semi-continuous field property can be read in the existence of a continuous covariant surjection $q : \Sigma \to T$; if this one is open, then lower semi-continuity also holds. This is explained in Section 2.

Using these facts, in the final sections, we prove spectral continuity. We start with families of elements belonging to the abstract Rieffel algebras. Then we outline a setting in which these algebras admit interesting faithful representations in a unique Hilbert space, thus getting spectral continuity for families of pseudodifferential-like operators. Making suitable adaptations of the dynamical system, we also include an outer continuity result for *essential spectra* of Rieffel pseudodifferential operators. As an example, we are going to show that our results cover families of zero order standard pseudodifferential operators and this is new up to or knowledge. Spectral continuity for families of elliptic strictly positive order Hamiltonians (even including variable magnetic fields) is known; see [1, 2, 13, 20]. But the methods of these articles do not extend in some obvious way to zero-order operators. The resolvent of an elliptic operator of order $m > 0$ is a pseudodifferential operator of strictly negative order and this helps a lot. In the framework of [1] for instance, it allows using a certain form of crossed product C^*-algebras, which form semi-continuous fields by well-known results [19, 22, 23]; this is not available if $m = 0$. Continuity in Planck's constant $\hbar$, treated in [24] and in [16], is also special case of our general results but we shall not repeat this here.

The full strength of these spectral techniques would require an extension of Rieffel's calculus to suitable families of unbounded elements. Hopefully this will be achieved in the future and this would be the right opportunity to present detailed examples, which could include non-elliptic positive order pseudodiferential operators with variable magnetic fields.

1. Families of Rieffel quantized C^*-algebras

Let T be a locally compact space (always supposed Hausdorff); we denote dy $\mathcal{C}(T)$ the space of all complex continuous functions defined on T and vanishing at infinity.

Definition 1.1. (*see* [19, 23, 26] *and references therein*) *By* upper semi-continuous field of C^*-algebras *we mean a family* $\left\{\mathcal{B} \xrightarrow{\mathcal{P}(t)} \mathcal{B}(t) \mid t \in T\right\}$ *of epimorphisms of C^*-algebras indexed by the locally compact topological space T and satisfying:*

1. *For every $b \in \mathcal{B}$ one has $\| b \|_{\mathcal{B}} = \sup_{t\in T} \| \mathcal{P}(t)b \|_{\mathcal{B}(t)}$.*
2. *For every $b \in \mathcal{B}$ the map $T \ni t \mapsto \| \mathcal{P}(t)b \|_{\mathcal{B}(t)}$ is upper semi-continuous and vanishes at infinity.*
3. *There is a multiplication $\mathcal{C}(T) \times \mathcal{B} \ni (\varphi, b) \to \varphi * b \in \mathcal{B}$ such that*

$$\mathcal{P}(t)[\varphi * b] = \varphi(t)\,\mathcal{P}(t)b\,, \qquad \forall\, t \in T\,,\ \varphi \in \mathcal{C}(T)\,,\ b \in \mathcal{B}\,.$$

If the map $t \mapsto \| \mathcal{P}(t)b \|_{\mathcal{B}(t)}$ is upper semi-continuous for every $b \in \mathcal{B}$, we say that $\left\{\mathcal{B} \xrightarrow{\mathcal{P}(t)} \mathcal{B}(t) \mid t \in T\right\}$ *is* an upper semi-continuous field of C^*-algebras.

One can identify $\mathcal{B}$ with a C^*-algebra of sections of the field. It will always be assumed that $\mathcal{B}(t) \neq \{0\}$ for all $t \in T$.

We go on by describing briefly Rieffel quantization [24]. Let $(\Xi, [\![\cdot,\cdot]\!])$ be a $2n$-dimensional symplectic vector space and $(\mathcal{A}, \Theta, \Xi)$ a C^*-*dynamical system*, meaning that Ξ acts strongly continuously by automorphisms of the C^*-algebra $\mathcal{A}$. We denote by $\mathcal{A}^\infty$ the family of elements f such that the mapping $\Xi \ni X \mapsto \Theta_X(f) \in \mathcal{A}$ is C^∞; it is a dense *-algebra of $\mathcal{A}$. Inspired by Weyl's pseudodifferential calculus, one keeps the involution unchanged but introduce on $\mathcal{A}^\infty$ the product

$$f \# g := \pi^{-2n} \int_\Xi \int_\Xi dY dZ \, e^{2i[\![Y,Z]\!]} \, \Theta_Y(f) \, \Theta_Z(g) \ , \tag{1.1}$$

defined by oscillatory integral techniques. One gets a *-algebra $(\mathcal{A}^\infty, \#, ^*)$, which admits a C^*-completion $\mathfrak{A}$ in a C^*-norm $\| \cdot \|_{\mathfrak{A}}$ as described in [24]. The action Θ leaves $\mathcal{A}^\infty$ invariant and extends [24, Prop. 5.11] to a strongly continuous action of the C^*-algebra $\mathfrak{A}$, that will also be denoted by Θ. The space $\mathfrak{A}^\infty$ of C^∞-vectors coincide with $\mathcal{A}^\infty$, cf [24, Th. 7.1].

Let $(\mathcal{A}_j, \Theta_j, \Xi, [\![\cdot,\cdot]\!])$, $j = 1, 2$, be two data as above and let $\mathcal{R} : \mathcal{A}_1 \to \mathcal{A}_2$ be a Ξ-morphism, *i.e.*, a (C^*-)morphism intertwining the two actions Θ_1, Θ_2. Then $\mathcal{R}$ sends $\mathcal{A}_1^\infty$ into $\mathcal{A}_2^\infty$ and extends to a morphism $\mathfrak{R} : \mathfrak{A}_1 \to \mathfrak{A}_2$ that also intertwines the corresponding actions.

Let now T be a locally compact Hausdorff space and let $\left\{ \mathcal{A} \xrightarrow{\mathcal{P}(t)} \mathcal{A}(t) \mid t \in T \right\}$ be a field of C^*-algebras. We are given actions Θ of Ξ on $\mathcal{A}$ and $\Theta(t)$ of Ξ on $\mathcal{A}(t)$ satisfying $\Theta(t)_X \circ \mathcal{P}(t) = \mathcal{P}(t) \circ \Theta_X$ for each $t \in T$ and $X \in \Xi$. One can say that $\left\{ \mathcal{A} \xrightarrow{\mathcal{P}(t)} \mathcal{A}(t) \mid t \in T \right\}$ is *a covariant field of C^*-algebras*. Then, by Rieffel quantization, one constructs the new covariant field $\left\{ \mathfrak{A} \xrightarrow{\mathfrak{P}(t)} \mathfrak{A}(t) \mid t \in T \right\}$.

Theorem 1.2. *Rieffel quantization transforms covariant semi-continuous fields of C^*-algebras into covariant semi-continuous fields of C^*-algebras.*

It is understood that the statement holds separately for upper and for lower semi-continuity. In the remaining part of this section we are going to present a proof of this result, different from that of [6].

First define

$$\kappa : \Xi \times \Xi \to \mathbb{T} := \{\lambda \in \mathbb{C} \mid |\lambda| = 1\} \, , \qquad \kappa(X,Y) := \exp\left(-\frac{i}{2} \, [\![X,Y]\!] \right) \tag{1.2}$$

and notice that it is a group 2-cocycle, i.e., for all $X, Y, Z \in \Xi$ one has

$$\kappa(X,Y) \, \kappa(X+Y,Z) = \kappa(Y,Z) \, \kappa(X,Y+Z) \, , \qquad \kappa(X,0) = 1 = \kappa(0,X) \, .$$

Thus the initial data is converted into $(\mathcal{A}, \Theta, \Xi, \kappa)$, a very particular case of *twisted C^*-dynamical system* [21, 22]. To any twisted C^*-dynamical system one associates

canonically a C^*-algebra $\mathcal{A} \rtimes^{\kappa}_{\Theta} \Xi$ (called *twisted crossed product*). This is the enveloping C^*-algebra of the Banach *-algebra $\left(L^1(\Xi;\mathcal{A}), \diamond, ^{\diamond}, \|\cdot\|_1\right)$, where

$$\| F \|_1 := \int_{\Xi} dX \, \| F(X) \|_{\mathcal{A}}, \qquad F^{\diamond}(X) := F(-X)^*$$

and (symmetrized version of the standard form)

$$(F_1 \diamond F_2)(X) := \int_{\Xi} dY \, \kappa(X,Y) \, \Theta_{(Y-X)/2} \left[F_1(Y)\right] \, \Theta_{Y/2} \left[F_2(X-Y)\right]. \tag{1.3}$$

In the same way, for each $t \in T$, to $(\mathcal{A}(t), \Theta(t), \Xi, \kappa)$ one associates the twisted crossed product $\mathcal{A}(t) \rtimes^{\kappa}_{\Theta(t)} \Xi$. Let us use the abbreviations $\mathfrak{C} := \mathcal{A} \rtimes^{\kappa}_{\Theta} \Xi$ and $\mathfrak{C}(t) := \mathcal{A}(t) \rtimes^{\kappa}_{\Theta(t)} \Xi$. The epimorphism $\mathcal{P}(t) : \mathcal{A} \to \mathcal{A}(t)$ raises canonically to an epimorphism $\mathcal{P}(t)^{\rtimes} : \mathfrak{C} \to \mathfrak{C}(t)$. As a consequence of results in [19, 22, 23] (see [23, Sect. 3] for instance), if $\left\{ \mathcal{A} \xrightarrow{\mathcal{P}(t)} \mathcal{A}(t) \mid t \in T \right\}$ is an upper (or lower, respectively) semi-continuous field, then $\left\{ \mathfrak{C} \xrightarrow{\mathcal{P}(t)^{\rtimes}} \mathfrak{C}(t) \mid t \in T \right\}$ is also an upper (resp. lower) semi-continuous field.

Thus it would be enough to have an efficient connection between Rieffel quantized C^*-algebras and twisted crossed products. We present some consequences of results from [7]. We recall first that the Schwartz space $\mathcal{S}(\Xi)$ is a *-algebra under complex conjugation and the Weyl product

$$(h \sharp k)(X) := \pi^{-2n} \int_{\Xi} \int_{\Xi} dY dZ \, e^{2i[\![Y,Z]\!]} \, h(X+Y) \, k(X+Z). \tag{1.4}$$

Fix now an element $h \in \mathcal{S}(\Xi) \setminus \{0\}$ satisfying $h \sharp h = h = \overline{h}$ and define for each $f \in \mathcal{A}^{\infty} = \mathfrak{A}^{\infty}$ and any $X \in \Xi$

$$\left[M_h(f)\right](X) := \int_{\Xi} dY \, e^{-i[\![X,Y]\!]} h(Y) \Theta_Y(f). \tag{1.5}$$

It is shown in [7] that M_h can be extended as an injective C^*-morphism $M_h : \mathfrak{A} \to \mathfrak{C} \equiv \mathcal{A} \rtimes^{\kappa}_{\Theta} \Xi$. We recall that injective C^*-morphisms are isometric. The construction can be repeated with $(\mathcal{A}, \Theta)$ replaced by $(\mathcal{A}(t), \Theta(t))$, so for each $t \in T$ one gets an isometry $M(t)_h : \mathfrak{A}(t) \to \mathfrak{C}(t) \equiv \mathcal{A}(t) \rtimes^{\kappa}_{\Theta(t)} \Xi$. In addition, by [7] one has $M(t)_h \circ \mathfrak{P}(t) = \mathcal{P}(t)^{\rtimes} \circ M_h$. Then, for any $f \in \mathfrak{A}$

$$\| \mathfrak{P}(t) f \|_{\mathfrak{A}(t)} = \| M(t)_h [\mathfrak{P}(t) f] \|_{\mathfrak{C}(t)} = \| \mathcal{P}(t)^{\rtimes} \left[M_h(f)\right] \|_{\mathfrak{C}(t)} .$$

Therefore, under the right assumption, the mapping $t \mapsto \| \mathfrak{P}(t) f \|_{\mathfrak{A}(t)}$ has the desired semi-continuity properties. The first condition in the definition of a semi-continuous field of C^*-algebras is checked analogously:

$$\begin{aligned} \| f \|_{\mathfrak{A}} &= \| M_h(f) \|_{\mathfrak{C}} = \sup_t \| \mathcal{P}(t)^{\rtimes} \left[M_h(f)\right] \|_{\mathfrak{C}(t)} \\ &= \sup_t \| M(t)_h [\mathfrak{P}(t) f] \|_{\mathfrak{C}(t)} = \sup_t \| \mathfrak{P}(t) f \|_{\mathfrak{A}(t)} . \end{aligned}$$

Finally, one must define the mapping $\star : \mathcal{C}(T) \times \mathfrak{A} \to \mathfrak{A}$ that should be deduced from the already existing $* : \mathcal{C}(T) \times \mathcal{A} \to \mathcal{A}$. Let $\varphi \in \mathcal{C}(T)$ and $f \in \mathfrak{A}$. There is a sequence $(f_n)_{n\in\mathbb{N}} \in \mathfrak{A}^\infty = \mathcal{A}^\infty$ with $\| f - f_n \|_{\mathfrak{A}} \to 0$ for $n \to \infty$. One sets $\varphi \star f := \lim_n \varphi * f_n$. We leave to the reader the easy task to check that this limit exists in $\mathfrak{A}$ and that the identity $\mathfrak{P}(t)[\varphi \star f] = \varphi(t)\mathfrak{P}(t)f$ holds for every $t \in T$.

2. The Abelian case

We denote by $\mathcal{C}(\Sigma)$ the Abelian C^*-algebra of all complex continuous functions on the locally compact Hausdorff space Σ that are arbitrarily small outside large compact subsets. When Σ is compact, $\mathcal{C}(\Sigma)$ is unital. We indicate a framework leading naturally to fields of C^*-algebras.

We assume given a continuous surjection $q : \Sigma \to T$. Then we have the disjoint decomposition of Σ in closed subsets $\Sigma = \sqcup_{t\in T}\Sigma_t$, where $\Sigma_t := q^{-1}(\{t\})$. One has the canonical injections $j_t : \Sigma_t \to \Sigma$ and the restriction epimorphisms $\mathcal{R}(t) : \mathcal{C}(\Sigma) \to \mathcal{C}(\Sigma_t)$, with $\mathcal{R}(t)f := f|_{\Sigma_t} = f \circ j_t$, $\forall\, t \in T$. This is the right setting to get semi-continuous fields of Abelian C^*-algebras.

Proposition 2.1. *In the setting above* $\left\{ \mathcal{C}(\Sigma) \xrightarrow{\mathcal{R}(t)} \mathcal{C}(\Sigma_t) \mid t \in T \right\}$ *is an upper semi-continuous field of commutative C^*-algebras. If q is also open, the field is continuous.*

Proof. Obviously $\cap_{t\in T} \ker[\mathcal{R}(t)] = \{0\}$, since $f|_{\Sigma_t} = 0$, $\forall\, t \in T$ implies $f = 0$. On the other hand, setting

$$\varphi * f := (\varphi \circ q)f\,, \qquad \forall\, \varphi \in \mathcal{C}(T)\,,\ f \in \mathcal{C}(\Sigma)\,, \tag{2.1}$$

we get immediately $\mathcal{R}(t)(\varphi * f) = \varphi(t)\,\mathcal{R}(t)f$, $\forall\, t \in T$.

We need to study continuity properties of the mapping

$$\begin{aligned} T \ni t \mapsto n_f(t) := \|\mathcal{R}(t)f\|_{\mathcal{C}(\Sigma_t)} &= \sup_{\sigma\in\Sigma_t} |f(\sigma)| \\ &= \inf\left\{ \|f + h\|_{\mathcal{C}(\Sigma)} \ \mid\ h \in \mathcal{C}(\Sigma),\ h|_{\Sigma_t} = 0 \right\} \in \mathbb{R}_+\,. \end{aligned}$$

The last expression for the norm can be justified directly easily, but it also follows from the canonical isomorphism $\mathcal{C}(\Sigma_t) \cong \mathcal{C}(\Sigma)/\mathcal{C}_{\Sigma_t}(\Sigma)$, where $\mathcal{C}_{\Sigma_t}(\Sigma)$ is the ideal of functions $h \in \mathcal{C}(\Sigma)$ such that $h|_{\Sigma_t} = 0$.

We first assume that q is only continuous. For every $S \subset T$ we set $\Sigma_S := q^{-1}(S)$. It is easy to see by the Stone-Weierstrass Theorem that

$$\mathcal{C}_{(t)}(\Sigma) := \{h \in \mathcal{C}(\Sigma) \mid \exists \text{ an open neighborhood } U \text{ of } t \text{ such that } h|_{\Sigma_{\overline{U}}} = 0\}$$

is a self-adjoint 2-sided ideal dense in $\mathcal{C}_{\Sigma_t}(\Sigma)$. Let $t_0 \in T$ and $\varepsilon > 0$; by density and the definition of inf

$$\exists\, h \in \mathcal{C}_{(t_0)}(\Sigma) \ \text{ such that } \ n_f(t_0) + \varepsilon \ \geq\ \|f + h\|_{\mathcal{C}(\Sigma)}\,.$$

Let U be the open neighborhood of t_0 for which $h|_{\Sigma_{\overline{U}}} = 0$. For any $t \in U$ one also has $h \in \mathcal{C}_{(t)}(\Sigma)$, so

$$n_f(t) = \inf\left\{\|f+g\|_{\mathcal{C}(\Sigma)} \;\middle|\; g \in \mathcal{C}_{(t)}(\Sigma)\right\} \;\leq\; \|f+h\|_{\mathcal{C}(\Sigma)} \;\leq\; n_f(t_0)+\varepsilon$$

and this is upper semi-continuity.

Let us also suppose q open, let $t_0 \in T$ and $\varepsilon > 0$. By the definition of sup, there exists $\sigma_0 \in \Sigma_{t_0}$ such that $|f(\sigma_0)| \geq n_f(t_0) - \varepsilon/2$. Since f is continuous, there is a neighborhood V of σ_0 in Σ such that

$$|f(\sigma)| \geq |f(\sigma_0)| - \varepsilon/2 \geq n_f(t_0) - \varepsilon, \qquad \forall\, \sigma \in V.$$

Since q is open, $U := q(V)$ is a neighborhood of t_0. For every $t \in U$ we have $\Sigma_t \cap V \neq \emptyset$, so for such t

$$n_f(t) \geq \sup\{|f(\sigma)| \mid \sigma \in \Sigma_t \cap V\} \geq n_f(t_0) - \varepsilon$$

and this is lower semi-continuity. □

Suppose now that a continuous action Θ of Ξ by homeomorphisms of Σ is also given. For $(\sigma, X) \in \Sigma \times \Xi$ we are going to use all the notations

$$\Theta(\sigma, X) = \Theta_X(\sigma) = \Theta_\sigma(X) \in \Sigma \tag{2.2}$$

for the X-transformed of the point σ. The function Θ is continuous and the homeomorphisms Θ_X, Θ_Y satisfy $\Theta_X \circ \Theta_Y = \Theta_{X+Y}$ for every $X, Y \in \Xi$.

The action Θ of Ξ on Σ induces an action of Ξ on $\mathcal{C}(\Sigma)$ (also denoted by Θ) given by $\Theta_X(f) := f \circ \Theta_X$. This action is strongly continuous, *i.e.*, for any $f \in \mathcal{C}(\Sigma)$ the mapping

$$\Xi \ni X \mapsto \Theta_X(f) \in \mathcal{C}(\Sigma) \tag{2.3}$$

is continuous; thus we are placed in the setting presented in the first section. We denote by $\mathcal{C}(\Sigma)^\infty \equiv \mathcal{C}^\infty(\Sigma)$ the set of elements $f \in \mathcal{C}(\Sigma)$ such that the mapping (2.3) is C^∞; it is a dense *-algebra of $\mathcal{C}(\Sigma)$. The general theory supplies a non-commutative C^*-algebra $\mathfrak{A} \equiv \mathfrak{C}(\Sigma)$, acted continuously by the group Ξ, with smooth vectors $\mathfrak{C}^\infty(\Sigma) = \mathcal{C}^\infty(\Sigma)$.

To insure covariance for the emerging families of C^*-algebras, we impose a condition of compatibility between the action Θ and the mapping q.

Definition 2.2. *We say that the surjection q* is Θ-covariant *if it satisfies the equivalent conditions:*

1. *Each Σ_t is Θ-invariant.* 2. *For each $X \in \Xi$ one has $q \circ \Theta_X = q$.*

Recall now the Rieffel-quantized C^*-algebras $\mathfrak{C}(\Sigma)$ and $\mathfrak{C}(\Sigma_t)$ as well as the epimorphisms $\mathfrak{R}(t) : \mathfrak{C}(\Sigma) \to \mathfrak{C}(\Sigma_t)$. Applying Theorem 1.2 and Proposition 2.1, one gets

Corollary 2.3. *Assume that $q : \Sigma \to T$ is a Θ-covariant continuous surjection. Then the covariant field of non-commutative C^*-algebras $\left\{\mathfrak{C}(\Sigma) \xrightarrow{\mathfrak{R}(t)} \mathfrak{C}(\Sigma_t) \,|\, t \in T\right\}$ is upper semi-continuous.*

If q is also open, then the field is continuous.

3. Spectral continuity for symbols

Let us introduce the concept of continuity for families of sets that will be useful below.

Definition 3.1. *Let T be a Hausdorff locally compact topological space and let $\{S(t) \mid t \in T\}$ be a family of compact subsets of $\mathbb{R}$.*

1. *The family is called* outer continuous *if for any $t_0 \in T$ and any compact subset K of $\mathbb{R}$ such that $K \cap S(t_0) = \emptyset$, there exists a neighborhood V of t_0 with $K \cap S(t) = \emptyset$, $\forall t \in V$.*
2. *The family $\{S(t) \mid t \in T\}$ is called* inner continuous *if for any $t_0 \in T$ and any open subset A of $\mathbb{R}$ such that $A \cap S(t_0) \neq \emptyset$, there exists a neighborhood W of t_0 with $A \cap S(t) \neq \emptyset$, $\forall t \in W$.*
3. *If the family is both inner and outer continuous, we say simply that it is* continuous.

In applications the sets $S(t)$ are spectra of some self-adjoint elements $f(t)$ of (non-commutative) C^*-algebras $\mathfrak{A}(t)$. The next result states technical conditions under which one gets continuity of such families of spectra. It is taken from [1] and it has been inspired by the treatment in [3]. We include the proof for the convenience of the reader.

Proposition 3.2. *For any $t \in T$ let $f(t)$ be a self-adjoint element in a C^*-algebra $\mathfrak{A}(t)$ with norm $\|\cdot\|_{\mathfrak{A}(t)}$ and inversion $g \mapsto g^{(-1)_{\mathfrak{A}(t)}}$. We denote by $S(t) \subset \mathbb{R}$ the spectrum of $f(t)$ in $\mathfrak{A}(t)$.*

1. *Assume that for any $z \in \mathbb{C} \setminus \mathbb{R}$ the mapping*
$$T \ni t \mapsto \left\| (f(t) - z)^{(-1)_{\mathfrak{A}(t)}} \right\|_{\mathfrak{A}(t)} \in \mathbb{R}_+ \tag{3.1}$$
is upper semi-continuous. Then the family $\{S(t) \mid t \in T\}$ is outer continuous.
2. *Assume that for any $z \in \mathbb{C} \setminus \mathbb{R}$ the mapping (3.1) is lower semi-continuous. Then the family $\{S(t) \mid t \in T\}$ is inner continuous.*

Proof. We use the functional calculus for self-adjoint elements in the C^*-algebra $\mathfrak{A}(t)$ to define $\chi[f(t)]$ for every continuous function $\chi : \mathbb{R} \to \mathbb{C}$ vanishing at infinity. Notice that
$$(f(t) - z)^{(-1)_{\mathfrak{A}(t)}} = \chi_z[f(t)]\,, \quad \text{with} \quad \chi_z(\lambda) := (\lambda - z)^{-1}\,.$$
By a standard argument relying on Stone-Weierstrass Theorem, one deduces that the map $t \mapsto \|\chi[f(t)]\|_{\mathfrak{A}(t)}$ has the same continuity properties (upper or lower semi-continuity, respectively) as (3.1).

Let us suppose now upper semi-continuity in t_0 and assume that $S(t_0) \cap K = \emptyset$ for some compact set K. By Urysohn's Lemma, there exists $\chi \in \mathcal{C}(\mathbb{R})_+$ with $\chi|_K = 1$ and $\chi|_{S(t_0)} = 0$, so $\chi\,[f(t_0)] = 0$. Choose a neighborhood V of t_0 such that for $t \in V$
$$\|\,\chi[f(t)]\,\|_{\mathfrak{A}(t)} \leq \|\,\chi[f(t_0)]\,\|_{\mathfrak{A}(t_0)} + \frac{1}{2} = \frac{1}{2}\,.$$

If for some $t \in V$ there exists $\lambda \in K \cap S(t)$, then

$$1 = \chi(\lambda) \leq \sup_{\mu \in S(t)} \chi(\mu) = \| \chi[f(t)] \|_{\mathfrak{A}(t)} \leq \frac{1}{2},$$

which is absurd.

Let us assume now lower semi-continuity in t_0. Pick an open set $A \subset \mathbb{R}$ such that $S(t_0) \cap A \neq \emptyset$ and let $\lambda \in S(t) \cap A$. By Urysohn's Lemma there exist a positive function $\chi \in \mathcal{C}(\mathbb{R})$ with $\chi(\lambda) = 1$ and $\mathrm{supp}(\chi) \subset A$; thus $\| \chi[f(t_0)] \|_{\mathfrak{A}(t_0)} \geq 1$. Suppose moreover that for any neighborhood $W \subset T$ of t_0 there exists $t \in W$ such that $S(t) \cap A = \emptyset$ and thus $\chi[f(t)] = 0$. This clearly contradicts the lower semi-continuity of $t \mapsto \| \chi[f(t)] \|_{\mathfrak{A}(t)}$. We conclude thus the inner continuity property for the family $S(t)$. □

Proving these properties of the resolvents is a priori a difficult task, since this involves working both with norms and composition laws that depend on t. But putting together the information obtained until now, we get our abstract result concerning spectral continuity:

Theorem 3.3. *Let* $\left\{ \mathcal{A} \xrightarrow{\mathcal{P}(t)} \mathcal{A}(t) \mid t \in T \right\}$ *be a covariant upper semi-continuous field of* C^**-algebras indexed by a Hausdorff locally compact space* T *and let* f *be a smooth self-adjoint element of* $\mathcal{A}$*. For any* $t \in T$ *we denote by* $\mathfrak{A}(t)$ *the Rieffel quantization of* $\mathcal{A}(t)$ *and consider* $f(t) := \mathcal{P}(t)f$ *as an element of* $\mathcal{A}(t)^\infty = \mathfrak{A}(t)^\infty \subset \mathfrak{A}(t)$*, with spectrum* $S(t)$ *computed in* $\mathfrak{A}(t)$*. Then the family* $\{S(t) \mid t \in T\}$ *is outer continuous.*

If the field is continuous, the family of subsets will also be continuous.

Proof. Theorem 1.2 allows us to conclude that the quantized field

$$\left\{ \mathfrak{A} \xrightarrow{\mathfrak{P}(t)} \mathfrak{A}(t) \mid t \in T \right\}$$

has the same continuity properties as the original one.

For any $z \in \mathbb{C} \setminus \mathbb{R}$ one has $(f - z)^{(-1)_{\mathfrak{A}}} \in \mathfrak{A}$ and $(f(t) - z)^{(-1)_{\mathfrak{A}(t)}} = \mathfrak{P}(t)\left[(f - z)^{(-1)_{\mathfrak{A}}}\right]$. Therefore the assumptions of Proposition 3.2 are fulfilled both in the upper semi-continuous and in the lower semi-continuous case, so we obtain the desired continuity properties for the family of sets $\{S(t) \mid t \in T\}$. □

Of course, the conclusion also holds for non-smooth self-adjoint elements $f \in \mathfrak{A}$. Very often they are much less "accessible" than the smooth elements, being obtained by an abstract completion procedure, so we only make the statements for C^∞ vectors.

Specializing to the Abelian case and using the notations of Section 2, one gets

Corollary 3.4. *Assume that* $q : \Sigma \to T$ *is a* Θ*-covariant continuous surjection. Let* $f \in \mathcal{C}^\infty(\Sigma)$ *a real function and for each* $t \in T$ *denote by* $S(t)$ *the spectrum of* $f(t) := f|_{\Sigma_t} \in \mathcal{C}^\infty(\Sigma_t) = \mathfrak{C}^\infty(\Sigma_t)$ *seen as an element of the non-commutative* C^**-algebra* $\mathfrak{C}(\Sigma_t)$.

Then the family $\{S(t) \mid t \in T\}$ *of compact subsets of* $\mathbb{R}$ *is outer continuous. If* q *is also open, the family of subsets is continuous.*

Remark 3.5. One can use [24, Ex. 10.2] to identify quantum tori as Rieffel-type quantizations of usual tori. One is naturally placed in the setting above and can reproduce some known spectral continuity results [8, 3] on generalized Harper operators.

4. Spectral continuity for operators

The standard approach of Quantum Mechanics asks for Hilbert space operators. This can be achieved by representing faithfully the C^*-algebras $\mathfrak{A}(t)$ in a Hilbert space of L^2-functions in a way that generalizes the Schrödinger representation. We are going to get continuity results for both spectra and essential spectra of the emerging self-adjoint operators. We work in the following

Framework

1. $(\mathcal{C}(\Sigma), \Theta, \Xi)$ is an Abelian C^*-dynamical system, with Σ compact.
2. Ξ is symplectic, given in a Lagrangean decomposition $\Xi = \mathscr{X} \times \mathscr{X}^* \ni X = (x, \xi)\,,\ Y = (y, \eta)\,$, where $\mathscr{X}$ is a n-dimensional real vector space, $\mathscr{X}^*$ is its dual and the symplectic form on Ξ is given in terms of the duality between $\mathscr{X}$ and $\mathscr{X}^*$ by $[\![(x, \xi), (y, \eta)]\!] := y \cdot \xi - x \cdot \eta\,.$
3. $q : \Sigma \to T$ is a Θ-covariant continuous surjection. We also assume that each $\Sigma_t := q^{-1}(\{t\})$ is *a quasi-orbit*, i.e., there is a point $\sigma \in \Sigma_t$ such that the orbit $\mathcal{O}_\sigma := \Theta_\Xi(\sigma)$ is dense in Σ_t (we say that σ *generates the quasi-orbit* Σ_t).
4. We fix a real element $f \in \mathcal{C}^\infty(\Sigma)\,.$ For each $t \in T$ and for any point σ generating the quasi-orbit Σ_t we define $f(t) := f|_{\Sigma_t}$ and $f_\sigma(t) := f(t) \circ \Theta_\sigma : \Xi \to \mathbb{R}\,.$
5. We set $H_\sigma(t) := \mathfrak{Op}\left[f_\sigma(t)\right]$ (self-adjoint operator in the Hilbert space $\mathcal{H} := L^2(\mathscr{X})$), by applying to $f_\sigma(t)$ the usual Weyl pseudodifferential calculus. We denote by $S(t)$ the spectrum of $H_\sigma(t)\,.$

Some explanations are needed. It is easy to see that each $f_\sigma(t)$ belongs to $BC^\infty(\Xi)$, i.e., it is a smooth function with bounded derivatives of any order. Therefore, using oscillatory integrals, one can define the self-adjoint operator in $L^2(\mathscr{X}) \ni u$

$$\begin{aligned}\left[H_\sigma(t)u\right](x) &\equiv \left[\mathfrak{Op}(f_\sigma(t))u\right](x)\\ &:= (2\pi)^{-n} \int_{\mathscr{X}} \mathrm{d}y \int_{\mathscr{X}^*} \mathrm{d}\xi\, e^{i(x-y)\cdot\xi}\, \left[f_\sigma(t)\right]\left(\frac{x+y}{2}, \xi\right) u(y)\,.\end{aligned}$$

This operator is bounded by the Calderón-Vaillancourt Theorem [9]. Using the notation (2.2), we see that for every $X \in \Xi$ one has $\left[f_\sigma(t)\right](X) := f\left[\Theta_X(\sigma)\right]$; this

depends on $t \in T$ through σ and only involves the values of f on the dense subset $\mathcal{O}_\sigma$ of Σ_t. The same is true about $H_\sigma(t)$, which can be written

$$[H_\sigma(t)u](x) = (2\pi)^{-n} \int_{\mathscr{X}} \mathrm{d}y \int_{\mathscr{X}^*} \mathrm{d}\xi \, e^{i(x-y)\cdot\xi} f\left[\Theta_{\left(\frac{x+y}{2},\xi\right)}(\sigma)\right] u(y)\,. \tag{4.1}$$

It is shown in [16] that if σ and σ' are both generating the same quasi-orbit Σ_t, then the operators $H_\sigma(t)$ and $H_{\sigma'}(t)$ are isospectral (but not unitarily equivalent in general). Thus the compact set $S(t)$ only depends on t and not on the choice of the generating element σ.

Theorem 4.1. *Assume the Framework above. Then the family $\{S(t) \mid t \in T\}$ is outer continuous.*

If q is also open, than the family is continuous.

Proof. By Corollary 3.4, it would be enough to show for every t that $S(t)$ coincides with the spectrum of $f(t) \in \mathfrak{C}(\Sigma_t)$. For this we define

$$\mathcal{N}_\sigma : \mathcal{C}^\infty(\Sigma_t) \to BC^\infty(\Xi), \qquad \mathcal{N}_\sigma(g) := g \circ \Theta_\sigma$$

and then set

$$\mathfrak{Op}_\sigma := \mathfrak{Op} \circ \mathcal{N}_\sigma : \mathcal{C}^\infty(\Sigma_t) \to \mathbb{B}(\mathcal{H})\,.$$

Then one has $H_\sigma(t) := \mathfrak{Op}[f_\sigma(t)] = \mathfrak{Op}_\sigma[f(t)]$. It is not quite trivial, but it has been shown in [16], that $\mathfrak{Op}_\sigma$ extends to a faithful representation of the Rieffel quantized C^*-algebra $\mathfrak{C}(\Sigma_t)$ in $\mathcal{H}$. Faithfulness is implied by the fact that σ generates the quasi-orbit Σ_t, which results in the injectivity of $\mathcal{N}_\sigma$, conveniently extended to $\mathfrak{C}(\Sigma_t)$. It follows then that $\mathrm{sp}[H_\sigma(t)] = \mathrm{sp}[f(t)]$, as required, so the family $\{S(t) \mid t \in T\}$ has the desired continuity properties. □

We recall that *the essential spectrum* of an operator is the part of the spectrum composed of accumulation points or infinitely-degenerated eigenvalues. Let us denote by $S^{\mathrm{ess}}(t)$ the essential spectrum of $H_\sigma(t)$; once again this only depends on t. To discuss the continuity properties of this family of sets we are going to need some preparations relying mainly on results from [16].

First we write each Σ_t as a disjoint Θ-invariant union $\Sigma_t = \Sigma_t^{\mathrm{g}} \sqcup \Sigma_t^{\mathrm{n}}$. The elements σ_1 of Σ_t^{g} are *generic points for* Σ_t, meaning that each of them is generating Σ_t. The points $\sigma_2 \in \Sigma_t^{\mathrm{n}}$ are *non-generic*, i.e., the closure of the orbit $\mathcal{O}_{\sigma_2}$ is strictly contained in Σ_t.

Let us now fix a point $t \in T$ and a generating element $\sigma \in \Sigma_t$. The monomorphism $\mathcal{N}_\sigma$ extends to an isomorphism between $\mathcal{C}(\Sigma_t)$ and a C^*-subalgebra $\mathcal{B}_\sigma(t)$ of the C^*-algebra $BC_{\mathrm{u}}(\Xi)$ of all the bounded uniformly continuous complex functions on Ξ. It is shown in Lemma 2.2 from [16] that only two possibilities can occur, and this is independent of σ: either $\mathcal{C}(\Xi) \subset \mathcal{B}_\sigma(t)$ (and then t is called *of the first type*), or $\mathcal{C}(\Xi) \cap \mathcal{B}_\sigma(t) = \{0\}$ (and then we say that t is *of the second type*). Correspondingly, one has the disjoint decomposition $T = T_I \sqcup T_{II}$.

Theorem 4.2. *Assume the Framework above. Then the family $\{S^{\mathrm{ess}}(t) \mid t \in T\}$ is outer continuous.*

Proof. One must rephrase the essential spectrum $S^{\rm ess}(t) := {\rm sp}_{\rm ess}[H_\sigma(t)]$ in convenient C^*-algebraic terms. Assume first that t is of the second type. By [16, Prop. 3.4], the discrete spectrum of $H_\sigma(t)$ is void, thus one has $S^{\rm ess}(t) = S(t)$. If t is of the first type, the subset $\Sigma_t^{\rm n}$ is invariant under the action Θ and it is also closed by [16, Prop. 2.5]. Denoting by $f^{\rm n}(t)$ the restriction of $f(t)$ to $\Sigma_t^{\rm n}$, one gets an element of $\mathcal{C}^\infty(\Sigma_t^{\rm n}) \subset \mathfrak{C}(\Sigma_t^{\rm n})$ with spectrum $S^{\rm n}(t)$. But [16, Th. 3.7] states among others that $S^{\rm n}(t)$ coincides with $S^{\rm ess}(t)$.

We need to construct now a suitable restricted dynamical system. Let us consider the decomposition

$$\Sigma = \big(\bigsqcup_{t\in T_I}\Sigma_t\big) \sqcup \big(\bigsqcup_{t\in T_{II}}\Sigma_t\big) = \big(\bigsqcup_{t\in T_I}\Sigma_t^{\rm g}\big) \sqcup \big\{\big(\bigsqcup_{t\in T_I}\Sigma_t^{\rm n}\big) \sqcup \big(\bigsqcup_{t\in T_{II}}\Sigma_t\big)\big\} =: \Sigma^{\rm d} \sqcup \Sigma^{\rm ess}\,.$$

One might set $\Sigma_t^{\rm ess} := \Sigma_t^{\rm n}$ if $t \in T_I$ and $\Sigma_t^{\rm ess} := \Sigma_t$ if $t \in T_{II}$. Notice that each $\Sigma_t^{\rm ess}$ is not void. This is clear for $t \in T_{II}$, since q has been supposed surjective. If $t \in T_I$ and $\Sigma_t^{\rm n} = \emptyset$, then $\Sigma_t = \Sigma_t^{\rm g}$ is minimal and compact, so $t \in T_{II}$ by Lemma 2.3 in [16], which is absurd. The disjoint union $\Sigma^{\rm ess} := \sqcup_{t\in T}\Sigma_t^{\rm ess}$ (with the topology induced from Σ) is a compact dynamical system under the restriction of the action Θ of Ξ and $q^{\rm ess} := q|_{\Sigma^{\rm ess}} : \Sigma^{\rm ess} \to T$ is a covariant continuous surjection. Thus we can apply the previous results and conclude that $\{\mathfrak{C}(\Sigma^{\rm ess}) \to \mathfrak{C}(\Sigma_t^{\rm ess}) \mid t \in T\}$ is an upper semi-continuous field of C^*-algebras; the arrows are Rieffel quantizations of obvious restriction maps.

From all these applied to $f|_{\Sigma^{\rm ess}} \in \mathfrak{C}^\infty(\Sigma^{\rm ess})$ it follows that

$$\big\{S^{\rm ess}(t) = {\rm sp}\,\big[f(t)|_{\Sigma^{\rm ess}(t)}\big] \mid t \in T\big\}$$

is outer continuous. □

Remark 4.3. Even in simple situations, the surjective restriction of a continuous open surjection may not be open. So $q^{\rm ess}$ may fail to be open and in general we don't obtain inner continuity for the family of essential spectra. On the other hand, if openness of the restriction $q^{\rm ess}$ is required explicitly, one clearly gets the inner continuity. Since only the dynamical system $(\Sigma^{\rm ess}, \Theta, \Xi)$ is involved in controlling the family of essential spectra, some assumptions weaker than those above would suffice.

Example 4.4. To show that our results cover families of zero-order standard pseudodifferential operators, one has to make some simple choices. Recall that $BC_{\rm u}(\Xi)$, the unital C^*-algebra of all bounded uniformly continuous functions on Ξ, is stable under the action θ of Ξ by translations. The *-algebra of smooth elements is $BC^\infty(\Xi)$, formed of smooth functions with bounded derivatives; such functions can be regarded as zero-order symbols in the sense of Hörmander. By Gelfand theory, $BC_{\rm u}(\Xi)$ is isomorphic to $\mathcal{C}(\Omega)$ for a compactification Ω of Ξ. Actually, if $g \in BC_{\rm u}(\Xi)$, its image $\hat{g}$ in $\mathcal{C}(\Omega)$ is just the extension of g from the dense subset Ξ to the entire Ω. The action by translations θ of Ξ on itself extends to an action by homeomorphisms of Ω.

Let now T be a locally compact space and for each $t \in T$ let $g(t)$ be a real element of $BC^\infty(\Xi)$ and $\hat{g}(t)$ its continuous extension to Ω. We are also requiring that the map $T \ni t \mapsto g(t) \in BC_{\mathrm{u}}(\Xi)$ be continuous. Denote by $H(t) := \mathfrak{Op}[g(t)]$ the zero-order pseudodifferential operator obtained by Weyl quantization. We claim that both the spectra $S(t)$ and the essential spectra $S^{\mathrm{ess}}(t)$ of these operators form inner and outer continuous families of compact subsets of $\mathbb{R}$.

To see this, construct the locally compact space $\Sigma := \Omega \times T$ and endow it with the action $\Theta_X(\omega, t) := (\theta_X(\omega), t)$. Of course, $q : \Sigma \to T,\ q(\omega, t) := t$ is a Θ-covariant continuous open surjection. Each quasi-orbit $\Sigma_t := q^{-1}(\{t\}) = \Omega \times \{t\}$ is of the first type and can be identified with Ω. The generic points of Ω are the elements of Ξ, while the non-generic ones are those of $\Omega \setminus \Xi$. The restriction of q to $\Sigma^{\mathrm{ess}} = (\Omega \setminus \Xi) \times T$ is still (continuous and) open.

We use the family $\{g(t) \mid t \in T\}$ to define a function $f : \Sigma \to \mathbb{R}$ by $f(\omega, t) := [\hat{g}(t)](\omega)$. One checks easily that $f \in \mathcal{C}^\infty(\Sigma)$. Choosing the generating point $\sigma := (0, t) \in \Sigma_t$, one gets $f_{(0,t)} = g(t)$, so $H_\sigma(t) := \mathfrak{Op}[f_\sigma(t)] = \mathfrak{Op}[g(t)] =: H(t)$. So the continuity of the families $\{S(t) \mid t \in T\}$ and $\{S^{\mathrm{ess}}(t) \mid t \in T\}$ follows from Theorems 4.1 and 4.2. Obviously, the result for essential spectra still holds if to each Hamiltonian $H(t)$ one adds a compact perturbation $V(t)$.

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Stability of Matter

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Abstract. These are extended notes based on a series of four lectures on the Stability of Matter, given by the author at the "Spectral Days" conference in Santiago de Chile in September, 2010.

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Mais ce n'est pas tout; la Physique ne nous donne pas
seulement l'occasion de résoudre des problèmes;
elle nous aide à en trouver les moyens, et cela de deux manières.
Elle nous fait présentir la solution;
elle nous suggère des raisonaments.
Conference of H. Poincaré at the ICM, in Zürich, 1897, see [57], p. 340.

1. Introduction: The stability of quantum systems: A historical overview

Stability properties of two or more particle systems interacting among themselves via one over distance potentials (i.e., via Coulomb or Kepler interactions) have been a central and recurrent theme in Physics since the second half of the 17th century. After the introduction of the universal law of gravitation by Newton in 1687 [56], many people studied the stability of the solar system. These studies not only shed light on the physical properties of a multiple body system interacting via Kepler potentials but, in fact, produced fundamental advances in mathematics. On the one hand it triggered the introduction of perturbation theory in classical mechanics in terms of action and angle variables. On the other hand it triggered a whole realm of new mathematics centered around dynamical systems, which

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ultimately produced the Kolmogorov-Arnold-Moser theory (see, e.g., the classical book of Siegel and Moser [64]).

Stability also played a fundamental role in atomic physics during the early XXth century. At the beginning of the century several people (e.g., Thomson [69], Nagaoka [55], Rutherford [59, 60]) introduced different models of atoms (basically neutral systems with positive and negative charge distributions interacting via a Coulomb potential). The early models of Nagaoka and later of Rutherford had a strong influence from their gravitational counterpart. Soon after their introduction, they realized that (at least in the framework of classical physics) these systems were unstable. In the Rurtherford model, the accelerated electron loosing energy via electromagnetic radiation, would fall into the nucleus in a very short time. It was partly because of the (classical) instability of the Rutherford atom that Bohr introduced his model [8, 9, 10, 11], that gave birth to the *old quantum mechanics* in 1913. At the beginning of the *old quantum mechanics*, Jeans observed: *There seems to be no difficulty about the supposition that at very small distances the law of force is different from the inverse square. On the contrary, there would be a very real difficulty in supposing the law* $1/r^2$ *held down to zero values of* r*. For the force between two charges at zero distance would be infinite; we should have charges of opposite sign continuously rushing together and, when once together, no force would be adequate to separate them... Thus the matter in the universe would tend to shrink into nothing or to diminish indefinitely in size. The observed permanence of matter precludes any such hypothesis... We should be wrong in regarding a molecule as a cluster of electrons and positive charges. A more likely suggestion, put forward by Larmor and others is that the molecule may consist, in part at least, of rings of electrons in rapid orbital motion.* (see, [32], p. 168). The old quantum mechanics was successful in explaining the observed spectrum of the hydrogen atom, but failed in explaining the spectra of more complicated atomic structures. Following the de Broglie's [17] suggestion that matter had also a wave-like behavior, Schrödinger in 1926 [63] introduced his (now classical) wave equation for the electron. The solution of the time independent Schrödinger equation for the Hydrogen atom (i.e., with a potential $V(x) = -Z/|x|$) reproduced the known spectra of this system. It is easy to see, either by exact computations or by using Heisenberg's *uncertainty principle* (with the help of Hardy's or better Sobolev's inequality) that the spectrum of the Hydrogen atom is bounded below (and thus, this one particle system is *stable*). For a more complex system one not only needs to prove a similar lower bound on the ground state energy, but more important, one needs to prove that the energy per particle of the system is bounded below. This last property is what one understands as the *Stability of Matter*. Speculations about matter's stability go back to the early days of quantum mechanics. In 1931, Paul Ehrenfest observed that someone holding a piece of metal or stone should be *astonished that this quantity of matter should occupy so large a volume. Admittedly*, Ehrenfest remarked, *the molecules are packed tightly together and likewise the atoms within each molecule. But why are the atoms themselves so big?* For an answer, he summoned a principle first stated by Wolfgang Pauli: No two particles

of the same kind can occupy the same quantum state at the same time. Pauli's principle means that electrons can't all fall into the lowest energy, smallest orbital around an atomic nucleus but have to fill successively larger orbitals. *That is why atoms are so unnecessarily big, and why metal and stone are so bulky,* Ehrenfest concluded. It took forty years after the Schrödinger equation to have the first proof of the Stability of Matter in the context of Nonrelativistic Quantum Mechanics. This was accomplished by Freeman Dyson and Andrew Lenard [20, 37]. What Dyson and Lenard proved was that for a system of fermions interacting via Coulomb forces the ground state energy per particle of the system is bounded from below by a constant. The constant in their proof was unnecessarily large. In 1975, Lieb and Thirring [51] provided a simpler proof, based on the fact that the Thomas–Fermi energy is a good approximation to the Quantum Mechanical energy [50], and that in the Thomas–Fermi model there are no molecules [67]. The lower bound to the energy per particle in the proof of Lieb and Thirring is much more realistic (of the order of a few Rydbergs per particle). After the proof of Lieb and Thirring there has been a huge literature on the subject, with extensions to many different physical situations. There are several reviews (e.g., [39, 45, 54, 49, 61]) on the subject. In these lectures I will start by reviewing the now classical proof the Stability of non-relativistic matter by Lieb and Thirring. Then I will review some basic facts about Lieb–Thirring inequalities and finally I will give the details of the proof of stability of a Relativistic toy model. It is a pleasure to thank the organizers of "Spectral Days – 2010" for their kind invitation and support.

2. Stability of Matter: The classical proof of Lieb and Thirring

In this section we will introduce some notation and definitions and we will review the classical proof of Elliott Lieb and Walter Thirring of the stability of matter in nonrelativistic quantum mechanics.

In *Nonrelativistic Quantum Mechanics* we consider a system of N electrons and K fixed nuclei, described by the Hamiltonian,

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_i - e^2\sum_{i=1}^{N}V(x_i) + e^2\sum_{1\le i<j\le N}\frac{1}{|x_i - x_j|} + U, \tag{1}$$

acting on $L^2(\mathbb{R}^{3N}; C^{2^N})$ (bosons) or on the space $\bigwedge^N L^2(\mathbb{R}^3, C^2)$ (fermions). Here,

$$V(x) = \sum_{j=1}^{k}\frac{z_j}{|x - R_j|} \tag{2}$$

is (minus) the electrostatic potential created by the K fixed nuclei in $x \in \mathbb{R}^3$. Here, the nuclei are located at the positions $R_1, R_2, \ldots, R_k$, and have electric charge $ez_1, ez_2, \ldots, ez_k$ respectively, where e is the absolute value of the charge of

the electron. Moreover, m is the mass of the electron. Finally,

$$U = e^2 \sum_{1 \le i < j \le k} \frac{z_i \, z_j}{|R_i - R_j|}. \tag{3}$$

denotes the interaction energy between the nuclei. We denote as

$$E_\psi = \frac{(\psi, H\psi)}{(\psi, \psi)}, \tag{4}$$

the expectation value of the Hamiltonian in the state $\psi \in \bigwedge^N L^2(\mathbb{R}^3, C^2)$, and

$$E(N, k, \underline{Z}, \underline{R}) = \inf_{\psi} E_\psi. \tag{5}$$

Here, $\underline{Z} = (Z_1, Z_2, \ldots, Z_N)$, etc. Now, if we minimize over all possible configurations of the nuclei we get the ground state energy of the system of k nuclei and N electrons, which we denote by,

$$E(N, k, \underline{Z}) = \inf_{\underline{R}} E(N, k, \underline{Z}, \underline{R}). \tag{6}$$

There are two notions of **Stability**:

(A) Stability of the first type
$E(N, k, \underline{Z}, \underline{R})$ is finite for all N, k, $\underline{Z}$, $\underline{R}$.

The stability of the first type amounts to the fact that the Hamiltonian given by (1) is bounded below.

(B) Stability of the second type
$E(N, k, \underline{Z}) \ge -A(z)(N + k)$, assuming that each $z_i \le z$. In Nature, $z_j \le 92$.

The stability of the second kind amounts to the fact that in the configuration of least energy, the energy per particle is bounded below by a constant (i.e., the constant $A(z)$).

2.1. Stability of the hydrogen atom in non-relativistic Quantum Mechanics

As we discussed in the Introduction, the stability of atoms was one of the reasons that gave rise to quantum mechanics at the beginning of the XXth century. By *stability of atoms* one means the fact that the energy of the ground state of an atom is finite. Let us first consider the Hamiltonian of the Hydrogen atom,

$$H = -\frac{1}{2}\Delta - \frac{Z}{|x|}, \tag{7}$$

acting on $L^2(\mathbb{R}^3)$. Here, we have chosen Hartree Atomic Units (au), i.e., units in which $\hbar = 1$, $m = 1$, $|e| = 1$. Let E_0 the bottom of the spectrum of H. Of course, one knows (by exact calculations) that $E_0 = -Z^2/2$ [Ha] $= -Z^2$ [Ry] (in Hatree Atomic Units, the unit of energy is a Hartree, which is equivalent to $= 27,2$ [eV], or, in other words, 2 Rydbergs). However, we can pretend for a moment that we do not know this exact value and we will use functional analytic inequalities to estimate E_0 from below. We will use three different inequalities (Hardy's, Sobolev's and

the Coulomb's Uncertainty Principle), yielding different lower bounds. Just a few years before the Schrödinger equation, Hardy [28] proved the following inequality

$$\int_{\mathbb{R}^3} |\nabla\psi|^2\, dx > \frac{1}{4}\int_{\mathbb{R}^3} \frac{\psi^2}{|x|^2}\, dx, \tag{8}$$

for all $\psi \in H^1(\mathbb{R}^3)$. Using the Rayleigh–Ritz principle, one has

$$E_0 = \inf \frac{(\psi, H\psi)}{(\psi,\psi)} = \inf \frac{(1/2)\int_{\mathbb{R}^3} |\nabla\psi|^2\, dx - Z\int_{\mathbb{R}^3} \psi^2|x|^{-1}\, dx}{\int_{\mathbb{R}^3}\psi^2\, dx}, \tag{9}$$

where the infimum is taken over all $\psi \in H^1(\mathbb{R}^3)$. Using Hardy's inequality (8) in (9), we obtain,

$$E_0 = \inf \frac{\int_{\mathbb{R}^3} \psi^2(a^2/8 - a\,Z)\, dx}{\int_{\mathbb{R}^3}\psi^2\, dx}, \tag{10}$$

where we have set $a = 1/|x|$. Finally, using the estimate $a^2/8 - aZ \geq -2\,Z^2$, one gets from (10) that

$$E_0 \geq -2\,Z^2 \text{ [Ha]}. \tag{11}$$

This estimate is way too low (it is four times the actual value), but it is simple to obtain and it proves that the bottom of the spectrum of the Hydrogen atom is bounded below, and that the atom is *stable*. One can get an improved lower bound if we use Sobolev's inequality [65], i.e.,

$$\int_{\mathbb{R}^3} (\nabla\psi)^2\, dx \geq K_s \left(\int_{\mathbb{R}^3} \psi^6\, dx\right)^{1/3}, \tag{12}$$

with $K_s = 3\left(\frac{\pi}{2}\right)^{4/3} \approx 5,478\ldots$. Using this in (9) we get,

$$(\psi, H\psi) \geq (K_s/2)\left(\int \rho^3\, dx\right)^{1/3} - \int \frac{Z}{|x|}\rho\, dx \equiv h(\rho), \tag{13}$$

where we have set $\rho = \psi^2$. From the previous equation we have that for all $\psi \in L^2(\mathbb{R}^3)$, normalized (i.e., such that $\int \psi^2\, dx = 1$),

$$(\psi, H\psi) \geq \min_{\rho} h(\rho),$$

where

$$h(\rho) \equiv (K_s/2)\left(\int \rho^3\, dx\right)^{1/3} - Z\int \frac{\rho}{|x|}\, dx, \tag{14}$$

with $\rho \geq 0$, and $\int \rho\, dx = 1$. It is straightforward to find the function ρ that minimizes the functional $h(\rho)$ subject to these constraints. It is given by

$$\hat{\rho}(x) = C\left(\frac{1}{|x|} - \frac{1}{R}\right)^{1/2},$$

for $|x| \leq R$, and $\hat{\rho}(x) = 0$, for $|x| \geq R$, where $R = 3/(2Z)$. From here, it follows that,

$$\min_{\rho} h(\rho) = h(\hat{\rho}) = -\frac{2}{3}Z^2 \qquad \text{[Ha]},$$

and, therefore,

$$E_0 \equiv \inf_{\psi} \frac{(\psi, H\psi)}{(\psi,\psi)} \geq -\frac{2}{3}Z^2 \qquad \text{[Ha]}, \tag{15}$$

which is a better approximation to the actual value $E_0 = -Z^2/2$ [Ha].

There is a somewhat different way to estimate the ground state energy of the hydrogen atom. The new way, although gives a slightly worse bound, can be easily generalized to the case of N electrons. In fact, let us consider *Hölder's inequality*,

$$\left| \int f(x)\, g(x)\, dx \right| \leq \left(\int |f(x)|^p\, dx \right)^{1/p} \left(\int |g(x)|^q\, dx \right)^{1/q}, \tag{16}$$

with p and q such that $(1/p) + (1/q) = 1$, and $p \geq 1$. Using (16) with $f = \rho$, $g = \rho^{2/3}$, $p = 3$, and $q = 3/2$, one gets,

$$\int \rho^{5/3}\, dx \leq \left(\int \rho(x)^3\, dx \right)^{1/3} \left(\int \rho(x)\, dx \right)^{2/3}. \tag{17}$$

Now, using Sobolev's inequality together with (17) we have,

$$\int (\nabla \psi^2)\, dx \geq K_s \int \rho_\psi(x)^{5/3}\, dx. \tag{18}$$

Here, $\rho_\psi \equiv \psi^2$, is such that $\int \rho_\psi\, dx = 1$.

Remark. Of course, one can study directly the minimization problem:

$$K_1 \equiv \min_{\psi} \frac{\int (\nabla\psi)^2\, dx}{\int \psi(x)^{10/3}\, dx} \qquad \text{subject to } \int \psi^2\, dx = 1. \tag{19}$$

We leave this minimization problem as an exercise to the reader. Numerically one finds $K_1 \approx 9,578\ldots$. For reasons that will be clear below, it is convenient at this point to introduce the constant (c here stand for *classical*)

$$K_c \equiv \frac{3}{5}(6\pi^2)^{2/3} \approx 9,116\ldots \tag{20}$$

Numerically, $K_1 > K_c > K_s$. Using this bound, i.e.,

$$\int (\nabla\psi)^2\, dx \geq K_c \int \psi^{10/3}\, dx = K_c \int \rho^{5/3}\, dx, \tag{21}$$

in order to estimate from below the expectation value of the kinetic energy of the electron one gets.

$$(\psi, H\psi) \geq h_c(\rho),$$

with,

$$h_c(\rho) = (K_c/2) \int \rho^{5/3}\, dx - Z \int \frac{\rho}{|x|}\, dx.$$

One is lead to the minimization problem,

$$\min_{\rho} \left\{ h_c(\rho) \;\middle|\; \rho(x) \geq 0, \qquad \int \rho(x)\, dx \right\}. \tag{22}$$

The minimizer of $h_c(\rho)$ is given by

$$\rho_c(x) = \left(\left(\frac{6}{5} \frac{Z}{K_c} \right) \left(\frac{1}{|x|} - \frac{1}{R} \right) \right)^{3/2}, \tag{23}$$

for $|x| \leq R$ while $\rho_c(x) = 0$ for $|x| > R$. The radius R is determined by the condition $\int \rho(x)\, dx = 1$ and it turns our to be

$$R = \frac{K_c}{2\, Z} \left(\frac{2}{\pi} \right)^{4/3}.$$

Also, the value of $\min h_c(\rho) = h(\rho_c)$ is given by $-3^{1/3} Z^2/2$ [Ha]. So, finally, using this variational principle one gets,

$$E_0 \geq -\frac{3^{1/3}}{2} Z^2 \qquad \text{[Ha]}.$$

So far, we have discussed (as in [39]) the use of Hardy's and Sobolev's inequalities in order to prove the *stability* of the Hydrogen atom. This discussion has some relevance in particular to make the connection with the N-particle case. Of course the sharp (exact) lower bound (for the Hydrogen atom) is obtained using the *Coulomb Uncertainty Principle*:

Theorem 2.1 (Coulomb Uncertainty Principle (see, e.g., [46] and [54, p. 14])). *Let $\psi \in L^2(\mathbb{R}^3)$, such that $\nabla\psi \in L^2(\mathbb{R}^3)$, then,*

$$\int_{\mathbb{R}^3} \frac{1}{|x|} \psi^2\, dx \leq \|\nabla\psi\|_2 \|\psi\|_2. \tag{24}$$

Equality is attained in (24) *if and only if $\psi(x) = A \exp -c|x|$, for any $A \in \mathbb{R}$, and $c > 0$.*

Proof. There are many ways of proving this sharp result. Perhaps the simplest proof (see [54], p. 14) uses commutator techniques. Here I will use rearrangements (see the Bibliographical Remarks i) at the end of this chapter for references on rearrangements). If we denote by ψ^* the *symmetric decreasing rearrangement* of ψ (i.e., a radially symmetric, non increasing function equi-measurable to ψ), one has that $\|\psi\|_2 = \|\psi^*\|_2$ (in general L^p norms stay the same under rearrangements) and $\|\nabla\psi\|_2 \geq \|\nabla\psi^*\|_2$. Moreover, since $1/|x|$ is symmetric decreasing, one also has,

$$\int_{\mathbb{R}^3} \frac{1}{|x|} \psi(x)^2\, dx \leq \int_{\mathbb{R}^3} \frac{1}{|x|} \psi(x)^{*\,2}\, dx.$$

Because of these three facts, it is enough to prove (24) for radially symmetric functions. For radially symmetric functions, (24) follows by integration by parts and Schwarz's inequality. In fact. if $\psi(x) = \psi(r)$, with $r = |x|$, we have,

$$\begin{aligned} &\textstyle\int_{\mathbb{R}^3} |x|^{-1} \psi(x)^2\, dx = 4\pi \int_0^\infty \psi^2(r)\, r\, dr = -4\pi \int_0^\infty \psi(r)\, \psi'(r)\, r^2\, dr \\ &\leq \left(\textstyle\int_0^\infty \psi^2(r)\, 4\pi r^2\, dr \right)^{1/2} \left(\int_0^\infty \psi'^2(r)\, 4\pi r^2\, dr \right)^{1/2} = \|\psi\|_2 \|\nabla\psi\|_2. \end{aligned} \tag{25}$$

One has equality, if and only if $\psi'(r) = -c\psi(r)$, i.e., if $\psi(r) = A \exp -cr$. □

Remarks.

i) *It follows immediately from* (24) *that* $E_0 = -Z^2/2$ [Ha] (*and the infimum in* (9) *is actually attained at* $\psi(x) = A \exp -Z|x|$).

ii) *Coulomb Uncertainty Principles play an important role in most of the proofs of Stability of Matter, since they provide a way of controlling the Coulomb singularities with the help of the kinetic energy term* (*see, e.g., Theorem* 4.2, *below, for an example of the use of a Coulomb Uncertainty Principle in a simple relativistic toy model*).

2.2. Stability of a system of N electrons in non-relativistic Quantum Mechanics

Consider now a system of N noninteracting fermions in a cubic box of volume V, with Dirichlet boundary conditions. (In the rest of this chapter we will switch to units in which $\hbar^2/(2m) = 1$ and $e = 1$.) It is well known that for large values of N the ground state energy of this system, which we will denote by T_V, (the Hamiltonian of this system in these units is just $-\sum_{i=1}^{N} \Delta_i$, acting on $\bigwedge^N L^2(\mathbb{R}^3, C^2)$), is approximately given by

$$T_V \approx q^{-2/3} K_c V \rho^{5/3} \tag{26}$$

where $\rho = N/V$ and q is the number of spin states (as usual, $q = 2$ for electrons). In other words, T_V is proportional to $N^{5/3}$ for fermions. On the other hand, T_V is proportional to N in the case of bosons. As we have seen above (see equation (21)), the expectation value of the kinetic energy of one electron satisfies,

$$T_\psi \geq K_c \int \rho_\psi(x)^{5/3}\, dx, \tag{27}$$

and (26) suggests that for a system of N electrons,

$$T_\psi \approx q^{-2/3} K_c \int \rho_\psi(x)^{5/3}\, dx. \tag{28}$$

In some sense this intuition is correct. In 1975, Lieb and Thirring [51] proved that the right side of (28) with a smaller constant is in fact a lower bound to the expectation of the kinetic energy of a system of N fermions (see, (32)) below.

A system of N electrons is described by the wavefunction

$$\psi(x_1, x_2, \ldots, x_N; \sigma_1, \sigma_2, \ldots, \sigma_N) \tag{29}$$

with $x_i \in \mathbb{R}^3$, $\sigma_i \in \{1, 2, \ldots, q\}$. Because of the *Pauli Principle*, the function ψ must be antisymmetric in the pairs (x_i, σ_i). The norm of ψ is given by

$$(\psi, \psi) \equiv \sum_{\sigma_i=1}^{q} \int |\psi(x_1, x_2, \ldots, x_N; \sigma_1, \sigma_2, \ldots, \sigma_N)|^2\, dx_1\, dx_2\, \ldots\, dx_N.$$

Also, the expectation value of the kinetic energy of the fermions is given by

$$T_\psi = \sum_{i=1}^{N} \sum_{\sigma_i=1}^{q} \int |\nabla_i \psi(x_1, x_2, \ldots, x_N; \sigma_1, \sigma_2, \ldots, \sigma_N)|^2\, dx_1\, dx_2\, \ldots\, dx_N. \tag{30}$$

Recall that the kinetic energy of the system of N fermions is given by $-\sum_{i=1}^{N} \Delta_i$, in the units we are using in this section. The *single particle density* of this system of N fermions is defined, as usual, as

$$\rho_\psi(x) = N \sum_{\sigma_i=1}^{q} \int |\psi(x, x_2, \ldots, x_N; \sigma_1, \sigma_2, \ldots, \sigma_N)|^2 \, dx_2 \ldots dx_N. \tag{31}$$

and, it is normalized in such a way that $\int \rho_\psi(x)\, dx = N$. In 1975, Lieb and Thirring [51] proved that if ψ is normalized (so that $(\psi, \psi) = 1$), and the single particle density is given by (31), then one has

$$T_\psi \geq (4\pi)^{-2/3} q^{-2/3} K_c \int \rho_\psi(x)^{5/3}\, dx. \tag{32}$$

The numerical value of $(4\pi)^{-2/3}$ is approximately 0.185 (this constant was later improved to 0.277).

In order to prove this theorem, Lieb and Thirring devised a new type of functional inequalities that we describe in Chapter 2 below. The study of these inequalities, together with their extensions in many directions, has developed greatly in the last 35 years. The whole subject is now generically known under the name *Lieb Thirring inequalities*. For the problem at hand we only need the following special case: Consider the Schrödinger operator $H = -\Delta + V$ acting on $L^2(\mathbb{R}^3)$, where $V(x) \leq 0$. Let $e_1 \leq e_2 \leq \cdots \leq 0$ denote the negative eigenvalues of H. Then one has

$$\sum_j |e_j| \leq \frac{4\pi}{15\pi^2} \int |V(x)|^{5/2}\, dx. \tag{33}$$

Notice that if we were to use the semiclassical approximation, one would approximate

$$\sum_j |e_j| \approx \frac{1}{(2\pi)^3} \int (p^2 + V)_-\, dx\, dp = \frac{1}{(2\pi)^3} \int \left[4\pi \int_0^{|V(x)|^{1/2}} (p^2 + V)_- p^2\, dp \right] dx$$

where $f(x)_- \equiv \max(0, -f(x))$ denotes the negative part of the function f. The integral on p can be done explicitly, and one gets the semiclassical estimate

$$\sum_j |e_j| \approx \frac{1}{15\pi^2} \int |V(x)|^{5/2}\, dx,$$

which differs from the upper bound (33) by the factor (4π).

Central to the discussion here is the physical intuition that in average a single electron "feels" the (electrostatic) potential generated by the nuclei plus the average potential generated by the whole cloud of electrons. In fact, each single electron will "feel" the Thomas–Fermi potential associated to the single particle density. It is this physical intuition plus an appropriate Lieb–Thirring inequality that allows to find a lower bound on the kinetic energy of the N electrons in terms

of a functional of the single particle ρ_ψ. With that in mind consider the single particle Hamiltonian for the ith electron, given by

$$h_i = p_i^2 - g\rho_\psi^{2/3}, \tag{34}$$

where g is a coupling constant to be determined. Also, consider the following N-particle Hamiltonian,

$$\hat{H} = \sum_{i=1}^{N} h_i. \tag{35}$$

Then, the ground state energy of this N particle Hamiltonian, E_0 say, satisfies

$$E_0 \leq (\psi, \hat{H}\psi) = T - g \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3}\, dx. \tag{36}$$

On the other hand (by Pauli's principle) E_0 is greater than or equal to the sum of negative eigenvalues of $\hat{H}$, sum that can be estimated using the Lieb–Thirring inequality (33). Thus, one gets,

$$E_0 \geq -\frac{4}{15\pi} g^{5/2} \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3}\, dx. \tag{37}$$

Combining (36) and (37), one finally gets,

$$T \geq (g - \frac{4}{15\pi} g^{5/2}) \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3}\, dx. \tag{38}$$

Maximizing over g, one obtains,

$$T \geq \frac{3}{5} \left(\frac{3\pi}{2}\right)^{2/3} \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3}\, dx, \tag{39}$$

which is the desired lower bound on the kinetic energy of the system in terms of a functional of the single particle density.

2.3. Stability of a many particle system via Thomas–Fermi

In the previous paragraphs we have seen how to use the uncertainty principle (either using Hardy's inequality, Sobolev's inequality, or better the Coulomb Uncertainty Principle) to show that in non-relativistic Quantum Mechanics the energy of an atom with one electron is bounded below (and that therefore there is no collapse). For atoms with many electrons, the proof of the stability of matter (understood as above) is more difficult, and it was accomplished by F. Dyson and A. Lenard. In 1975, Lieb and Thirring [51] gave a different proof, with a major improvement on the lower bound for the energy per particle. The proof of Lieb and Thirring relied on two physical facts:

i) That the energy of the Thomas–Fermi model of atoms is a good approximation to the groundstate energy of the non-relativistic Hamiltonian of the system of N electrons, and
ii) that in the Thomas–Fermi model there are no molecules (Teller's Theorem).

As pointed above, in order to use this physical intuition, Lieb and Thirring used what it is nowadays known as *Lieb–Thirring inequalities* to find a lower bound to the quantum mechanical energy in terms of the Thomas–Fermi model.

The Thomas–Fermi model (introduced independently by Thomas [68] and Fermi [26]) is defined through the energy functional [38]

$$\xi(\rho) = q^{-2/3} K_c \int_{\mathbb{R}^3} \rho^{5/3}\, dx - \int_{\mathbb{R}^3} V(x)\rho(x)\, dx + \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\rho(x)\rho(y)}{|x-y|}\, dx\, dy + U \quad (40)$$

where $\rho(x) \geq 0$ denotes the electronic density. On the other hand,

$$V(x) = \sum_{i=1}^{K} \frac{z_i}{|x - R_i|},$$

denotes the Coulomb potential created by the K fixed nuclei of charge $z_i > 0$, located at R_i, $i = 1, \ldots, K$. Finally,

$$U = \sum_{1 \leq i < j \leq K} \frac{z_i\, z_j}{|R_i - R_j|}$$

denotes the repulsion energy between the nuclei. The term $\int \rho^{5/3}$ in (40) represents the kinetic energy of the electrons, and takes into account the Fermi statistics of them. The energy of the system of λ electrons and K nuclei in this model is given by

$$E_{TF}(\lambda) = \inf\left\{ \xi(\rho) \;\middle|\; \rho \geq 0, \int \rho\, dx = \lambda \right\}, \quad (41)$$

The corresponding Euler equation, i.e., the *Thomas–Fermi equation*, is given by,

$$\frac{5}{3} K_c q^{-2/3} \rho^{5/3} \equiv \max(\phi(x) - \mu, 0), \quad (42)$$

with

$$\phi(x) = V(x) - \int \rho(y) \frac{1}{|x-y|}\, dy. \quad (43)$$

Here, μ, the *chemical potential*, is a Lagrange multiplier that is introduced to take into account the constraint $\int \rho(x)\, dx = \lambda$. The equation (42) has a solution if and only if $\lambda \leq \sum_{i=1}^{k} z_i$. The Thomas–Fermi energy of an isolated *neutral atom* of nuclear charge Z (i.e., with $K = 1$ and $\lambda = Z$) is found numerically to be

$$E_{TF}(Z) = -2.21 q^{2/3} \frac{1}{K_c} Z^{7/3}. \quad (44)$$

One of the main inputs in the proof of stability by Lieb and Thirring is Teller's *no binding* theorem [67] that asserts that "there are no molecules in the Thomas–Fermi model". If there are at least two nuclei, decompose

$$V(x) = \sum_{i=1}^{K} z_i \frac{1}{|x - R_i|} = V^1 + V^2,$$

with

$$V^1(x) = \sum_{i=1}^{m} z_i \frac{1}{|x - R_i|},$$

with $m < K$. Let $E^1_{TF}(\lambda)$ be the TF energy for a system of λ electrons in the presence of the nuclei $1, \ldots, m$ and respectively $E^2_{TF}(\lambda)$ for the nuclei $m+1, \ldots, K$. Given λ, let $\lambda_1 \geq 0$ and $\lambda_2 \equiv \lambda - \lambda_1 \geq 0$ be chosen in such a way that $E^1_{TF}(\lambda_1) + E^2_{TF}(\lambda_2)$ is minimized. Then, Teller's theorem says that

$$E_{TF}(\lambda) \geq E^1_{TF}(\lambda_1) + E^2_{TF}(\lambda_2), \tag{45}$$

i.e., there is *no binding*.

Using the *no binding* theorem of Teller one has that for all $\lambda \geq 0$ and $Z \equiv \sum_{i=1}^{K} z_i$,

$$E_{TF}(\lambda) \geq E_{TF}(Z) \geq -2.21 q^{2/3} \frac{1}{K_c} \sum_{j=1}^{K} z_j^{7/3}. \tag{46}$$

The first inequality in (46) follows from the fact that the Thomas–Fermi energy is a decreasing function on the number of electrons and that the absolute minimum of the energy functional without a restriction on the number of electrons is attained at neutrality (i.e., when $\lambda = Z$). The second inequality in (46) follows from (44) and Teller's Theorem.

Using (46), Lieb and Thirring realized that taking all the nuclear charges $z_i = 1$, and replacing K_c by γ, one has that for all $\rho(x) > 0$ with $\int \rho(x)\,dx < \infty$ and $\int \rho(x)^{5/3}\,dx < \infty$,

$$\begin{aligned} \textstyle\sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|} &\geq -\tfrac{1}{2} \textstyle\int \rho(x) \frac{1}{|x-y|} \rho(y)\,dx\,dy \\ &+ \textstyle\int \rho(y) V_X(y)\,dy - 2.21 \frac{N}{\gamma} - \gamma \int \rho(x)^{5/3}\,dx \end{aligned} \tag{47}$$

where $V_X(y) \equiv \sum_{j=1}^{N} 1/|y - x_j|$. Taking the expectation value of the equation (47) with respect to a normalized antisymmetric function ψ, and setting $\rho(x) = \rho_\psi(x)$ (i.e., the *single particle density* associated to ψ), one readily gets,

$$\begin{aligned} &\left(\psi, \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|} \psi \right) \\ &\geq \frac{1}{2} \int \rho_\psi(x) \frac{1}{|x-y|} \rho_\psi(y)\,dx\,dy - 2.21 \frac{N}{\gamma} - \gamma \int \rho_\psi(x)^{5/3}\,dx. \end{aligned} \tag{48}$$

To control the expectation value of the kinetic energy we use (32). Collecting terms we have,

$$E^Q_\psi \geq \alpha \int \rho_\psi^{5/3} - \int V(x) \rho_\psi(x)\,dx + \frac{1}{2} \int \rho_\psi(x) \frac{1}{|x-y|} \rho_\psi(y)\,dx\,dy + U - 2.21 \frac{N}{\gamma}, \tag{49}$$

with $\alpha \equiv (4\pi q)^{-2/3} K_c - \gamma$. So far, γ was arbitrary. From now on we restrict its value so that $\alpha > 0$, and later one optimizes over γ. From Teller's no binding theorem, one has,

$$E_\psi^Q \geq -2.21 \left\{ \frac{N}{\gamma} + \frac{1}{\alpha} \sum_{j=1}^{K} z_j^{7/3} \right\}.$$

One can optimize the right side of this equation with respect to γ. The optimal γ is given by

$$\gamma = (4\pi q)^{-2/3} K_c \left[1 + \left(\sum_{j=1}^{K} z_j^{7/3} / N \right)^{1/2} \right]^{-1},$$

and thus one gets,

$$E_N^Q \geq -2.21 \frac{(4\pi q)^{2/3} N}{K_c} \left(1 + a^{1/2} \right)^2,$$

with $a \equiv \sum_{j=1}^{K} z_j^{7/3}/N$. Using Schwarz, one has $(1 + a^{1/2})^2 \leq 2 + 2a$; therefore,

$$E_N^Q \geq -4.42 (4\pi q)^{2/3} \frac{1}{K_c} \left(N + \sum_{j=1}^{K} z_j^{7/3} \right). \tag{50}$$

Thus, if the nuclear charges z_j are bounded above by some fixed z, E_N^Q is bounded below by a constant times the *Total Number* of particles, $N+K$. If $z_j = 1$ (i.e., one has a bunch of hydrogen atoms) and $N = K$ (i.e., we are in the case of neutrality) (50) implies

$$E_N^Q \geq -22.24 N \qquad [\text{Ry}].$$

In the previous formulas, the q dependence is kept in purpose in order to say something about *bosons*. In fact, if $q = N$, the requirement of antisymmetry on ψ is no restriction at all. In this case $E_N^Q = \inf \text{spec} H_N$ over all $L^2(\mathbb{R}^{3N})$. Hence,

$$E_N^Q \geq -\frac{2.21}{K_c} (4\pi)^{2/3} N^{5/3} \left[1 + \left(\sum_{j=1}^{K} \frac{z_j^{7/3}}{N} \right)^{1/2} \right]^2. \tag{51}$$

2.4. Bibliographical Remarks

i) Rearrangements of functions were introduced by G. Hardy and J.E. Littlewood. Their results are contained in the classical book, G.H. Hardy, J.E. Littlewood, J.E., and G. Pólya, *Inequalities*, 2d ed., Cambridge University Press, 1952. The fact that the L^2 norm of the gradient of a function decreases under rearrangements was proven by Faber and Krahn [24, 33, 34]. A more modern proof as well as many results on rearrangements and their applications to PDE's can be found in [66]. The reader may want to see also the article by E.H. Lieb, *Existence and uniqueness of the minimizing*

solution of Choquard's nonlinear equation, Studies in Appl. Math. **57**, 93–105 (1976/77), for an alternative proof of the fact that the L^2 norm of the gradient decreases under rearrangements using heat kernel techniques. An excellent expository review on rearrangements of functions (with a good bibliography) can be found in Talenti, G., *Inequalities in rearrangement invariant function spaces*, in *Nonlinear analysis, function spaces and applications, Vol.* 5 (*Prague,* 1994), 177–230, Prometheus, Prague, 1994 (available at the website: http://www.emis.de/proceedings/Praha94/). See also, Chapter 3, *Rearrangement Inequalities* of [46], and also Lecture 2 of my recent lecture notes [2].

ii) Since the work of Dyson and Lenard and later of Lieb and Thirring, many new alternative proofs of the stability of matter have appeared. In particular, many of the recent proofs do not use the Thomas–Fermi model as a physical and mathematical tool. Instead, the use of electrostatic inequalities initiated by Onsager in the thirties is perhaps the most common method nowadays. See for example [54, 49, 61] and the references therein.

3. Lieb–Thirring inequalities

The Lieb–Thirring inequalities (LT for short) originated in the proof of the stability of matter of Elliott Lieb and Walter Thirring [51] in 1975, and have given place to a vast mathematical literature since then. Consider a Schrödinger operator

$$H = -\Delta + V(x), \tag{52}$$

acting on $L^2(\mathbb{R}^n)$, and denote $e_1 \leq e_2 \leq \cdots < 0$ its negative eigenvalues. Then, the Lieb–Thirring inequalities amount to the fact that

$$\sum_j |e_j|^\gamma \leq L_{\gamma,n} \int_{\mathbb{R}^n} V_-(x)^{\gamma+n/2}\, dx \tag{53}$$

where $V_-(x) = \max(-V(x), 0)$ s the negative part of $V(x)$, for suitable values of γ. The range of possible values of γ depend on n. For $n = 1$, LT inequalities hold for all $\gamma \geq 1/2$ (the case $\gamma = 1/2$ was proved in [73]). For $n = 2$, they hold for all $\gamma > 0$, and for dimensions larger or equal to 3 they hold for all $\gamma \geq 0$. Notice that the case $\gamma = 0$ in (53) yields the number of negative eigenvalues of the operator H. The LT in this special case (i.e., the LT inequality with $\gamma = 0$, $n \geq 3$) was obtained independently by Cwickel [15], Lieb, [40] and Rosenbljum [58], and it is usually referred to as the CLR bound (see also [13] for an alternative proof of the CLR bound). Associated with (53) is the semiclassical estimate for $\sum_j |e_j|^\gamma$ which in fact motivates it. Using the *Planck dictum* (with $\hbar = 1$),

$$\sum_{j\geq 1} |e_j|^\gamma \approx (2\pi)^{-n} \int_{\mathbb{R}^n \times \mathbb{R}^n} (p^2 + V(x))_-^\gamma\, dp\, dx = L^c_{\gamma,n} \int_{\mathbb{R}^n} V_-(x)^{\gamma+n/2}\, dx, \tag{54}$$

where

$$L^c_{\gamma,n} = \left(\frac{1}{4\pi}\right)^{n/2} \frac{\Gamma(\gamma+1)}{\Gamma(\gamma+1+(n/2))}. \tag{55}$$

By considering $V(x) = \lambda W(x)$ with W sufficiently smooth and letting the coupling constant $\lambda \to \infty$ (which is equivalent to letting $\hbar \to 0$ in the usual semiclassical picture) one concludes that

$$L_{\gamma,n} \geq L^c_{\gamma,n}. \tag{56}$$

Since the original paper of Lieb and Thirring there have been many results concerning the sharp values of the constants $L_{\gamma,n}$. In 1978, Aizenman and Lieb [1] proved that

$$R_{\gamma,n} \equiv \frac{L_{\gamma,n}}{L^c_{\gamma,n}}, \tag{57}$$

is a monotonically non-increasing function of γ, and thus, if there is a value of γ, say $\hat{\gamma}$ for which $R_{\hat{\gamma},n} = 1$, then,

$$L_{\gamma,n} = L^c_{\gamma,n},$$

for all $\gamma \geq \hat{\gamma}$. Using the Buslaev–Faddeev–Zakharov trace formula [12, 25], Lieb and Thirring [52] proved that

$$L_{3/2,1} = L^c_{3/2,1} = \frac{3}{16}$$

(see also the proof of this fact below, using commutation methods). Hence, $L_{\gamma,1} = L^c_{\gamma,1}$ for all $\gamma \geq 3/2$. The corresponding result

$$L_{\gamma,n} = L^c_{\gamma,n},$$

for $\gamma \geq 3/2$ and all $n \geq 2$ was established by Laptev and Weidl [36] (see also [5] for an alternative proof). The fact that

$$L_{1/2,1} = 2\, L^c_{1/2,1} = \frac{1}{2}, \tag{58}$$

was established in [30]. It is still an open problem to determine the sharp values of $L_{\gamma,n}$ for $1/2 < \gamma < 3/2$ in one dimension and for $\gamma < 3/2$ in higher dimensions. However, there is a conjecture due to Lieb and Thirring [52], which says that $L_{\gamma,n}$, for $\gamma \leq 3/2$, should be given by

$$L^1_{\gamma,n} = \sup \frac{|e_1|^\gamma}{\int_{\mathbb{R}^n} V_-(x)^{\gamma+n/2}\, dx} \tag{59}$$

where the supremum is taken over all potentials V such that $V_- \in L^{\gamma+n/2}(\mathbb{R}^n)$. In dimension $n = 1$ this maximization problem had been solved by Keller [35], who found

$$L^1_{\gamma,1} = \frac{1}{\sqrt{\pi}((\gamma-\frac{1}{2})} \frac{\Gamma(\gamma+1)}{\Gamma(\gamma+\frac{1}{2})} \left(\frac{\gamma-\frac{1}{2}}{\gamma+\frac{1}{2}}\right)^{\gamma+(1/2)},$$

using the direct method of the calculus of variations (see [6] for an alternative method of determining $L^1_{\gamma,1}$). This conjecture has only been proved in the case $\gamma = 1/2$, $n = 1$ [30], where $L^1_{1/2,1} = 1/2$.

In their original proof of the LT inequalities [51] (i.e., in the special case $\gamma = 1$ and $n = 3$) Lieb and Thirring used the Birman–Schwinger kernel together with the counting function $N_{-\alpha}(V)$ (i.e., the number of negative eigenvalues of $H = -\Delta + V$ acting on $L^2(\mathbb{R}^3)$ which lie below $-\alpha$, $\alpha > 0$) to derive it. Se also the review articles [54, 61] and the book [49] for details. In what follows I will present two different alternative methods that have been used to obtain LT inequalities:

i) The *commutation method*, and ii) The Eden–Foias method.

3.1. Use of commutation methods to prove the Lieb–Thirring inequality for $\gamma = 3/2$ in dimension 1

Commutation methods were introduced by Jacobi in the 1837 [31], and later by Darboux [16] to derive spectral properties of Sturm–Liouville operators, and since then, they have had a long history. Its modern appearance seems to be due to Crum [14]. For a rigorous discussion of the use of commutation methods we refer to [18] and [27]. Here we will present the proof of (58), using commutation methods as given in [5]. Let $-\lambda_1$ be the lowest eigenvalue of the one-dimensional Schrödinger operator

$$H = -\frac{d^2}{dx^2} + V(x),$$

acting on $L^2(\mathbb{R})$. Here we assume for simplicity that $V(x)$ has compact support, which lies in $[-a, a]$. It is well known that the lowest eigenvalue is not degenerate and the corresponding eigenfunction ϕ_1 can be chosen to be strictly positive. Moreover, outside the support of the potential we have,

$$\phi_1(x) = \begin{cases} \text{const. } e^{-\sqrt{\lambda_1}\,x}, & \text{if } x > a, \\ \text{const. } e^{+\sqrt{\lambda_1}\,x}, & \text{if } x < -a. \end{cases} \tag{60}$$

Thus the logarithmic derivative,

$$F(x) = \frac{\phi_1'(x)}{\phi_1(x)}, \tag{61}$$

is defined and satisfies the Riccati equation,

$$F' + F^2 = V + \lambda_1, \tag{62}$$

together with the conditions

$$F(x) = \begin{cases} -\sqrt{\lambda_1}\,x, & \text{if } x > a, \\ +\sqrt{\lambda_1}\,x, & \text{if } x < -a. \end{cases} \tag{63}$$

A simple computation shows that the Hamiltonian H can be written as

$$H = D^* D - \lambda_1, \tag{64}$$

where

$$D = \frac{d}{dx} - F, \tag{65}$$

and

$$D^* = -\frac{d}{dx} - F. \tag{66}$$

It is a general fact [18, 27] that the operators $D^* D$ and $D D^*$ acting on $L^2(\mathbb{R})$ have the same spectrum with the possible exception of the zero eigenvalue. Note that $D^* D$ has a zero eigenvalue which corresponds to the ground state of H. The operator $D D^*$ does not have a zero eigenvalue. This follows from the fact that the corresponding eigenfunction ψ satisfies

$$\psi' = -F\psi,$$

and hence $\psi(x) = c/\phi_1(x)$ (where c is a constant) which grows exponentially and is not normalizable. Thus, the new Schrödinger operator,

$$\tilde{H} = D D^* - \lambda_1 = -\frac{d^2}{dx^2} - F' + F^2 - \lambda_1 = -\frac{d^2}{dx^2} + V - 2F', \tag{67}$$

has, except for the eigenvalue $-\lambda_1$, precisely the same eigenvalues as H. Also, notice that the potential $V - 2F'$ is smooth and has compact support in the same interval as the potential V. Next, we compute using the Riccati equation (62)

$$\int (V - 2F')^2 \, dx = \int V^2 \, dx + 4 \int (\lambda_1 - F^2) F' \, dx. \tag{68}$$

The last term can be computed explicitly using (63) and we obtain,

$$\int (V - 2F')^2 \, dx = \int V^2 \, dx - \frac{16}{3} \lambda_1^{3/2}. \tag{69}$$

Thus,

$$\sum_{k=1}^{L} \lambda_k^{3/2} - \frac{3}{16} \int V^2 \, dx = \sum_{k=2}^{L} \lambda_k^{3/2} - \frac{3}{16} \int (V - 2F')^2 \, dx \tag{70}$$

and the Schrödinger operator with the potential $V - 2F'$ has precisely the eigenvalues $-\lambda_2, \ldots, -\lambda_L$. Continuing this process we remove one eigenvalue after another. After the last one is removed a manifestly negative quantity is left over, and this proves Theorem 1 in the scalar case.

3.2. The Eden–Foias bound [21]

A completely different approach to derive LT inequalities was introduced by Eden and Foias in 1991, [21]. This method yields the best (not sharp) LT constants to date in the $n = \gamma = 1$ case. Recently it has been extended also to cover the n-dimensional case with $\gamma = 1$ (see, [19], where the best constants up to date for the case $n \geq 1$ and $\gamma = 1$ are obtained).

Lemma 3.1 (An L^∞ bound for functions $f \in L^2(\mathbb{R})$ and $f' \in L^2(\mathbb{R})$). *If $f \in L^2(\mathbb{R})$ and $f' \in L^2(\mathbb{R})$, then,*

$$f(x)^2 \leq \|f\|_2 \|f'\|_2 \tag{71}$$

Proof. Using the fundamental theorem of calculus we write,

$$f(x)^2 = \int_{-\infty}^{x} \frac{d}{ds} f^2(s)\, ds = 2\int_{-\infty}^{x} f(s)f'(s)\, ds$$
$$\leq \alpha \int_{-\infty}^{x} f^2(s)\, ds + \frac{1}{\alpha}\int_{-\infty}^{x} f'^2(s)\, ds,$$

for any constant $\alpha > 0$. Analogously, we have,

$$f(x)^2 \leq \beta \int_{x}^{\infty} f^2(s)\, ds + \frac{1}{\beta}\int_{x}^{\infty} f'^2(s)\, ds,$$

for any $\beta > 0$. We choose $\beta = \alpha$, and add the last two equations to get,

$$2f(x)^2 \leq \alpha \|f\|_2^2 + \frac{1}{\alpha}\|f'\|_2^2,$$

and the result follows optimizing the right side in α, i.e., choosing $\alpha = \|f'\|_2/\|f\|_2$. □

Now, consider an orthonormal set $\{u_n\}_{n=1}^N$ of functions in $L^2(\mathbb{R})$, and introduce the function

$$K(x,y) = \sum_{n=1}^{N} u_n(x)u_n(y), \tag{72}$$

In the sequel we use the result of Lemma 3.1, with the function $f_y(x) \equiv K(x,y)$, i.e., we consider $K(x,y)$ as a function of x with y as a parameter. Thus, setting $f_y(x) = K(x,y)$, we compute first,

$$\|f_y\|_2^2 = \sum_{n,m=1}^{N} \int_{\mathbb{R}} u_n(x)u_n(y)u_m(x)u_m(y)\, dx = \sum_{n=1}^{N} u_n(y)^2, \tag{73}$$

where the last equality follows from the orthonormality of the set $\{u_n\}_{n=1}^N$. Analogously, one can compute,

$$\|f_y'\|^2 = \sum_{n,m=1}^{N} u_n(y)u_m(y) \int_{\mathbb{R}} u_n'(x)u_m'(x)\, dx \tag{74}$$

Using (71) with the function $f_y(x)$, squaring, using (73) and (74), and choosing $x = y$ on the right side of the result, we finally get,

$$\left[\sum_{n=1}^{N} u_n(y)^2\right]^4 \leq \sum_{n=1}^{N} u_n(y)^2 \sum_{n,m=1}^{N} u_n(y)u_m(y) \int_{\mathbb{R}} u_n'(x)u_m'(x)\, dx. \tag{75}$$

Simplifying one gets,

$$\left[\sum_{n=1}^{N} u_n(y)^2\right]^3 \leq \sum_{n,m=1}^{N} u_n(y)u_m(y) \int_{\mathbb{R}} u_n'(x)u_m'(x)\, dx.$$

Finally, integrating the above inequality in y over the whole line, one obtains,

$$\int_{\mathbb{R}} \left[\sum_{n=1}^{N} u_n(y)^2 \right]^3 dy \leq \int_{\mathbb{R}} \sum_{n=1} u_n'(y)^2 \, dy, \tag{76}$$

where we have used again the orthonormality of the set $\{u_n\}_{n=1}^N$.

Now, one can use the result embodied in (76) to derive a Lieb–Thirring inequality with exponent $\gamma = 1$ in one dimension. In fact, consider the Schrödinger operator,

$$H = -\frac{d^2}{dx^2} - V(x), \tag{77}$$

acting on $L^2(\mathbb{R})$. Here the potential $V(x) \geq 0$ goes to *zero* at $\pm\infty$. Let $-\lambda_1 < -\lambda_2 < \cdots$ the eigenvalues of H, where $\lambda_n \geq 0$, all n. Also, denote by u_n the corresponding (normalized) eigenfunctions. Thus, we have,

$$-u_n'' - V u_n = -\lambda_n u_n, \tag{78}$$

Since H is self adjoint, the set $\{u_n\}_{n=1}^N$ is an orthonormal set (where N is the number of eigenvalues; without loss of generality we can always assume that V is of compact support, so the number of negative eigenvalues (i.e., N) is finite. Multiplying (78) by u_n and integrating in x over the line $\mathbb{R}$, one has,

$$\lambda_n = \int_{\mathbb{R}} V u_n^2 \, dx - \int_{\mathbb{R}} (u_n')^2 \, dx. \tag{79}$$

Summing (78) over n, we get,

$$\sum_{n=1}^{N} \lambda_n = \int_{\mathbb{R}} V \left(\sum_n u_n^2 \right) dx - \int_{\mathbb{R}} V \left(\sum_n {u'}_n^2 \right) dx. \tag{80}$$

Now, for any positive θ, we have the point-wise bound,

$$V(x)\theta \leq \theta^3 + \left(\frac{2}{3\sqrt{3}} \right) V(x)^{3/2}. \tag{81}$$

From (76), (80) and (81) we finally conclude that

$$\sum_{n=1}^{N} \lambda_n \leq \frac{2}{3\sqrt{3}} \int_{\mathbb{R}} V(x)^{3/2} \, dx. \tag{82}$$

The constant $c = 1/(3\sqrt{3}) \approx 0.3849$ is the best constant to date, but is almost sixty percent larger than the conjectured value $L^1_{1,1} = 4/(3\pi\sqrt{3}) \approx 0.2450$.

3.3. Bibliographical Remarks

The function $K(x, y)$ used in the proof of the Eden–Foias bound (i.e., equation (72) above) appears frequently in the proof of many results concerning orthogonal polynomials, in particular in connection with the Christoffel–Darboux formula (see, e.g., [29], p. X).

Lieb–Thirring inequalities are not only important in connection to the mathematics of the stability of matter. They have also connections to interesting geometrical problems. Just to mention one particular problem in that direction, Benguria and Loss [6] proved that the following geometrical problem for ovals in the plane is related to the Lieb–Thirring conjecture in the case $n = 1$, $\gamma = 1$: Denote by C a closed curve in the plane, of length 2π, with positive curvature κ, and let

$$H(C) \equiv -\frac{d^2}{ds^2} + \kappa^2 \tag{83}$$

acting on $L^2(C)$ with periodic boundary conditions. Let $\lambda_1(C)$ denote the lowest eigenvalue of $H(C)$. Certainly, $\lambda_1(C)$ depends on the geometry of the curve C. In [6] it is proven that a particular case of the Lieb–Thirring conjecture for $\gamma = 1$ and $n = 1$ is equivalent to proving that

$$\lambda_1(C) \geq 1, \tag{84}$$

with equality if and only if C belongs to a one-parameter family of ovals which include the circle (in fact the one-parameter family of curves is characterized by a curvature given by $\kappa(s) = 1/(a^2 \cos^2(s) + a^{-2} \sin^2(s))$[6]). It is a simple matter to see that if C is a circle of length 2π, the lowest eigenvalue of $H(C)$ is precisely 1. The fact that there is degeneracy of the conjectured minimizers makes the problem much harder.

The conjecture (84) is still open. Concerning (nonoptimal) lower bounds, Benguria and Loss proved [6]

$$\lambda_1(C) \geq 1/2, \tag{85}$$

and more recently Linde [45] found the best lower bound to date,

$$\lambda_1(C) > \left(1 + \frac{\pi}{\pi + 8}\right)^{-2} \approx 0.60847. \tag{86}$$

4. The stability of matter for a relativistic toy model

In the last lecture I will consider the stability of a relativistic model. The model I will consider here is rather a toy model. There are two reasons for considering the stability of matter for this simple relativistic toy model. The first one is that it is simple but at the same time one uses, in studying its stability, most of the known techniques needed in order to prove stability for relativistic Coulomb systems. The second is that recently we used the analog two-dimensional version of this model as a basic tool to get a Lieb–Oxford type bound for the exchange energy in two dimensions (see [4]).

The zero mass limit of the relativistic Thomas–Fermi–Weizsäcker (henceforth ultrarelativistic TFW) energy functional for nuclei of charges $z_i > 0$ (which need not be integral) located at R_i, $i = 1, \ldots, K$ is defined by [22, 23]

$$\xi(\rho) = a^2 \int_{\mathbb{R}^3} (\nabla \rho^{1/3})^2 \, dx + b^2 \int_{\mathbb{R}^2} \rho^{4/3} \, dx - \int_{\mathbb{R}^3} V(x)\rho(x) \, dx + D(\rho, \rho) + U, \tag{87}$$

where the potential V is given by,

$$V(x) = \sum_{i=1}^{K} \frac{z_i}{|x - R_i|}, \tag{88}$$

which is the Coulomb potential generated by K point particles (nuclei) of charge $z_i > 0$, located at $R_i \in \mathbb{R}^3$ (with $i = 1, \dots K$). Here, the function $\rho(x) \geq 0$ is the electronic density of a system of N electrons, and

$$D(\rho, \rho) = \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \rho(x) \frac{1}{|x - y|} \rho(y)\, dx\, dy, \tag{89}$$

the electronic repulsion energy. Finally,

$$U = \sum_{1 \leq i < j \leq K} \frac{z^2}{|R_i - R_j|} \tag{90}$$

is the repulsion energy between the nuclei. The powers of the first two terms in (87), i.e.,

$$\mathrm{T}(\rho) = \mathrm{a}^2 \int_{\mathbb{R}^2} (\nabla \rho^{1/3})^2 \,\mathrm{dx} + \mathrm{b}^2 \int_{\mathbb{R}^3} \rho^{4/3} \,\mathrm{dx}, \tag{91}$$

are such that $T(\rho_\alpha) = \alpha\, T(\rho)$, where $\rho_\alpha(x) = \alpha^3 \rho(\alpha x)$ (with $\alpha > 0$) is such that $\int_{\mathbb{R}^3} \rho_\alpha\, dx = \int_{\mathbb{R}^3} \rho(x)\, dx$. In other words, the kinetic energy of the electrons scales like one over a length, i.e., in the same way as the potential energy. Then, as usual in this situation, the values of the coupling constant (i.e., the values of the nuclear charges) will be crucial to insure stability of the system. Our main result in this section is the following stability theorem [7]. In the sequel we will set all the nuclear charges equal to a given value z. By a standard convexity argument one can reduce the general case to this situation.

Theorem 4.1. *For any $a, b > 0$, and $R_i \in \mathbb{R}^3$, $i = 1, \dots, K$, and for all $\rho \geq 0$ (with $\rho \in L^{4/3}(\mathbb{R}^3)$ and $\nabla \rho^{1/3} \in L^2(\mathbb{R}^3)$), we have that*

$$\xi(\rho) \equiv a^2 \int_{\mathbb{R}^3} (\nabla \rho^{1/3})^2\, dx + b^2 \int_{\mathbb{R}^3} \rho^{4/3}\, dx - \int_{\mathbb{R}^3} V(x) \rho(x)\, dx + D(\rho, \rho) + U \geq 0, \tag{92}$$

where V, D, and U are defined by (88), (89), *and* (90), *respectively, provided,*

$$0 \leq z \leq z_c(a, b) \equiv \frac{4\, a\, b}{3} \sqrt{1 - \sigma}. \tag{93}$$

Here $0 < \sigma < 1$ is the only positive root of the quartic equation

$$\frac{\sigma^3}{(1 - \sigma)} = \frac{117\, \pi}{8} \frac{a^2}{b^4} \tag{94}$$

on the interval $(0, 1)$.

In the rest of this section we will give the proof of this theorem (which is taken from Theorem 1.2 in [7]). Notice that the upper limit $z_c(a, b)$ on z to insure stability is not sharp; in other words, there could still be values of z above our z_c for which $\xi(\rho) \geq 0$. We start with an appropriate *Coulomb uncertainty principle.*

Theorem 4.2. *For any smooth function f on the closed ball B_R, of radius R, and for all a, $b \in \mathbb{R}$, we have*

$$a^2 \int_{B_R} |\nabla f(x)|^2 \, dx + b^2 \int_{B_R} f(x)^4 \, dx \geq ab \int_{B_R} \left(\frac{4}{3|x|} - \frac{2}{R} \right) f(x)^3 \, dx.$$

The proof of this theorem is given in Theorem 2.1 in [7], which we reproduce here for completeness. We start with the following preliminary result which is of independent interest.

Lemma 4.3. *Let $u = u(|x|)$ be a smooth function on the interval $(0, R)$, such that $u(R) = 0$. Then the following uncertainty principle holds*

$$\left| \int_{B_R} [3u(|x|) + |x|u'(|x|)] f(x)^3 \, dx \right| \leq 3 \left(\int_{B_R} |\nabla f(x)|^2 \, dx \right)^{1/2} \left(\int_{B_R} u(|x|)^2 |x|^2 f(x)^4 \, dx \right)^{1/2}. \tag{95}$$

In (95) *there is equality if and only if*

$$f(x) = \frac{1}{\lambda \int_0^{|x|} s u(s) \, ds + C}, \tag{96}$$

for some constants C and λ.

Proof. Set $g_j(x) = u(|x|)x_j$. Then we have,

$$\begin{aligned} \int_{B_R} [3u(|x|) + |x|u'(|x|)] f(x)^3 \, dx &= \sum_{j=1}^{3} \int_{B_R} [\partial_j g_j(x)] f(x)^2 \, dx \\ &= \sum_j \int_{B_R} f(x) \partial_j [g_j(x) f(x)^2] \, dx - 2 \sum_j \int_{B_R} f(x)^2 g_j(x) \partial_j f(x) \, dx \\ &= -3 \int_{B_R} \langle \nabla f(x), \, x \rangle u(|x|) f(x)^2 \, dx. \end{aligned}$$

In the last equality we integrated by parts and made use of the fact that u vanishes on the boundary ∂B_R. Next, the Schwarz inequality implies,

$$\left| \int_{B_R} [3u(|x|) + |x|u'(|x|)] f(x)^3 \, dx \right| \leq 3 \left(\int_{B_R} |\nabla f(x)|^2 \, dx \right)^{1/2} \left(\int_{B_R} u(|x|)^2 |x|^2 f(x)^4 \, dx \right)^{1/2}.$$

In the last expression, equality is obtained if and only if

$$\partial_j f(x) = -\lambda x_j u(|x|) f(x)^2,$$

which after an integration yields the function given by (96) above. □

Proof of Theorem 4.2. Choosing $u(r) = (r^{-1} - R^{-1})/2$ in (95), we conclude

$$ab \left| \int_{B_R} \left(\frac{4}{3|x|} - \frac{2}{R} \right) f(x)^3 dx \right| \leq 2ab \left(\int_{B_R} |\nabla f(x)|^2 \, dx \right)^{1/2} \left(\int_{B_R} f(x)^4 \, dx \right)^{1/2}$$
$$\leq a^2 \int_{B_R} |\nabla f(x)|^2 \, dx + b^2 \int_{B_R} f(x)^4 \, dx. \qquad \square$$

To prove our main result of this section, i.e., Theorem 4.1, we will also need the following auxiliary lemma.

Lemma 4.4. *Let* $B_L(x_0) = \{x \in \mathbb{R}^3 \mid |x - x_0| < L\}$ *and* H *be a half-space such that* $\operatorname{dist}(x_0, \partial H) = L$ *and* $x_0 \in H$. *Then*

$$\int\limits_{H \setminus B_L(x_0)} \frac{1}{|x - x_0|^4} \, dx = \frac{3\pi}{L}.$$

Proof. Let us shift the origin of the coordinates to x_0, and the z axis perpendicular to the plane ∂H. Then in the respective spherical coordinates $(\varrho, \theta.\varphi)$,

$$\int\limits_{H \setminus B_L(x_0)} \frac{1}{|x - x_0|^4} \, dx = 2\pi \int_0^{\pi/2} \int_L^{\frac{L}{\cos\theta}} \frac{1}{\varrho^2} \, d\varrho \, \sin\theta \, d\theta + 2\pi \int_{\pi/2}^{\pi} \int_L^{\infty} \frac{1}{\varrho^2} \, d\varrho \, \sin\theta \, d\theta$$

from which the assertion of the lemma follows by a straightforward integration. $\square$

In the sequel we need some notation. We introduce the nearest neighbor, or Voronoi, cells [71] (see also the review [49]), $\{\Gamma_j\}_{j=1}^K$, defined by

$$\Gamma_j = \{x \mid |x - R_j| \leq |x - R_k|\}. \tag{97}$$

The boundary of Γ_j, $\partial\Gamma_j$, consists of a finite number of planes. We also define the distance

$$D_j = \operatorname{dist}(R_j, \partial\Gamma_j) = \frac{1}{2} \min\{|R_k - R_j| \mid k \neq j\}. \tag{98}$$

Finally, we denote by B_j the ball of radius D_j centered at R_j, $j = 1, \ldots, K$.

One of the key ingredients we need in the sequel is an electrostatic inequality of Lieb and Yau [47, 48]. Define the piecewise function $\Phi(x)$ on $\mathbb{R}^3$ with the aid of the Voronoi cells mentioned above. In the cell Γ_j, $\Phi(x)$ equals the electrostatic potential generated by all the nuclei except for the nucleus situated in Γ_j itself, i.e., for $x \in \Gamma_j$,

$$\Phi(x) = \sum_{\substack{i=1 \\ i \neq j}}^{K} \frac{z}{|x - R_i|}. \tag{99}$$

Then, one has (see, e.g., [47, 48]),

$$D(\rho, \rho) - \int_{\mathbb{R}^3} \Phi(x) \rho(x) \, dx + U \geq \frac{z^2}{8} \sum_{j=1}^{K} \frac{1}{D_j}. \tag{100}$$

With the help of the Coulomb uncertainty principle and the electrostatic inequality (100), we are ready to prove the following estimate.

Lemma 4.5. *For any $\rho \in L^{4/3}(\mathbb{R}^3)$ such that $\nabla\rho^{1/3} \in L^2(\mathbb{R}^3)$; for all $b_1 > 0$, and $b_2 > 0$ such that $b_1^2 + b_2^2 = b^2$ we have,*

$$\xi(\rho) \geq \sum_{j=1}^{K} \frac{1}{D_j} \left[\frac{z^2}{8} - \frac{27}{256\, b_1^6} \left(3\pi z^4 + \pi \frac{64}{3} a^4 b_2^4 \right) \right]. \tag{101}$$

Proof. Setting $f(x)^3 = \rho(x)$, splitting $\mathbb{R}^3$ as the disjoint union of the Voronoi cells Γ_j, using Theorem 4.2 in each disk B_j, and discarding the kinetic energy terms (which are positive) in the complements $\Gamma_j \setminus B_j$ we conclude,

$$\xi(\rho) \geq b_1^2 \int_{\mathbb{R}^3} \rho^{4/3}\, dx - \int_{\mathbb{R}^3} V\rho\, dx + ab_2 \sum_{j=1}^{K} \int_{B_j} \left(\frac{4}{3|x - R_j|} - \frac{2}{D_j} \right) \rho(x)\, dx + D(\rho,\rho) + U. \tag{102}$$

It is convenient to define the piecewise function $W(x)$ as

$$W(x) = \begin{cases} \Phi(x) + \dfrac{z}{|x - R_j|} = V(x) & \text{if } x \in \Gamma_j \setminus B_j \\ \Phi(x) + \dfrac{2\, ab_2}{D_j} & \text{if } x \in B_j, \end{cases} \tag{103}$$

Provided $z \leq 4\, a\, b_2/3$ (which we assume from here on), we can estimate from below the sum of the second and third integrals in (102) in terms of $W(x)$ as follows,

$$\begin{aligned} & ab_2 \sum_{j=1}^{K} \int_{B_j} \left(\frac{4}{3|x - R_j|} - \frac{2}{D_j} \right) \rho(x)\, dx - \int_{\mathbb{R}^3} V\rho\, dx \\ & \quad = ab_2 \sum_{j=1}^{K} \int_{B_j} \left(\frac{4}{3|x - R_j|} - \frac{2}{D_j} \right) \rho(x)\, dx - z \sum_{i,j=1}^{K} \int_{\Gamma_j \setminus B_j} \frac{\rho(x)}{|x - R_i|}\, dx \\ & \qquad - z \sum_{\substack{i,j=1 \\ i \neq j}}^{K} \int_{B_j} \frac{\rho(x)}{|x - R_i|}\, dx - z \sum_{j=1}^{K} \int_{B_j} \frac{\rho(x)}{|x - R_j|}\, dx \\ & \quad = -\int_{\mathbb{R}^3} W(x)\rho(x)\, dx + \sum_{j=1}^{K} \int_{B_j} \left(\frac{4\, ab_2}{3} - z \right) \frac{\rho(x)}{|x - R_j|}\, dx \geq -\int_{\mathbb{R}^3} W(x)\rho(x)\, dx. \end{aligned}$$

Thus, we can write

$$\xi(\rho) \geq \xi_1(\rho) + \xi_2(\rho), \tag{104}$$

with

$$\xi_1(\rho) = b_1^2 \int_{\mathbb{R}^3} \rho^{4/3}\, dx - \int_{\mathbb{R}^3} (W - \Phi)(x)\rho(x)\, dx \qquad \text{and,}$$

$$\xi_2(\rho) = D(\rho,\rho) - \int_{\mathbb{R}^3} \Phi(x)\rho(x)\, dx + U.$$

From the definition of $\xi_1(\rho)$, it is clear that $\xi_1(\rho) \geq \xi_1(\hat{\rho})$, where $\hat{\rho}(x) = 27(W(x) - \Phi(x))_+^3/(64\, b_1^6)$, where as usual $u_+ = \max(u, 0)$. Hence,

$$\begin{aligned}\xi_1(\rho) &\geq -\frac{27}{256\, b_1^6} \int_{\mathbb{R}^2} (W - \Phi)_+^4 \, dx \\ &= -\frac{27}{256\, b_1^6} \sum_{j=1}^{K} \left(\int_{\Gamma_j \setminus B_j} \frac{z^4}{|x - R_j|^4} \, dx + \int_{B_j} \left(\frac{2\, a b_2}{D_j} \right)^4 dx \right),\end{aligned}$$

where the last equality follows from the definition (103) of W. As any Γ_j is contained in a half-space, we may estimate the first integral above with the help of Lemma 4.4. This way we get

$$\xi_1(\varrho) \geq -\frac{27}{256\, b_1^6} \left[3\pi z^4 + \pi \frac{64}{3} a^4 b_2^4 \right] \sum_{j=1}^{K} \frac{1}{D_j}. \tag{105}$$

The lower bound for $\xi_2(\rho)$ follows at once from (100), i.e.,

$$\xi_2(\varrho) \geq \frac{z^2}{8} \sum_{j=1}^{N} \frac{1}{D_j}. \tag{106}$$

Putting (104), (105), and (106) together the assertion of the lemma immediately follows. □

We end this section with the proof of Theorem 4.1.

Proof of Theorem 4.1. Let $M(z)$ stand for the right side of (101). Then $M(z) \geq 0$ if and only if

$$1 \geq \frac{27}{32 z^2 b_1^6} \left(3\pi z^4 + \frac{64}{3} \pi a^4 b_2^4 \right). \tag{107}$$

Since $(4\, a b_2/3) \geq z$, it follows from (107) that

$$1 \geq \frac{81}{128} (13\pi) \frac{z^2}{b_1^6} \tag{108}$$

Let $\sigma = b_1^2/b^2$, hence $b_2 = b\sqrt{1 - \sigma}$. In terms of σ, the conditions $z \leq 4a\, b_2/3$ and (108), can be expressed, as $z \leq (4\, a\, b/3)\sqrt{1 - \sigma}$ and $z \leq \sqrt{128}/(9\sqrt{13\pi})\sigma^{3/2} b^3$, respectively. That is,

$$z \leq h(\sigma) = \min \left\{ \frac{4}{3} ab\sqrt{1 - \sigma}, \frac{\sqrt{128}}{9\sqrt{13\pi}} \sigma^{3/2} b^3 \right\}$$

The maximum of $h(\sigma)$ in the interval $(0, 1)$ is attained at the (unique) solution $\hat{\sigma}$ of

$$\frac{\sigma^3}{(1 - \sigma)} = \frac{117\pi}{8} \frac{a^2}{b^4},$$

and $\xi(\rho) \geq 0$ for all $0 < z \leq (4ab/3)\sqrt{1 - \hat{\sigma}}$. □

4.1. Bibliographical Remarks

i) The stability of matter of several relativistic models has been studied since the eighties. In particular, see the original articles of Lieb and Yau [47, 48]. For a review up to the recent literature on the subject see the review article of Michael Loss [54] and the recent monograph of Lieb and Seiringer [49]. See also [45], which contains many articles on different aspects of the stability of relativistic matter.

ii) In realistic Relativistic Models, one not only needs bounds on the nuclear charges to insure stability, but also one needs upper bounds on the values of the *fine structure constant* α. In the toy model that I have discussed in this lecture, there is no need of such a bound on the fine structure constant to ensure its stability. This is due to the absence of the exchange term in the present model.

iii) Recently [4], we have used an analog of the toy model considered in this lecture to obtain a lower bound on the exchange energy of a system of electrons confined to live in a two-dimensional system.

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On the Regularity of the Hausdorff Distance Between Spectra of Perturbed Magnetic Hamiltonians

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Abstract. We study the regularity properties of the Hausdorff distance between spectra of continuous Harper-like operators. As a special case we obtain Hölder continuity of this Hausdorff distance with respect to the intensity of the magnetic field for a large class of magnetic elliptic (pseudo)differential operators with long range magnetic fields.

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1. Introduction

Analytic perturbation theory tells us that if V is relatively bounded to H_0, then the spectrum of $H_\lambda = H_0 + \lambda V$ is at a Hausdorff distance of order $|\lambda|$ from the spectrum of H_0. This property is not true for singular perturbations (like for example the magnetic perturbation coming from a constant field), neither in the discrete nor in the continuous case.

Maybe the first proof of spectral stability of discrete Harper operators with respect to the variation of the intensity $b \geq 0$ of the external magnetic field is due to Elliott [9]. The result is refined in [7] where it is shown that the gap boundaries are $\frac{1}{3}$-Hölder continuous in b. Later results by Avron, van Mouche and Simon [4], Helffer and Sjöstrand [13, 14], and Haagerup and Rørdam [11] pushed the exponent up to $\frac{1}{2}$. In fact they prove more, they show that the Hausdorff distance between spectra behaves like $|b-b_0|^{\frac{1}{2}}$. These results are optimal in the sense that the Hölder constant is independent of the length of the eventual gaps, and it is known that these gaps can close down precisely like $|b-b_0|^{\frac{1}{2}}$ near rational values of b_0 [14, 12]. Note that Nenciu [27] proves a similar result for a much larger class of discrete

Harper-like operators. Many other spectral properties of Harper operators can be found in a paper by Herrmann and Janssen [15].

In the continuous case, the stability of gaps for Schrödinger operators was first shown by Avron and Simon [3], and Nenciu [26]. In [16] a very general result is obtained for perturbations of the anisotropic Laplacian. In [2] spectral continuity is proven for a large class of Hamiltonians defined by elliptic symbols. Nenciu's result implicitly gives a $\frac{1}{2}$-Hölder continuity in b for the Hausdorff distance between spectra. Then in [6] the Hölder exponent of gap edges was pushed up to $\frac{2}{3}$.

The first proof of Lipschitz continuity of gap edges for discrete Harper-like operators was given by Bellissard [5] (later on Kotani [19] extended his method to more general regular lattices and dimensions larger than two). Very recently a completely different proof was given in [8].

Our main technical result in this paper is Theorem 1.1, extending a previous result of Nenciu [27] and asserting Hölder continuity of a specific order for a class of bounded self-adjoint operators having a locally integrable integral kernel satisfying a weighted Schur-Holmgren estimate (1.1). This result, combined with the magnetic quantization [20, 22, 24] and the associated magnetic pseudodifferential calculus developed in [23, 17, 18, 21], allow us to we prove Theorem 3.1 stating Hölder continuity of order 1/2 of the spectrum of resolvents associated to a large class of elliptic Hamiltonians in a BC^∞ magnetic field, with respect to the intensity of the magnetic field. The case of unbounded operators will be considered elsewhere.

1.1. The setting and the main result

Consider the Hilbert space $L^2(\mathbb{R}^d)$ with $d \geq 2$. Let $\langle x\rangle := \sqrt{1+|\mathbf{x}|^2}$ and let $\alpha \geq 0$. We consider bounded integral operators $T \in B(L^2(\mathbb{R}^d))$ to which we can associate a locally integrable kernel $T(\mathbf{x},\mathbf{x}')$ which is continuous outside the diagonal and obeys the following weighted Schur-Holmgren estimate:

$$||T||_{1,\alpha} := \max\Big\{ \sup_{\mathbf{x}'\in\mathbb{R}^d} \int_{\mathbb{R}^d} |T(\mathbf{x},\mathbf{x}')|\langle \mathbf{x}-\mathbf{x}'\rangle^\alpha d\mathbf{x}, \sup_{\mathbf{x}\in\mathbb{R}^d} \int_{\mathbb{R}^d} |T(\mathbf{x},\mathbf{x}')|\langle \mathbf{x}-\mathbf{x}'\rangle^\alpha d\mathbf{x}' \Big\} < \infty. \tag{1.1}$$

Let us denote the set of all these operators with $\mathcal{C}_{1,\alpha}$. When $\alpha = 0$, we need to introduce a uniformity condition. Let χ be the characteristic function of the interval $[0,1]$ and define

$$\mathbb{R}^d \times \mathbb{R}^d \ni (\mathbf{x},\mathbf{x}') \mapsto \chi_M(\mathbf{x},\mathbf{x}') := \chi(|\mathbf{x}-\mathbf{x}'|/M), \quad M \geq 1. \tag{1.2}$$

If $T \in \mathcal{C}_{1,0}$ we denote by T_M the operator given by the integral kernel $\chi_M(\mathbf{x},\mathbf{x}')T(\mathbf{x},\mathbf{x}')$. Then we define $\mathcal{C}_{\text{unif}}$ to be the subset of $\mathcal{C}_{1,0}$ consisting of operators obeying the estimate

$$\lim_{M\to\infty} ||T - T_M||_{1,0} = 0. \tag{1.3}$$

Note that if we only consider kernels $T(\mathbf{x},\mathbf{x}')$ which are dominated by L^1 functions of $\mathbf{x}-\mathbf{x}'$, then $\mathcal{C}_{\text{unif}} = \mathcal{C}_{1,0}$.

For $T \in \mathcal{C}_{1,\alpha}$, we are interested in a family of Harper-like operators $\{T_b\}_{b\in\mathbb{R}}$ given by kernels of the form $e^{ib\varphi(\mathbf{x},\mathbf{x}')}T(\mathbf{x},\mathbf{x}')$ with $\varphi : \mathbb{R}^d \times \mathbb{R}^d \mapsto \mathbb{R}$ a continuous phase function satisfying the two properties:

$$\varphi(\mathbf{x},\mathbf{x}') = -\varphi(\mathbf{x}',\mathbf{x}) \quad \text{and} \quad |\varphi(\mathbf{x},\mathbf{y}) + \varphi(\mathbf{y},\mathbf{x}') - \varphi(\mathbf{x},\mathbf{x}')| \leq |\mathbf{x}-\mathbf{y}|\,|\mathbf{y}-\mathbf{x}'|. \tag{1.4}$$

Clearly, $\{T_b\}_{b\in\mathbb{R}} \subset \mathcal{C}_{1,\alpha}$.

The Hausdorff distance between two real compact sets A and B is defined as:

$$d_H(A,B) := \max\left\{\sup_{x\in A}\inf_{y\in B}|x-y|,\ \sup_{y\in B}\inf_{x\in A}|x-y|\right\}. \tag{1.5}$$

And here is our main technical result:

Theorem 1.1. *Let H be self-adjoint and consider a family of Harper-like operators $\{H_b\}_{b\in\mathbb{R}}$ as above. Then the map*

$$\mathbb{R} \ni b \mapsto d_H(\sigma(H_b),\sigma(H)) \in \mathbb{R}_+$$

is continuous if $H \in \mathcal{C}_{\text{unif}}$. Moreover, if $H \in \mathcal{C}_{1,\alpha}$ with $\alpha > 0$, then the above map is Hölder continuous with exponent $\beta := \min\{1/2, \alpha/2\}$. More precisely, for all b_0 we can find a constant $C > 0$ such that:

$$d_H(\sigma(H_{b_0+\delta}),\sigma(H_{b_0})) \leq C\,|\delta|^{\beta}. \tag{1.6}$$

Remark 1. Denoting by $\delta = b - b_0$, then according to our notations we have that $H_b = (H_{b_0})_\delta$. It means that it is enough to prove the theorem at $b_0 = 0$.

Remark 2. It is natural to ask if the condition $H \in \mathcal{C}_{1,\alpha}$ is optimal in order to insure a Hölder continuity of order $\min\{1/2, \alpha/2\}$; we believe in any case that if α becomes smaller and smaller, one cannot expect the Hölder coefficient to remain $1/2$. Similarly, if $\alpha = 0$ it is unlikely to expect more than continuity of the Hausdorff distance.

2. Proof of Theorem 1.1

Let $g \in C_0^\infty(\mathbb{R}^d)$ with $0 \leq g \leq 1$, $g(\mathbf{x}) = 1$ if $|\mathbf{x}| \leq 1/2$ and $g(\mathbf{x}) = 0$ if $|\mathbf{x}| \geq 2$. If $\mathbf{y} \in \mathbb{R}^d$, denote by $g_{\mathbf{y}}(\mathbf{x}) = g(\mathbf{x}-\mathbf{y})$. By standard arguments, we may assume that $\sum_{\gamma\in\mathbb{Z}^d} g_\gamma^2(\mathbf{x}) = 1$ for all $\mathbf{x} \in \mathbb{R}^d$. For each g_γ there is a finite number of neighbors whose supports are not disjoint from $\text{supp}(g_\gamma)$, uniformly in γ.

Denote by $g_{\mathbf{y},b}(\mathbf{x}) := g_{\mathbf{y}}(b^{1/2}\mathbf{x}) = g(b^{1/2}\mathbf{x}-\mathbf{y})$. In this way we constructed a locally finite, quadratic partition of unity obeying

$$\sum_{\gamma\in\mathbb{Z}^d} g_{\gamma,b}^2(\mathbf{x}) = 1, \quad \mathbf{x} \in \mathbb{R}^d, \tag{2.1}$$

and if $V_{\gamma,b}$ denotes the set of functions $g_{\gamma',b}$ whose supports are not disjoint from the support of $g_{\gamma,b}$, then $\sup_{\gamma\in\mathbb{Z}^d}\ \#\{V_{\gamma,b}\}$ is independent of b. Moreover, if $\chi_{\gamma,b}$ is the characteristic function of the support of $g_{\gamma,b}$ we have:

$$\mathrm{supp}(g_{\gamma,b})\subset\{\mathbf{x}\in\mathbb{R}^d:\ |\mathbf{x}-b^{-1/2}\gamma|\leq 2b^{-1/2}\},\tag{2.2}$$

$$|g_{\gamma,b}(\mathbf{x})-g_{\gamma,b}(\mathbf{y})|\leq||\ |\nabla g|\ ||_\infty^\epsilon\ b^{\epsilon/2}|\mathbf{x}-\mathbf{y}|^\epsilon\ \{\chi_{\gamma,b}(\mathbf{x})+\chi_{\gamma,b}(\mathbf{y})\},\quad 0\leq\epsilon\leq 1.\tag{2.3}$$

Lemma 2.1. *Let $\{T_\gamma\}_{\gamma\in\mathbb{Z}^d}\subset B(L^2(\mathbb{R}^d))$ possibly depending on b such that*

$$|||T|||_\infty:=\sup_{\gamma\in\mathbb{Z}^d}||T_\gamma||<\infty.\tag{2.4}$$

Define on compactly supported functions the maps

$$\psi\mapsto\Gamma(T)(\psi):=\sum_{\gamma\in\mathbb{Z}^d}\chi_{\gamma,b}\ T_\gamma\ \chi_{\gamma,b}\psi,\quad\tilde{\Gamma}(T)(\psi):=\sum_{\gamma\in\mathbb{Z}^d}\chi_{\gamma,b}\ |T_\gamma\ \chi_{\gamma,b}\psi|\,.$$

Then both $\Gamma(T)$ and $\tilde{\Gamma}(T)$ can be extended by continuity to bounded maps on $L^2(\mathbb{R}^d)$ and there exists a constant C independent of b such that $\max\{||\tilde{\Gamma}(T)||,\ ||\Gamma(T)||\}\leq C\ |||T|||_\infty$.

Proof. Let $\psi\in L^2(\mathbb{R}^d)$ with compact support. We have:

$$\begin{aligned}||\Gamma(T)(\psi)||^2&\leq\sum_{\gamma\in\mathbb{Z}^d}\sum_{\gamma'\in V_{\gamma,b}}|\ \langle\chi_{\gamma',b}\ T_{\gamma'}\ \chi_{\gamma',b}\psi,\chi_{\gamma,b}\ T_\gamma\ \chi_{\gamma,b}\psi\rangle\ |\\&\leq\sum_{\gamma\in\mathbb{Z}^d}\sum_{\gamma'\in V_{\gamma,b}}||T_{\gamma'}\ \chi_{\gamma',b}\psi||\ ||T_\gamma\ \chi_{\gamma,b}\psi||\\&\leq\frac{|||T|||_\infty^2}{2}\sum_{\gamma\in\mathbb{Z}^d}\sum_{\gamma'\in V_{\gamma,b}}\left(||\chi_{\gamma',b}\psi||^2+||\chi_{\gamma,b}\psi||^2\right)\leq C\ |||T|||_\infty^2||\psi||^2,\end{aligned}\tag{2.5}$$

where in the last inequality we used:

$$\sum_{\gamma\in\mathbb{Z}^d}\sum_{\gamma'\in V_{\gamma,b}}||\chi_{\gamma',b}\psi||^2=\int_{\mathbb{R}^d}|\psi(\mathbf{x})|^2\left\{\sum_{\gamma\in\mathbb{Z}^d}\sum_{\gamma'\in V_{\gamma,b}}\chi_{\gamma',b}(\mathbf{x})\right\}d\mathbf{x}\leq C||\psi||^2.$$

The same proof also works for $\tilde{\Gamma}(T)$ since the linearity is not used. Note that

$$||\tilde{\Gamma}(T)(\psi_1)-\tilde{\Gamma}(T)(\psi_2)||\leq||\tilde{\Gamma}(T)(\psi_1-\psi_2)||$$

which is enough for proving continuity. □

Lemma 2.2. *Let A be a positivity preserving bounded linear operator and define on compactly supported functions ψ the following positively homogeneous map:*

$$\hat{\Gamma}_A(T)(\psi):=\sum_{\gamma\in\mathbb{Z}^d}\chi_{\gamma,b}\ A\,|T_\gamma\ \chi_{\gamma,b}\psi|\,.$$

Then $\hat{\Gamma}_A(T)$ can be extended by continuity to a bounded map on the whole space and $||\hat{\Gamma}_A(T)||\leq C\ ||A||\ |||T|||_\infty$.

Proof. We note that:

$$\left|\hat{\Gamma}_A(T)(\psi_1) - \hat{\Gamma}_A(T)(\psi_2)\right| \leq \sum_{\gamma\in\mathbb{Z}^d} \chi_{\gamma,b}\ A\left|T_\gamma\ \chi_{\gamma,b}(\psi_1-\psi_2)\right| = \hat{\Gamma}_A(T)(\psi_1-\psi_2)$$

due to the positivity preserving of A. Thus boundedness implies continuity. But the proof of Lemma 2.1 can be repeated almost identically, and the proof is over. □

2.1. The case $\alpha > 0$

If $z \in \rho(H)$, denote by $R(z) = (H-z)^{-1}$. We construct the operators

$$T_\gamma(z) := e^{ib\varphi(\cdot,b^{-1/2}\gamma)} g_{\gamma,b} R(z) g_{\gamma,b} e^{-ib\varphi(\cdot,b^{-1/2}\gamma)}, \quad T(z) := \{T_\gamma(z)\}_{\gamma\in\mathbb{Z}}.$$

Then $|||T(z)|||_\infty \leq 1/\mathrm{dist}(z,\sigma(H))$. Introduce the notation

$$fl(\mathbf{x},\mathbf{y},\mathbf{x}') := \varphi(\mathbf{x},\mathbf{y}) + \varphi(\mathbf{y},\mathbf{x}') - \varphi(\mathbf{x},\mathbf{x}').$$

The operator $\Gamma(T(z))$ is bounded (see Lemma 2.1). If Id denotes the identity operator, we can compute (use (2.1)):

$$(H_b - z)\Gamma(T(z)) = \mathrm{Id} + S(z) \tag{2.6}$$

where

$$\begin{aligned}(S(z)\psi)(\mathbf{x}) :=& \sum_{\gamma\in\mathbb{Z}^d} e^{ib\varphi(\mathbf{x},b^{-1/2}\gamma)} \int_{\mathbb{R}^d} d\mathbf{x}' H(\mathbf{x},\mathbf{x}') \Big\{e^{ibfl(\mathbf{x},\mathbf{x}',b^{-\frac{1}{2}}\gamma)} - 1\Big\} g_{\gamma,b}(\mathbf{x}') \\ &\times \left\{R(z) g_{\gamma,b} e^{-ib\varphi(\cdot,b^{-\frac{1}{2}}\gamma)}\psi\right\}(\mathbf{x}') \\ &+ \sum_{\gamma\in\mathbb{Z}^d} e^{ib\varphi(\mathbf{x},b^{-1/2}\gamma)} \int_{\mathbb{R}^d} d\mathbf{x}' H(\mathbf{x},\mathbf{x}') \left\{g_{\gamma,b}(\mathbf{x}') - g_{\gamma,b}(\mathbf{x})\right\} \\ &\times \left\{R(z) g_{\gamma,b} e^{-ib\varphi(\cdot,b^{-\frac{1}{2}}\gamma)}\psi\right\}(\mathbf{x}') \\ =:& (S_1(z)\psi)(\mathbf{x}) + (S_2(z)\psi)(\mathbf{x}).\end{aligned} \tag{2.7}$$

Let us analyze the contribution of the first term $(S_1(z)\psi)(\mathbf{x})$. Using the inequality (see also (1.4))

$$\left|e^{ibfl(\mathbf{x},\mathbf{x}',b^{-\frac{1}{2}}\gamma)} - 1\right| \leq 2^{1-\epsilon} b^\epsilon |\mathbf{x}-\mathbf{x}'|^\epsilon |\mathbf{x}' - b^{-\frac{1}{2}}\gamma|^\epsilon, \quad 0 \leq \epsilon \leq 1,$$

we have:

$$\begin{aligned}|S_1(z)\psi(\mathbf{x})| \leq\ & 2^{1-\epsilon} b^\epsilon \int_{\mathbb{R}^d} d\mathbf{x}' |H(\mathbf{x},\mathbf{x}')|\ |\mathbf{x}-\mathbf{x}'|^\epsilon \\ &\times \sum_{\gamma\in\mathbb{Z}^d} g_{\gamma,b}(\mathbf{x}')\ |\mathbf{x}' - b^{-1/2}\gamma|^\epsilon \left|R(z) g_{\gamma,b} e^{-ib\varphi(\cdot,b^{-1/2}\gamma)}\psi\right|(\mathbf{x}').\end{aligned} \tag{2.8}$$

With the notation $L_\gamma := g_{\gamma,b}(\cdot)|\cdot - b^{-1/2}\gamma|^\epsilon R(z) g_{\gamma,b} e^{-ib\varphi(\cdot,b^{-1/2}\gamma)}$ we see that the above inequality can be written as:

$$|S_1(z)\psi(\mathbf{x})| \leq 2^{1-\epsilon} b^\epsilon \int_{\mathbb{R}^d} d\mathbf{x}' |H(\mathbf{x},\mathbf{x}')|\ |\mathbf{x}-\mathbf{x}'|^\epsilon \left\{\tilde{\Gamma}(L)\psi\right\}(\mathbf{x}').$$

Using the fact that on the support of $g_{\gamma,b}$ we have $|\mathbf{x}' - b^{-1/2}\gamma| \leq 2b^{-1/2}$ it follows that $|||L|||_\infty \leq Cb^{-\epsilon/2}||R(z)||$, thus:

$$||S_1(z)|| \leq C\ \frac{b^{\epsilon/2}}{\mathrm{dist}(z,\sigma(H))}\ ||H||_{1,\epsilon}. \tag{2.9}$$

Let us analyze the contribution from $S_2(z)$. Using (2.3) we can write:

$$\begin{aligned}
&|S_2(z)\psi|(\mathbf{x}) \qquad\qquad (2.10)\\
&\leq C\ b^{\epsilon/2} \sum_{\gamma\in\mathbb{Z}^d} \int_{\mathbb{R}^d} d\mathbf{x}' |H(\mathbf{x},\mathbf{x}')|\ |\mathbf{x}-\mathbf{x}'|^\epsilon \{\chi_{\gamma,b}(\mathbf{x}) + \chi_{\gamma,b}(\mathbf{x}')\}\\
&\qquad\qquad \times \left| R(z) g_{\gamma,b} e^{-ib\varphi(\cdot,b^{-1/2}\gamma)}\psi \right| (\mathbf{x}')\\
&\leq C\ b^{\epsilon/2} \sum_{\gamma\in\mathbb{Z}^d} \chi_{\gamma,b}(\mathbf{x}) \int_{\mathbb{R}^d} d\mathbf{x}' |H(\mathbf{x},\mathbf{x}')|\ |\mathbf{x}-\mathbf{x}'|^\epsilon \left| R(z) g_{\gamma,b} e^{-ib\varphi(\cdot,b^{-1/2}\gamma)}\psi \right| (\mathbf{x}')\\
&\quad + C\ b^{\epsilon/2} \int_{\mathbb{R}^d} d\mathbf{x}' |H(\mathbf{x},\mathbf{x}')|\ |\mathbf{x}-\mathbf{x}'|^\epsilon \sum_{\gamma\in\mathbb{Z}^d} \chi_{\gamma,b}(\mathbf{x}') \left| R(z) g_{\gamma,b} e^{-ib\varphi(\cdot,b^{-1/2}\gamma)}\psi \right| (\mathbf{x}').
\end{aligned}$$

Now denoting with A the operator with integral kernel $|H(\mathbf{x},\mathbf{x}')|\ |\mathbf{x}-\mathbf{x}'|^\epsilon$ and with $L_\gamma = R(z) g_{\gamma,b} e^{-ib\varphi(\cdot,b^{-1/2}\gamma)}$ we obtain $|S_2(z)\psi| \leq C\ b^{\epsilon/2} \left\{ \hat{\Gamma}_A(L)(\psi) + A\tilde{\Gamma}(L)(\psi) \right\}$ thus

$$||S_2(z)|| \leq C\ \frac{b^{\epsilon/2}}{\mathrm{dist}(z,\sigma(H))}\ ||H||_{1,\epsilon}. \tag{2.11}$$

Going back to (2.6) we obtain the estimate:

$$||S(z)|| \leq C\ \frac{b^{\epsilon/2}}{\mathrm{dist}(z,\sigma(H))}\ ||H||_{1,\epsilon}. \tag{2.12}$$

Now choose $0 < \epsilon = \min\{\alpha, 1\}$. It follows that $||S(z)|| \leq 1/2$ for every z with $\mathrm{dist}(z,\sigma(H)) \geq 2C\ b^{\epsilon/2}||H||_{1,\epsilon}$, and by a standard argument it follows from (2.6) that $z \in \rho(H_b)$. Thus for every $x \in \sigma(H_b)$ we must have $\mathrm{dist}(x,\sigma(H)) \leq 2C\ b^{\epsilon/2}||H||_{1,\epsilon}$, thus

$$\sup_{x\in\sigma(H_b)} \inf_{y\in\sigma(H)} |x-y| \ \leq\ 2C\ b^{\min\{\alpha/2,1/2\}} ||H||_{1,\min\{\alpha,1\}}.$$

Now we can interchange H_b with H because

$$H(\mathbf{x},\mathbf{x}') = e^{-ib\phi(\mathbf{x},\mathbf{x}')} \left\{ e^{ib\phi(\mathbf{x},\mathbf{x}')} H(\mathbf{x},\mathbf{x}') \right\} = e^{-ib\phi(\mathbf{x},\mathbf{x}')} H_b(\mathbf{x},\mathbf{x}')$$

and the $||\cdot||_{1,\alpha}$ norms are invariant with respect to the multiplication with a unimodular phase. Hence the Theorem is proved in the case $\alpha > 0$.

2.2. The case $\alpha = 0$

Due to our uniformity condition in (1.3) we can approximate H_b in operator norm (*uniformly in* b) with a sequence of operators $(H_b)_M$ which have strong localization near their diagonal. More precisely, given $\epsilon > 0$ there exists $M = M(\epsilon)$ large enough such that $||H_b - (H_b)_M|| \leq \epsilon/3$ for every $b \in \mathbb{R}$. If $d(z, \sigma(H_b)) > \epsilon/3$, then by writing

$$(H_b)_M - z = [\mathrm{Id} - (H_b - (H_b)_M)(H_b - z)^{-1}](H_b - z)$$

it follows that $z \notin \sigma((H_b)_M)$. It means that for every $x \in \sigma((H_b)_M)$ we must have $d(x, \sigma(H_b)) \leq \epsilon/3$. By reversing the roles of H_b and $(H_b)_M$ we conclude that $d_H(\sigma(H_b), \sigma((H_b)_M)) \leq \epsilon/3$, uniformly in $b \geq 0$. But now both $(H_b)_M$ and H_M have strong localization near the diagonal, thus we can apply the result from $\alpha > 0$, obtaining a $b(\epsilon) > 0$ such that for every $|b| \leq b(\epsilon)$ we have $d_H(\sigma(H_M), \sigma((H_b)_M)) \leq \epsilon/3$. The proof is finished by the triangle inequality. □

3. Magnetic Hamiltonians

Let us consider in $\mathbb{R}^d$ a magnetic field B with components of class $BC^\infty(\mathbb{R}^d)$, i.e., bounded, smooth and with all its derivatives bounded. Consider a Hamiltonian given by a real elliptic symbol h of class $S_1^m(\mathbb{R}^d \times \mathbb{R}^d)$ with $m > 0$, i.e., $h \in C^\infty_{\mathsf{pol}}(\mathbb{R}^d \times \mathbb{R}^d)$ verifying the estimates:

$$\forall (a, \alpha) \in \mathbb{N}^d \times \mathbb{N}^d,\ \exists C(a, \alpha) \in \mathbb{R}_+,$$
$$\sup_{(x,\xi) \in \mathbb{R}^d \times \mathbb{R}^d} \langle \xi \rangle^{|\alpha| - m} \left| \left(\partial_x^a \partial_\xi^\alpha h \right)(x, \xi) \right| \leq C(a, \alpha),$$
$$\exists (R, C) \in \mathbb{R}_+^2, \quad |\xi| \geq R \Rightarrow h(x, \xi) \geq C|\xi|^m,\ \forall x \in \mathbb{R}^d.$$

For our magnetic field B we can choose a vector potential A having components of class $C^\infty_{\mathsf{pol}}(\mathbb{R}^d)$; this can always be achieved by working with the transverse gauge:

$$A_j(x) := -\sum_{k=1}^{d} \int_0^1 ds\, B_{jk}(sx) s x_k.$$

Let us denote by $\mathfrak{Op}^A(h)$ the magnetic quantization of h defined as in [22]. Then, this operator is self-adjoint on the magnetic Sobolev space $H_A^m(\mathbb{R}^d)$ and essentially self-adjoint on the space of Schwartz test functions (see Definition 4.2 and Theorem 5.1 in [17]). Moreover this operator is lower semibounded and satisfies a Gårding type inequality (Theorem 5.3 in [17]). Thus for any $\mathfrak{z} \in \mathbb{C} \setminus [-a_0, +\infty)$, with $a_0 > 0$ large enough, we have that the following inverse exist

$$\left(\mathfrak{Op}^A(h) - \mathfrak{z}\mathbb{1} \right)^{-1} = \mathfrak{Op}^A\left(r_{\mathfrak{z}}^B \right)$$

and is defined by a symbol $r_{\mathfrak{z}}^B$ of class $S_1^{-m}(\mathbb{R}^d \times \mathbb{R}^d)$ (see Proposition 6.5 in [18]). But using now Lemma A.4 in [23] and the fact that evidently $S_1^m(\mathbb{R}^d \times \mathbb{R}^d) \subset S^m\left(\mathbb{R}^d; BC_u(\mathbb{R}^d)\right)$ with $S^m\left(\mathbb{R}^d; BC_u(\mathbb{R}^d)\right)$ as in Definition A.3 of [23], (or

Proposition 1.3.3 of [1]), we conclude that the symbol $r^B_\jmath$ has a partial Fourier transform (with respect to the second variable) of class $L^1\big(\mathbb{R}^d; BC_u(\mathbb{R}^d)\big)$. In fact looking closer to the proof of Lemma A.4 in [23] allows us to conclude (see also Proposition 1.3.6. in [1]) that the partial Fourier transform $\mathfrak{F}_2^{-1}\big[r^B_\jmath\big](\mathbf{x},\mathbf{y})$ has rapid decay in the second variable. Now, using formulas 3.28 and 3.29 in [22], we conclude that $\mathfrak{Op}^A\left(r^B_\jmath\right)$ is an integral operator with kernel

$$K^A(r^B_\jmath)(\mathbf{x},\mathbf{y}) := \left[\tilde{\Lambda}^A S^{-1}(\mathbf{1}\otimes\mathcal{F}_2^{-1})r^B_\jmath\right](\mathbf{x},\mathbf{y})$$

with

$$\tilde{\Lambda}^A(\mathbf{x},\mathbf{y}) := \exp\left\{-i\int_{\mathbf{x}}^{\mathbf{y}} A\right\}, \quad S^{-1}(\mathbf{x},\mathbf{y}) := \left(\frac{\mathbf{x}+\mathbf{y}}{2}, \mathbf{x}-\mathbf{y}\right).$$

In conclusion:

$$K^A(r^B_\jmath)(\mathbf{x},\mathbf{y}) = \exp\left\{-i\int_{\mathbf{x}}^{\mathbf{y}} A\right\}\left\{\left[\mathbf{1}\otimes\mathcal{F}_2^{-1}\right] r^B_\jmath\right\}\left(\frac{\mathbf{x}+\mathbf{y}}{2}, \mathbf{x}-\mathbf{y}\right).$$

Let us also notice that if we denote by $\langle 0,\mathbf{x},\mathbf{y}\rangle$ the triangle of vertices $0,\mathbf{x},\mathbf{y}$, we have that

$$\left|\int_{\mathbf{x}}^{\mathbf{y}} A + \int_{\mathbf{y}}^{\mathbf{x}'} A - \int_{\mathbf{x}}^{\mathbf{x}'} A\right| = \left|\int_{\langle \mathbf{x},\mathbf{y},\mathbf{x}'\rangle} B\right| \leq \|B\|_\infty |\mathbf{x}-\mathbf{y}|\ |\mathbf{x}'-\mathbf{y}|,$$

with $\|B\|_\infty := \max\limits_{j,k}\sup\limits_{\mathbf{x}\in\mathbb{R}^d}|B_{j,k}(\mathbf{x})|$.

Let us conclude that for any such magnetic field and elliptic symbol h, the resolvent $R = \big(\mathfrak{Op}^A(h)+a\big)^{-1}$ is a bounded self-adjoint operator having a locally integrable integral kernel of the form $e^{i\varphi_B(\mathbf{x},\mathbf{x}')}T_B(\mathbf{x},\mathbf{x}')$ with

$$\varphi_B(\mathbf{x},\mathbf{x}') := -\int_{\mathbf{x}}^{\mathbf{x}'} A, \qquad T_B(\mathbf{x},\mathbf{x}') := \big[S^{-1}(\mathbf{1}\otimes\mathcal{F}_2^{-1})r^B_\jmath\big](\mathbf{x},\mathbf{x}').$$

Now let us consider a magnetic field B_0 with components of class $BC^\infty(\mathbb{R}^d)$ and a small variation of it, in the same class, $B_b(\mathbf{x}) := B_0(\mathbf{x})+b\mathfrak{b}(\mathbf{x})$ with $b\in[0,1]$. Given an elliptic symbol h as before we now have two Hamiltonians $H := \mathfrak{Op}^{A_0}(h)$ and $H' := \mathfrak{Op}^A(h)$, with A_0 a vector potential for B_0 and A a vector potential for B. We can write $A(\mathbf{x}) = A_0(\mathbf{x}) + b\mathfrak{a}(\mathbf{x})$ with $\mathfrak{a}$ a vector potential for $\mathfrak{b}$. Then we have the following result:

Theorem 3.1. *For h, B_0 and B_b as above, consider $H = \mathfrak{Op}^{A_0}(h)$ and $H' = \mathfrak{Op}^A(h)$. For $a>0$ large enough we define the two associated resolvents as above:*

$$\begin{aligned} R &:= (H+a)^{-1} = \mathfrak{Op}^{A_0}(r^{B_0}_{-a}),\\ &\quad \textit{with integral kernel: } e^{-i\left[\int_{\mathbf{x}}^{\mathbf{x}'} A_0\right]}\big[S^{-1}(\mathbf{1}\otimes\mathcal{F}_2^{-1})r^{B_0}_{-a}\big](\mathbf{x},\mathbf{x}'),\\ R' &:= (H'+a)^{-1} = \mathfrak{Op}^{A_0}(r^{B_0}_{-a}),\\ &\quad \textit{with integral kernel: } e^{-i\left[\int_{\mathbf{x}}^{\mathbf{x}'} A\right]}\big[S^{-1}(\mathbf{1}\otimes\mathcal{F}_2^{-1})r^{B}_{-a}\big](\mathbf{x},\mathbf{x}'). \end{aligned}$$

Then there exists a constant C only depending on the symbol h and on the magnetic field B_0 such that we have the following estimate:

$$d_H\big(\sigma(R),\sigma(R')\big)\leq C\sqrt{b}.$$

Proof. Let us remark that the kernels $S^{-1}(\mathbf{1}\otimes\mathcal{F}_2^{-1})r_{-a}^{B_0}$ and $S^{-1}(\mathbf{1}\otimes\mathcal{F}_2^{-1})r_{-a}^{B}$ are the integral kernels of the operators given by the usual quantization (without magnetic field) $\mathfrak{Op}$ of the symbols $r_{-a}^{B_0}$ and resp. r_{-a}^{B}.

Proposition 3.2. *Being symbols of negative order, both $r_{-a}^{B_0}$ and r_{-a}^{B} define bounded operators on $L^2(\mathbb{R}^d)$ and we have that $\|\mathfrak{Op}(r_{-a}^{B_0})-\mathfrak{Op}(r_{-a}^{B})\|_{1,0}\leq Cb$.*

Proof. Using the ideas and results in [22] we shall use the magnetic Moyal composition $\sharp^B$ defined by the quantization associated to the field B. Let us compute (as tempered distributions):

$$(h+a)\sharp^B r_{-a}^{B_0}-1=(h+a)\sharp^B r_{-a}^{B_0}-(h+a)\sharp^{B_0} r_{-a}^{B_0}=:s_{-a}^{b}.$$

Due to the general theory developed in [17, 18] s_{-a}^{b} is defined by a symbol of class $S_1^0(\mathbb{R}^d\times\mathbb{R}^d)$ that can be computed by the following oscillating integral:

$$\begin{aligned}\big[(h+a)\sharp^B r_{-a}^{B_0}-1\big](\mathbf{x},\xi)&=(2\pi)^{-2d}\int_\Xi\int_\Xi d\mathbf{y}d\eta d\mathbf{x}'d\zeta\; e^{-2i(\langle\mathbf{x}',\eta\rangle-\langle\mathbf{y},\zeta\rangle)}\\&\quad\times\big[\omega^B(\mathbf{x},\mathbf{y}-\mathbf{x},\mathbf{x}'-\mathbf{x})-\omega^{B_0}(\mathbf{x},\mathbf{y}-\mathbf{x},\mathbf{x}'-\mathbf{x})\big]\\&\quad\times(h+a)(\mathbf{x}-\mathbf{y},\xi-\eta)r_{-a}^{B_0}(\mathbf{x}-\mathbf{x}',\xi-\zeta)\\&=ib(2\pi)^{-2d}\int_\Xi\int_\Xi d\mathbf{y}d\eta d\mathbf{x}'d\zeta\; e^{-2i(\langle\mathbf{x}',\eta\rangle-\langle\mathbf{y},\zeta\rangle)}\omega^{B_0}\\&\quad\times(\mathbf{x},\mathbf{y}-\mathbf{x},\mathbf{x}'-\mathbf{x})\theta_b(\mathbf{x},\mathbf{y}-\mathbf{x},\mathbf{x}'-\mathbf{x})\\&\quad\times(h+a)(\mathbf{x}-\mathbf{y},\xi-\eta)r_{-a}^{B_0}(\mathbf{x}-\mathbf{x}',\xi-\zeta),\end{aligned}$$

where

$$\theta_b(\mathbf{x},\mathbf{y}-\mathbf{x},\mathbf{x}'-\mathbf{x})=e^{-ib\int_{\langle\mathbf{x}+\mathbf{y}-\mathbf{x}',\mathbf{x}+\mathbf{x}'-\mathbf{y},\mathbf{x}-\mathbf{y}-\mathbf{x}'\rangle}\mathfrak{b}}-1$$

is a function of class $BC^\infty\big(\mathbb{R}^d;C^\infty_{\mathsf{pol}}(\mathbb{R}^d\times\mathbb{R}^d)\big)$ and we have the following estimates for its derivatives:

$$\big|\big(\partial_{\mathbf{x}}^{\rho}\partial_{\mathbf{y}}^{\mu}\partial_{\mathbf{x}'}^{\nu}\theta_b\big)(\mathbf{x},\mathbf{y}-\mathbf{x},\mathbf{x}'-\mathbf{x})\big|\leq C_{\rho,\mu,\nu}b^{1+|\rho+\mu+\nu}|\mathbf{y}|^{|\mu|}|\mathbf{x}'|^{|\nu|}.$$

Now using Proposition 8.45 in [18] we conclude that $(h+a)\sharp^B r_{-a}^{B_0}-1$ is a symbol of type $S_1^0(\mathbb{R}^d\times\mathbb{R}^d)$ with seminorms of order at least b and using Remark 3.3 in [17] we conclude that it defines a bounded operator with norm of order b. Thus for b small enough we can invert $1+s_{-a}^{b}$ and obtain that (using once again Proposition 8.45 in [18] and the Calderón-Vaillancourt Theorem [10])

$$r_{-a}^{B}=r_{-a}^{B_0}\sharp^B\big\{1+s_{-a}^{b}\big\}^{-_B},\quad r_{-a}^{B}-r_{-a}^{B_0}=-r_{-a}^{B}\sharp^B s_{-a}^{b},$$
$$\|\mathfrak{Op}(r_{-a}^{B_0})-\mathfrak{Op}(r_{-a}^{B})\|_{1,0}\leq Cb.$$

□

Now we shall consider the bounded self-adjoint operators R_b with the kernel $e^{-i\left[\int_{\mathbf{x}}^{\mathbf{x}'} A\right]}\left[S^{-1}(\mathbf{1}\otimes\mathcal{F}_2^{-1})r_{-a}^{B_0}\right](\mathbf{x},\mathbf{x}')$. Due to the above proposition, by replacing R' with R_b we make an error of order b in operator norm on $L^2(\mathbb{R}^d)$. Now we see that R_b is a Harper-type family, for which we can apply the results of Section 2. Here, $R = R_0$. We note that the integral kernels of R_b have a common factor independent of b which is of class $C_{1,\alpha}$ for any $\alpha \geq 0$. Moreover, the integral kernels of R_b only differ by a unimodular exponential factor $e^{ib\varphi(\mathbf{x},\mathbf{x}')}$ where $\varphi(\mathbf{x},\mathbf{x}') := -\int_{\mathbf{x}}^{\mathbf{x}'} \mathfrak{a}$ satisfies (1.4).

Therefore Theorem 1.1 implies that $d_H(\sigma(R_b),\sigma(R)) \leq C\ \sqrt{b}$, and since $d_H(\sigma(R_b),\sigma(R')) \leq C\ b$ it follows that

$$d_H(\sigma(R'),\sigma(R)) \leq C\ \sqrt{b}, \tag{3.1}$$

which finishes the proof of the theorem. □

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The Topological Bloch-Floquet Transform and Some Applications

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Abstract. We investigate the relation between the symmetries of a Schrödinger operator and the related topological quantum numbers. We show that, under suitable assumptions on the symmetry algebra, a generalization of the Bloch-Floquet transform induces a direct integral decomposition of the algebra of observables. More relevantly, we prove that the generalized transform selects uniquely the set of "continuous sections" in the direct integral decomposition, thus yielding a Hilbert bundle. The proof is constructive and provides an explicit description of the fibers. The emerging geometric structure is a rigorous framework for a subsequent analysis of some topological invariants of the operator, to be developed elsewhere [DFP12]. Two running examples provide an Ariadne's thread through the paper. For the sake of completeness, we begin by reviewing two related classical theorems by von Neumann and Maurin.

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1. Introduction

In view of the competition between different space-scales, magnetic Schrödinger operators with a periodic background exhibit striking features, as fractal spectrum and anomalous density of states. Beyond the spectrum and the density of states, other properties of these operators attracted the interest of physicists and, more recently, mathematicians: the so-called *Topological Quantum Numbers* (TQN), related to observable effects whose origin is geometric.

The prototypical example is the *Hall conductance* of a 2-dimensional gas of non-interacting electrons in a periodic background potential and a uniform orthogonal magnetic field. The dynamics of the single-electron wavefunction $\psi \in$

$L^2(\mathbb{R}^2, dx\,dy)$ is governed by the Hamiltonian operator

$$H_\beta = \frac{1}{2}\left[\left(-i\frac{\partial}{\partial x} - \frac{\beta}{2}y\right)^2 + \left(-i\frac{\partial}{\partial y} + \frac{\beta}{2}x\right)^2\right] + V_\Gamma(x,y) \tag{1}$$

where $V_\Gamma : \mathbb{R}^2 \to \mathbb{R}$ is periodic with respect to the lattice $\Gamma \cong \mathbb{Z}^2$ and β is proportional to the modulus of a uniform magnetic field in the direction orthogonal to the plane. More precisely, the magnetic flux through the unit cell of Γ is divided by the fundamental unit of flux to obtain the dimensionless parameter β.

If a current of intensity I is forced in the x-direction the charge carriers experience the Lorentz force, resulting in motion of the carriers and a non-zero equilibrium voltage V_H along the y-direction. The *Hall conductance* σ_H is experimentally defined as $\sigma_H = V_H/I$, its value depending on both the magnetic flux β and the density of carriers, which depends on the Fermi energy μ. While at room temperature the measured values of σ_H are in accordance with the predictions of classical electrodynamics, the same measurement performed at zero temperature show striking quantum features [vDP80], whose discovery deserved the Nobel Prize. The value of σ_H, when varying either β or μ, exhibit extremely accurate "plateaux" (which are flat up to an accuracy of one part over 10^7) corresponding to integer multiples of the constant e^2/h ($= 1/2\pi$ in the natural units used in (1)), where e is the charge of the electron and h the Planck constant.

By replacing (1) with a simplified Hamiltonian K_β (the Hofstadter operator [DP10]) a numerical simulation becomes feasible. For $\beta \in [0,1]$ and $\mu \in [0,4]$ the integer corresponding to $\sigma_H(\beta,\mu)$ is coded by a color (warm colors for positive integers, cold colors for negative integers and white for zero) yielding a beautiful picture known as the "colored Hofstadter butterfly" [OA01, Avr04]. It is assumed that μ is not in the spectrum of K_β, which appears for reader's convenience on the left-hand side of the Figure 1.

How are these integers (colors) related to the properties of the corresponding Schrödinger operators? How can one read these Topological Quantum Numbers from the Hamiltonian? The goal of this contribution is to provide a tool to investigate the simplest framework, namely the case of TQNs related to an abelian algebra of symmetries $\mathfrak{S}$ generated by a finite family of unitary operators. This framework includes the case of the Hall conductance for the Hamiltonian (1) which, as we shall see, is related to the algebra generated by the magnetic translations. It also includes the relevant examples of Hofstadter and Harper operators, which are discussed in [DFP12]. In particular, the latter paper exploits the methods here developed to prove properties of the Hall conductance corresponding to the operator K_β.

We firstly recall the standard construction. To simplify the notation, we assume that the lattice Γ in the definition of H_β is simply $\mathbb{Z}^2$. The unitary operators $T_{\beta,1}$ and $T_{\beta,2}$, acting on $\psi \in L^2(\mathbb{R}^2, dx\ dy)$ by

$$(T_{\beta,1}\psi)(x,y) = \mathrm{e}^{-i\frac{\beta}{2}y}\ \psi(x-1,y) \qquad (T_{\beta,2}\psi)(x,y) = \mathrm{e}^{i\frac{\beta}{2}x}\ \psi(x,y-1), \tag{2}$$

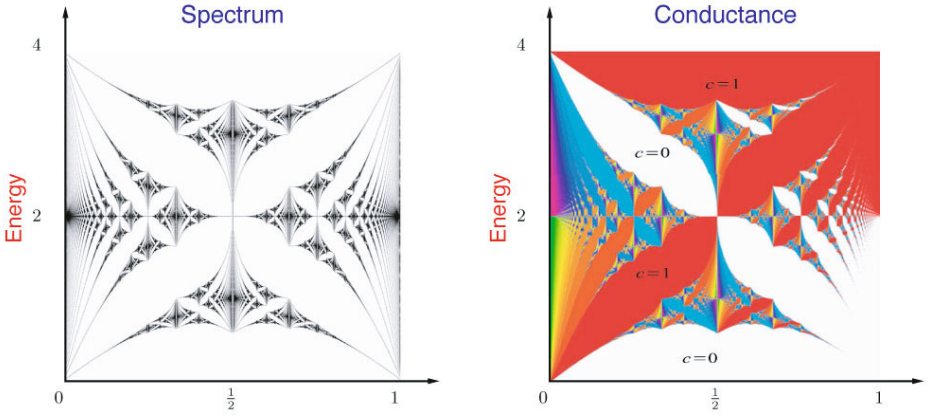


FIGURE 1. The black and white Hofstadter butterfly, showing the spectrum of the Hofstadter operator as a function of the parameter β, *versus* the colored Hofstadter butterfly, labeling the points of the resolvent set with a color corresponding to a suitable integer (Topological Quantum Number). The colored butterfly was originally obtained in [OA01].

describe symmetries of the Hamiltonian (1) in the sense that

$$[T_{\beta,1};\, H_\beta] = 0 = [T_{\beta,2};\, H_\beta].$$

The operators (2) are known as *magnetic translations*. Unfortunately, in general $T_{\beta,1}$ and $T_{\beta,2}$ do not commute and thus do not correspond to simultaneously implementable symmetries (except for $\beta \in 2\pi\mathbb{Z}$), indeed

$$T_{\beta,1}\, T_{\beta,2} = \mathrm{e}^{-i\beta}\, T_{\beta,2}\, T_{\beta,1}.$$

In particular, the map $(n_1, n_2) \mapsto T_{\beta,1}^{n_1}\, T_{\beta,2}^{n_2}$, with $(n_1, n_2) \in \mathbb{Z}^2$, provides only a projective unitary representation of the group $\mathbb{Z}^2$. Nevertheless, under the so-called *rational flux condition* $\beta \in 2\pi\mathbb{Q}$ it is still possible to recover a $\mathbb{Z}^2$-symmetry for H_β. We are mainly interested in this case. Let $\beta/2\pi = p/q$ with $p \in \mathbb{Z}$ and $q \in \mathbb{N}$ coprime. By replacing the standard lattice $\Gamma = \mathbb{Z}^2$ with the *super-lattice* $\Gamma' := (q\mathbb{Z})^2$, one obtains a unitary representation $(qn_1, qn_2) \mapsto {T'_{\beta,1}}^{n_1}\, {T'_{\beta,2}}^{n_2}$ of Γ' given by the commuting pair of unitary operators $T'_{\beta,j} := T_{\beta,j}^q$, $j = 1, 2$. Thus, assuming the rational flux condition, one can still define a $\mathbb{Z}^2$-symmetry for H_β implemented by the "gauged" translations $\{T'_{\beta,1}, T'_{\beta,2}\}$. One defines the magnetic *Bloch-Floquet* (BF) transform, initially for $\psi \in \mathcal{S}(\mathbb{R}^2)$, by posing

$$(\mathcal{U}_{\mathrm{BF}}\psi)(k, \cdot) := \sum_{n \in \mathbb{Z}^2} e^{-ik\cdot n} \big({T'_{\beta,1}}^{n_1}\, {T'_{\beta,2}}^{n_2}\psi\big)(\cdot), \qquad k \in \mathbb{R}^d, \tag{3}$$

where $n := (n_1, n_2)$. Definition (3) extends to a unitary operator

$$\mathcal{U}_{\mathrm{BF}} : L^2(\mathbb{R}^2) \longrightarrow \int_{\mathbb{T}^2}^{\oplus} \mathcal{H}(k)\, dk \tag{4}$$

where $\mathbb{T}^2 := \mathbb{R}^2/\Gamma^*$ corresponds to the first (magnetic) Brillouin zone in the physics literature, and

$$\mathcal{H}(k) := \left\{\varphi \in L^2_{\mathrm{loc}}(\mathbb{R}^2) : {T'_{\beta,1}}^{n_1}\, {T'_{\beta,2}}^{n_2}\varphi = e^{ik\cdot n}\varphi \quad \forall n \in \mathbb{Z}^2\right\}.$$

While we focused on the bidimensional case in view of its relevance for the Hall conductance, the definition of the magnetic translations and the magnetic BF transform effortlessly extend to any dimension $d \in \mathbb{N}$.

In the magnetic BF representation, the Fermi projector $P_\mu = \chi_{(-\infty,\mu)}(H_\beta)$, with χ_I the characteristic function of the set I, is a decomposable operator, in the sense that

$$\mathcal{U}_{\mathrm{BF}}\, P_\mu\, {\mathcal{U}_{\mathrm{BF}}}^{-1} = \int_{\mathbb{T}^2}^{\oplus} P_\mu(k)\, dk.$$

If μ lies in a spectral gap, the dimension of the range of $P_\mu(k)$ is constant. Thus it would be tempting to consider the *measurable* collection of vector spaces $\{\mathrm{Ran}\, P_\mu(k)\}_{k\in\mathbb{T}^2}$ as a vector bundle $\mathcal{E}$ over $\mathbb{T}^2$, and to consider its first Chern number $C_1(\mathcal{E}) \in \mathbb{Z}$ as a topological quantum number (analogously, for $d \geq 3$ one considers the first and the higher Chern numbers). However, as already emphasized, the decomposition (4) is a measure-theoretic object, yielding only a measurable collection of vector spaces, thus the Chern number might be undefined; even if one circumvents this obstacle, its value might not be invariant under unitary equivalence. In this paper we develop a construction that yields a *topological* decomposition analogous to (4). Moreover, the vector bundle $\mathcal{E}_{\mathfrak{S}} \to \mathbb{T}^d$ defined by this procedure is essentially unique, in the sense that it is invariant under any unitary equivalence commuting with the elements of $\mathfrak{S}$.

We formulate the result in a general framework: $\mathcal{H}$ is a separable Hilbert space which corresponds to the physical states; $\mathfrak{A} \subset \mathscr{B}(\mathcal{H})$ is a C^*-algebra of bounded operators which contains the relevant physical models (the self-adjoint elements of $\mathfrak{A}$ can be interpreted as Hamiltonians); the commutant $\mathfrak{A}'$ (the set of all the elements in $\mathscr{B}(\mathcal{H})$ which commute with $\mathfrak{A}$) can be seen as the set of all the physical symmetries; any commutative unital C^*-algebra $\mathfrak{S} \subset \mathfrak{A}'$ describes a set of simultaneously implementable physical symmetries.

Definition 1.1 (Physical frame). *A* physical frame *is a triple* $\{\mathcal{H}, \mathfrak{A}, \mathfrak{S}\}$ *where* $\mathcal{H}$ *is a separable Hilbert space,* $\mathfrak{A} \subset \mathscr{B}(\mathcal{H})$ *is a* C^**-algebra and* $\mathfrak{S} \subset \mathfrak{A}'$ *is a commutative unital* C^**-algebra. The physical frame* $\{\mathcal{H}, \mathfrak{A}, \mathfrak{S}\}$ *is called* irreducible *if* $\mathfrak{S}$ *is* maximal commutative. *Two physical frames* $\{\mathcal{H}_1, \mathfrak{A}_1, \mathfrak{S}_1\}$ *and* $\{\mathcal{H}_2, \mathfrak{A}_2, \mathfrak{S}_2\}$ *are* equivalent *if there exists a unitary map* $U : \mathcal{H}_1 \to \mathcal{H}_2$ *such that* $\mathfrak{A}_2 = U\,\mathfrak{A}_1\,U^{-1}$ *and* $\mathfrak{S}_2 = U\,\mathfrak{S}_1\,U^{-1}$.

We focus on triples $\{\mathcal{H}, \mathfrak{A}, \mathfrak{S}\}$ whose C^*-algebra $\mathfrak{S}$ describes symmetries with an intrinsic group structure. In particular, in this contribution, we focus on the case of the group $\mathbb{Z}^N$.

Definition 1.2 ($\mathbb{Z}^N$-algebra). *Let $\mathbb{Z}^N \ni n \mapsto U(n) \in \mathscr{U}(\mathcal{H})$ be a unitary representation of $\mathbb{Z}^N$ in the group $\mathscr{U}(\mathcal{H})$ of the unitary operators on $\mathcal{H}$. The representation is* faithful *if $U(n) = \mathbb{1}$ implies $n = 0$ and is* algebraically compatible *if the operators $\{U(n) \,:\, n \in \mathbb{Z}^N\}$ are linearly independent in $\mathscr{B}(\mathcal{H})$. Let $\mathfrak{S}(\mathbb{Z}^N)$ be the unital C^*-algebra generated by $\{U(n) \,:\, n \in \mathbb{Z}^N\}$. When the representation is faithful and algebraically compatible we say that $\mathfrak{S}(\mathbb{Z}^N)$ is a $\mathbb{Z}^N$-*algebra *in $\mathcal{H}$.*

In a nutshell, our main result is the following. Let $\{\mathcal{H}, \mathfrak{A}, \mathfrak{S}\}$ be a physical frame with $\mathfrak{S}$ a $\mathbb{Z}^N$-algebra satisfying the wandering property (see Definition 5.1). Then there exist (and one can explicitly construct):

- a Hermitian vector bundle $\mathcal{E}_{\mathfrak{S}} \to \mathbb{T}^N$, whose rank is equal to the cardinality of the wandering system;
- a unitary operator $\mathcal{F}_{\mathfrak{S}} : \mathcal{H} \to \Gamma_{L^2}(\mathcal{E}_{\mathfrak{S}} \to \mathbb{T}^N)$, the latter being the Hilbert space consisting of the L^2-sections of the Hermitian vector bundle $\mathcal{E}_{\mathfrak{S}} \to \mathbb{T}^N$;

such that the $*$-subalgebra $\mathfrak{A}^0 \subset \mathfrak{A}$, consisting of some adjointable operators in $\mathfrak{A}$ (see Proposition 7.13), satisfies

$$\mathcal{F}_{\mathfrak{S}} \; \mathfrak{A}^0 \; \mathcal{F}_{\mathfrak{S}}^{-1} \subset \Gamma(\mathrm{End}(\mathcal{E}_{\mathfrak{S}}) \to \mathbb{T}^N)$$

where $\Gamma(\cdot)$ is the space of the *continuous* sections of the vector bundle appearing as the argument. Moreover, if $\{\mathcal{H}, \mathfrak{A}_1, \mathfrak{S}_1\}$ and $\{\mathcal{H}, \mathfrak{A}_2, \mathfrak{S}_2\}$ are equivalent physical frames, then $\mathcal{E}_{\mathfrak{S}_1}$ and $\mathcal{E}_{\mathfrak{S}_2}$ are isomorphic Hermitian vector bundles. In particular, their topological invariants are the same, and can thus be considered a fingerprint of the physical frame.

Last but not least, it is physically interesting to consider the case of perturbed abelian symmetries, *e. g.*, to take into account the effects of disorder and impurities in the physical system, or, in the case of the Hamiltonian (1), an irrational value of the parameter $\beta/2\pi$. In this case the algebra of symmetries is replaced by a non-abelian C^*-algebra, and the related TQNs should be investigated either with the tools of Non Commutative Geometry [BSE94], or with other abstract methods [Gru01]. On the other hand, the aim of this paper is not to pursue the greatest generality, but rather to provide an explicit and manageable tool to define and to compute the TQNs hidden in the symmetries of Schrödinger operators.

The paper is organized as follows:

Section 2 introduces two relevant examples which will reappear later, as an Ariadne's thread through the paper.

In **Section 3 and 4** we review two cornerstones in the classical literature concerning the measurable decomposition of a physical frame: the *von Neumann's complete spectral theorem* (Theorem 3.1) and the *Maurin's nuclear spectral theorem* (Theorem 4.1).

Section 5 concerns the notion of *wandering property* for a commutative C^*-algebra generated by a finite family of operators. This notion is of particular relevance when the generators of the C^*-algebra are a finite set of unitary operators. In this case we prove that the wandering property assures that the C^*-algebra is a $\mathbb{Z}^N$-algebra with N the number of generators. Moreover the Gel'fand spectrum of the C^*-algebra is forced to be the dual group of $\mathbb{Z}^N$, i.e., the N-dimensional torus $\mathbb{T}^N$.

In **Section 6** we extend the decomposition (3) to the case of a $\mathbb{Z}^N$-algebra which satisfies the wandering property. This *generalized Bloch-Floquet transform* provides a concrete recipe to decompose the Hilbert space and the algebra $\mathfrak{A}$ according to the von Neumann and Maurin theorems.

Section 7 contains our novel results: we show that a *topological* decomposition of the algebra $\mathfrak{A}$ emerges in a canonical way from the generalized Bloch-Floquet transform, and we prove two decomposition theorems (Theorems 7.8 and 7.14). The topological structure is essentially unique, so the emerging information is a fingerprint of the given physical frame.

2. Some guiding examples

We elucidate the theory with two explicit examples, while other relevant applications are covered elsewhere [DFP12], [DL11].

Example 2.1 (Periodic systems, part one). Let H_Γ be a Γ-*periodic* operator defined on $L^2(\mathbb{R}^d)$. With the word Γ-periodic we mean that there exists a linear basis $\{\gamma_1, \dots, \gamma_d\}$ of $\mathbb{R}^d$ which spans the lattice $\Gamma \simeq \mathbb{Z}^d$ and d *gauged* translations $\{T_1, \dots, T_d\}$ defined by $(T_j\psi)(x) = g_j(x)\ \psi(x - \gamma_j)$, where $g_j(\cdot - \gamma) = g_j(\cdot)$ for all $\gamma \in \Gamma$, such that $[H_\Gamma; T_j] = 0$ for all $j = 1, \dots, d$. From the definition it follows that $[T_i; T_j] = 0$ for any i, j. Both the cases of the magnetic translations with rational flux condition (cf. Section 1) and the "genuine" translations (i.e., $g_j \equiv 1$) fit in this scheme.

The Gel'fand-Naĭmark Theorem shows that there exists an isomorphism between the commutative C^*-algebra $C_0(\sigma(H_\Gamma))$ and a commutative non-unital C^*-algebra $\mathfrak{A}_0(H_\Gamma)$ of bounded operators in $\mathcal{H}$. The elements of $\mathfrak{A}_0(H_\Gamma)$ are the operators $f(H_\Gamma) \in \mathscr{B}(\mathcal{H})$, for $f \in C_0(\sigma(H_\Gamma))$, obtained via the spectral theorem. Let $\mathfrak{A}(H_\Gamma)$ be the multiplier algebra of $\mathfrak{A}_0(H_\Gamma)$ in $\mathscr{B}(\mathcal{H})$. This is a unital commutative C^*-algebra which contains $\mathfrak{A}_0(H_\Gamma)$ (as an essential ideal), its Gel'fand spectrum is a (Stone-Čech) compactification of $\sigma(H_\Gamma)$ and the Gel'fand isomorphism maps $\mathfrak{A}(H_\Gamma)$ into the unital C^*-algebra of the continuous and bounded functions on $\sigma(H_\Gamma)$ denoted by $C_{\mathrm{b}}(\sigma(H_\Gamma))$ (see Appendix A for details). We assume that $\mathfrak{A}(H_\Gamma)$ is the C^*-algebra of physical models.

The C^*-algebra $\mathfrak{S}_T$ generated by the gauged translations T_j is clearly commutative. Since $[H_\Gamma; T_j] = 0$ it follows that $\mathfrak{S}_T \subset \mathfrak{A}(H_\Gamma)'$. Thus $\{L^2(\mathbb{R}^d), \mathfrak{A}(H_\Gamma), \mathfrak{S}_T\}$ is a physical frame. It is a convenient model to study the properties of an electron in a periodic medium. ◀▷

Example 2.2 (Mathieu-like Hamiltonians, part one). Let $\mathbb{T} := \mathbb{R}/(2\pi\mathbb{Z})$ be the one-dimensional torus. In the Hilbert space $L^2(\mathbb{T})$ consider the Fourier orthonormal basis $\{e_n\}_{n\in\mathbb{Z}}$ defined by $e_n(\theta) := (2\pi)^{-\frac{1}{2}} \mathrm{e}^{in\theta}$. Let $\mathfrak{u}$ and $\mathfrak{v}$ be the unitary operators defined, for $g \in L^2(\mathbb{T})$, by

$$(\mathfrak{u}g)(\theta) := \mathrm{e}^{i\theta}\, g(\theta), \qquad (\mathfrak{v}g)(\theta) := g(\theta - 2\pi\alpha), \qquad \mathfrak{u}\mathfrak{v} = \mathrm{e}^{i2\pi\alpha}\, \mathfrak{v}\mathfrak{u} \tag{5}$$

with $\alpha \in \mathbb{R}$. The last equation in (5) shows that the unitaries $\mathfrak{u}$ and $\mathfrak{v}$ satisfy the commutation relation of a *noncommutative torus* with deformation parameter α (see [Boc01] Chapter 1 or [GVF01] Chapter 12 for more details). We denote by $\mathfrak{A}_{\mathrm{M}}^{\alpha} \subset \mathscr{B}(L^2(\mathbb{T}))$ the unital C^*-algebra generated by $\mathfrak{u}$, $\mathfrak{v}$. We call $\mathfrak{A}_{\mathrm{M}}^{\alpha}$ the *Mathieu C^*-algebra*[(1)] and we refer to its elements as Mathieu-like operators. This name is due to the fact that the Hamiltonian $\mathfrak{h} := \mathfrak{u} + \mathfrak{u}^\dagger + \mathfrak{v} + \mathfrak{v}^\dagger \in \mathfrak{A}_{\mathrm{M}}^{\alpha}$ appears in the well-known (*almost-*)*Mathieu eigenvalue equation*

$$(\mathfrak{h}g)(\theta) \equiv g(\theta - 2\pi\alpha) + g(\theta + 2\pi\alpha) + 2\cos(\theta) g(\theta) = \varepsilon g(\theta). \tag{6}$$

The action of $\mathfrak{u}$ and $\mathfrak{v}$ on the Fourier basis is given explicitly by $\mathfrak{u}e_n = e_{n+1}$ and $\mathfrak{v}e_n = \mathrm{e}^{-i2\pi n\alpha} e_n$ for all $n \in \mathbb{Z}$.

We focus now on the commutant $\mathfrak{A}_{\mathrm{M}}^{\alpha\,\prime}$ of the Mathieu C^*-algebra. Let $\mathfrak{s} \in \mathscr{B}(L^2(\mathbb{T}))$ be a bounded operator such that $[\mathfrak{s}; \mathfrak{u}] = 0 = [\mathfrak{s}; \mathfrak{v}_\alpha]$ and let $\mathfrak{s}e_n = \sum_{m\in\mathbb{Z}} s_{n,m}\, e_m$ be the action of $\mathfrak{s}$ on the basis vectors. The relation $[\mathfrak{s}; \mathfrak{u}] = 0$ implies $s_{n+1,m+1} = s_{n,m}$ and the relation $[\mathfrak{s}; \mathfrak{v}_\alpha] = 0$ implies $\mathrm{e}^{-i2\pi(m-n)\alpha} s_{n,m} = s_{n,m}$ for all $n, m \in \mathbb{Z}$. If $\alpha \notin \mathbb{Q}$ then $\mathrm{e}^{-i2\pi(m-n)\alpha} \neq 1$ unless $n = m$, hence $s_{n,m} = 0$ if $n \neq m$ and the condition $s_{n+1,n+1} = s_{n,n}$ implies that $\mathfrak{s} = s\mathbb{1}$ with $s \in \mathbb{C}$. This shows that in the irrational case $\alpha \notin \mathbb{Q}$ the commutant of the Mathieu C^*-algebra is trivial.

To have a non trivial commutant we need to assume that $\alpha := {}^{p}\!/_{q}$ with p, q non zero integers such that $\gcd(q, p) = 1$. In this case the condition $\mathfrak{s} \in \left(\mathfrak{A}_{\mathrm{M}}^{p/q}\right)'$ implies that $s_{n,m} \neq 0$ if and only if $m - n = kq$ for some $k \in \mathbb{Z}$, moreover $s_{n,n+kq} = s_{0,kq} =: s'_k$ for all $n \in \mathbb{Z}$. Let $\mathfrak{w}$ be the unitary operator defined on the orthonormal basis by $\mathfrak{w}e_n := e_{n+q}$, namely $\mathfrak{w} = (\mathfrak{u})^q$. The relations for the commutant imply that $\mathfrak{s} \in \left(\mathfrak{A}_{\mathrm{M}}^{p/q}\right)'$ if and only if $\mathfrak{s} = \sum_{k\in\mathbb{Z}} s'_k\, \mathfrak{w}^k$. Then in the rational case the commutant of the Mathieu C^*-algebra is the von Neumann algebra generated in $\mathscr{B}(L^2(\mathbb{T}))$ as the strong closure of the family of finite polynomials in $\mathfrak{w}$. We will denote by $\mathfrak{S}_{\mathrm{M}}^{q}$ the unital commutative C^*-algebra generated by $\mathfrak{w}$. Observe that it does not depend on p. The triple $\{L^2(\mathbb{T}), \mathfrak{A}_{\mathrm{M}}^{q/p}, \mathfrak{S}_{\mathrm{M}}^{q}\}$ is an example of a physical frame. ◀▷

[(1)] Such an algebra is a representation of the rotation C^*-algebra and in particular it is a faithful representations when $\alpha \notin \mathbb{Q}$ [Boc01]. Since in this paper we focus on properties which *do* depend on the representation, we will adopt different names for images of the same abstract C^*-algebra under unitarily inequivalent representations.

Finally, we introduce some notation which will be useful in the following.

Remark 2.3 (Notation). The N-dimensional torus $\mathbb{T}^N := \mathbb{R}^N/(2\pi\mathbb{Z})^N$ is parametrized by the cube $[0, 2\pi)^N$: for every $t = (t_1, \dots, t_N)$ in the cube, $z(t) := (z_1(t), \dots, z_N(t))$, with $z_j(t) := \mathrm{e}^{it_j}$, is a point of $\mathbb{T}^N$. The normalized Haar measure is $dz(t) = {}^{dt_1 \dots dt_N}/_{(2\pi)^N}$. ♦◊

3. The complete spectral theorem by von Neumann

The complete spectral theorem is a useful generalization of the usual spectral decomposition of a normal operator on a Hilbert space. It shows that the symmetries reduce the description of the full algebra $\mathfrak{A}$ to a family of simpler representations. The main tool used in the theorem is the notion of the direct integral of Hilbert spaces (Appendix B). The "spectral" content of the theorem amounts to the characterization of the base space for the decomposition (the "set of labels") and of the measure which glues together the spaces so that the Hilbert space structure is preserved. This information emerges essentially from the Gel'fand theory (Appendix A). The definitions of decomposable and continuously diagonal operator are reviewed in Appendix B.

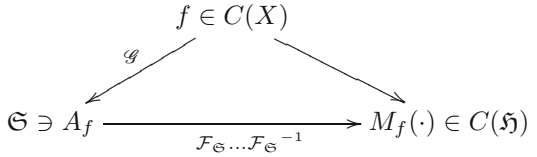
Theorem 3.1 (von Neumann's complete spectral theorem). *Let $\{\mathcal{H}, \mathfrak{A}, \mathfrak{S}\}$ be a physical frame and μ the basic measure carried by the spectrum X of $\mathfrak{S}$ (see Appendix A). Then there exist*

a) *a direct integral $\mathfrak{H} := \int_X^{\oplus} \mathcal{H}(x)\ d\mu(x)$ with $\mathcal{H}(x) \neq \{0\}$ for all $x \in X$,*

b) *a unitary map $\mathcal{F}_{\mathfrak{S}} : \mathcal{H} \to \mathfrak{H}$, called* $\mathfrak{S}$-Fourier transform[(2)]*,*

such that:

(i) *the unitary map $\mathcal{F}_{\mathfrak{S}}$ intertwines the Gel'fand isomorphism $C(X) \ni f \overset{\mathscr{G}}{\longmapsto} A_f \in \mathfrak{S}$ and the canonical isomorphism of $C(X)$ onto the continuously diagonal operators $C(\mathfrak{H})$, i.e., the following diagram commutes*



(ii) *the unitary conjugation $\mathcal{F}_{\mathfrak{S}} \dots \mathcal{F}_{\mathfrak{S}}^{-1}$ maps the elements of $\mathfrak{A}$ to decomposable operators on $\mathfrak{H}$; more precisely, there is a family $\{\pi_x\}_{x \in X}$ such that π_x is a representation of $\mathfrak{A}$ on $\mathcal{H}(x)$ and, for every $A \in \mathfrak{A}$, the map $x \mapsto \pi_x(A)$ is measurable and*

$$\mathcal{F}_{\mathfrak{S}}\, A\, \mathcal{F}_{\mathfrak{S}}{}^{-1} = \int_X^{\oplus} \pi_x(A)\ d\mu(x);$$

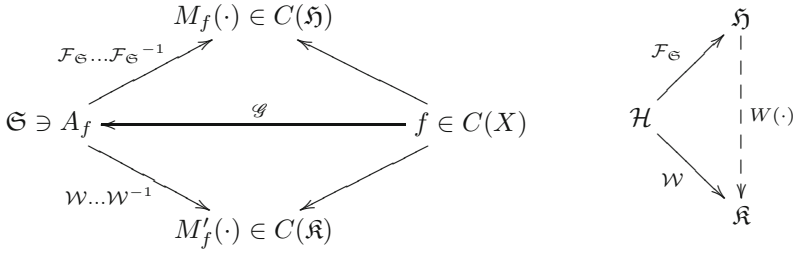
(2) According to the terminology used in [Mau68].

(iii) *the representations* π_x *are irreducible if and only if the physical frame* $\{\mathcal{H}, \mathfrak{A}, \mathfrak{S}\}$ *is irreducible.*

Remark 3.2. For a complete proof of the above theorem one can see [Mau68] (Theorem 25 in Chapter I and Theorem 2 in Chapter V) or [Dix81] (Theorem 1 in Part II, Chapter 6). For our purposes it is interesting to recall how the fiber Hilbert spaces $\mathcal{H}(x)$ are constructed. For $\psi, \varphi \in \mathcal{H}$ let $\mu_{\psi,\varphi} = h_{\psi,\varphi}\, \mu$ be the relation between the spectral measure $\mu_{\psi,\varphi}$ with the basic measure μ. For μ-almost every $x \in X$ the value of the Radon-Nikodym derivative $h_{\psi,\varphi}$ in x defines a semi-definite sesquilinear form on $\mathcal{H}$, i.e., $(\psi;\varphi)_x := h_{\psi,\varphi}(x)$. Let $\mathcal{I}_x := \{\psi \in \mathcal{H} \,:\, h_{\psi,\psi}(x) = 0\}$. Then the quotient space $\mathcal{H}/\mathcal{I}_x$ is a pre-Hilbert space and $\mathcal{H}'(x)$ is defined to be the its completion. By construction $\mathcal{H}'(x) \neq \{0\}$ for μ-almost every $x \in X$. Let $N \subset X$ be the μ- negligible set on which $\mathcal{H}'(x)$ is trivial or not well defined. Then $\mathfrak{H} := \int_X^{\oplus} \mathcal{H}(x)\, d\mu(x)$ with $\mathcal{H}(x) := \mathcal{H}'(x)$ if $x \in X \setminus N$ and $\mathcal{H}(x) := H$ if $x \in N$ where H is an arbitrary non trivial Hilbert space. ⧫◊

Given the triple $\{\mathcal{H}, \mathfrak{A}, \mathfrak{S}\}$, the direct integral decomposition invoked in the statement of Theorem 3.1 is essentially unique in measure-theoretic sense. The space X is unique up to homeomorphism: it agrees with the spectrum of $C(\mathfrak{H})$ in such a way that the canonical isomorphism of $C(X)$ onto $C(\mathfrak{H})$ may be identified with the Gel'fand isomorphism. As for the uniqueness of the direct integral decomposition, the following result holds true (see [Dix81] Theorem 3 in Part II Chapter 6).

Theorem 3.3 (Uniqueness). *With the notation of Theorem* 3.1*, let* ν *be a positive measure with support* X*,* $\prod_{x\in X} \mathcal{K}(x)$ *a field of non-zero Hilbert spaces over* X *endowed with a measurable structure,* $\mathfrak{K} := \int_X^{\oplus} \mathcal{K}(x)\, d\nu(x)$*,* $C(\mathfrak{K})$ *the commutative unital* C^**-algebra of continuously diagonal operators on* $\mathfrak{K}$ *and* $C(X) \to C(\mathfrak{K})$ *the canonical isomorphism. Let* $\mathcal{W}$ *be a unitary* (*antiunitary*) *map from* $\mathcal{H}$ *onto* $\mathfrak{K}$ *transforming by conjugation* $A_f \in \mathfrak{S}$ *into* $M'_f(\cdot) \in C(\mathfrak{K})$ *for all* $f \in C(X)$*, in such a way that the diagram on the right-hand side commutes.*



Then, μ *and* ν *are equivalent measures* (*so one can assume that* $\mu = \nu$ *up to a rescaling isomorphism*)*. Moreover there exists a decomposable unitary* (*antiunitary*) $W(\cdot)$ *from* $\mathfrak{H}$ *onto* $\mathfrak{K}$ *such that* $W(x) : \mathcal{H}(x) \to \mathcal{K}(x)$ *is a unitary* (*antiunitary*) *operator* μ*-almost everywhere and* $\mathcal{W} = W(\cdot) \circ \mathcal{F}_{\mathfrak{S}}$*, i.e., the diagram on the left-hand side commutes.*

Corollary 3.4 (Unitary equivalent triples). *Let* $\{\mathcal{H}_1, \mathfrak{A}_1, \mathfrak{S}_1\}$ *and* $\{\mathcal{H}_2, \mathfrak{A}_2, \mathfrak{S}_2\}$ *be two equivalent physical frames and* U *the unitary map which intertwines them. Let* $\mathfrak{H}_1$ *and* $\mathfrak{H}_2$ *denote the direct integral decomposition of the two triples and let* $\mathcal{F}_{\mathfrak{S}_1}$ *and* $\mathcal{F}_{\mathfrak{S}_2}$ *be the two* $\mathfrak{S}$*-Fourier transforms. Then* $W(\cdot) := \mathcal{F}_{\mathfrak{S}_2} \circ U \circ {\mathcal{F}_{\mathfrak{S}_1}}^{-1}$ *is a decomposable unitary operator from* $\mathfrak{H}_1$ *to* $\mathfrak{H}_2$*, so that* $W(x) : \mathcal{H}_1(x) \to \mathcal{H}_2(x)$ *is a unitary map for* μ*-almost every* $x \in X$*.*

4. The nuclear spectral theorem by Maurin

The complete spectral theorem by von Neumann shows that any physical frame $\{\mathcal{H}, \mathfrak{A}, \mathfrak{S}\}$ admits a representation in which the Hilbert space is decomposed (in a measure-theoretically unique way) into a direct integral $\int_X^{\oplus} \mathcal{H}(x)\ d\mu(x)$, the elements of $\mathfrak{S}$ are simultaneously diagonalized and the C^*-algebra $\mathfrak{A}$ is decomposed on the fibers. The contribution of Maurin is a characterization of the fiber spaces $\mathcal{H}(x)$ as common generalized eigenspaces for $\mathfrak{S}$.

A key ingredient of Maurin's theorem is the notion of (*nuclear*) *Gel'fand triple*. The latter is a triple $\{\Phi, \mathcal{H}, \Phi^*\}$ with $\mathcal{H}$ a separable Hilbert space, $\Phi \subset \mathcal{H}$ a norm-dense subspace such that Φ has a topology for which it is a nuclear space and the inclusion map $\imath : \Phi \hookrightarrow \mathcal{H}$ is continuous, and Φ^* is topological dual of Φ. By identifying $\mathcal{H}$ with its dual space $\mathcal{H}^*$ one gets an *antilinear* injection $\imath^* : \mathcal{H} \hookrightarrow \Phi^*$. Since the duality pairing between Φ and Φ^* is compatible with the scalar product on $\mathcal{H}$, namely $\langle \imath^*(\psi_1); \psi_2 \rangle = (\psi_1; \psi_2)_{\mathcal{H}}$ whenever $\psi_1 \in \mathcal{H}$ and $\psi_2 \in \Phi$, we write $\langle \psi_1; \psi_2 \rangle$ for $\langle \imath^*(\psi_1); \psi_2 \rangle$.
If A is a bounded operator on $\mathcal{H}$ such that $A^\dagger$ leaves invariant Φ and $A^\dagger : \Phi \to \Phi$ is continuous with respect to the nuclear topology of Φ, one defines $\hat{A} : \Phi^* \to \Phi^*$ by posing $\langle \hat{A}\, \eta; \varphi \rangle := \langle \eta; A^\dagger \varphi \rangle$ for all $\eta \in \Phi^*$ and $\varphi \in \Phi$. Then $\hat{A}$ is continuous and is an extension of A, defined on $\mathcal{H}$, to Φ^*.

Assume the notation of Theorem 3.1. Let $\{\xi_k(\cdot)\ :\ k \in I\}$ be a *fundamental family* of orthonormal measurable vector fields (see Appendix B) for the direct integral $\mathfrak{H}$ defined by the $\mathfrak{S}$-Fourier transform $\mathcal{F}_{\mathfrak{S}}$. Any square integrable vector field $\varphi(\cdot)$ can be written in a unique way as $\varphi(\cdot) = \sum_{k \in I} \widehat{\varphi}_k(\cdot)\ \xi_k(\cdot)$ where $\widehat{\varphi}_k \in L^2(X, d\mu)$ for all $k \in I$. Equipped with this notation, the scalar product in $\mathfrak{H}$ reads

$$\langle \varphi(\cdot); \psi(\cdot) \rangle_{\mathfrak{H}} = \int_X \sum_{k=1}^{\dim\ \mathcal{H}(x)} \overline{\widehat{\varphi}_k(x)}\ \widehat{\psi}_k(x)\ d\mu(x).$$

For any $\varphi \in \mathcal{H}$ let $\varphi(\cdot) := \mathcal{F}_{\mathfrak{S}} \varphi$ be the square integrable vector field obtained from φ by the $\mathfrak{S}$-Fourier transform. Denote by $A_f \in \mathfrak{S}$ the operator associated with $f \in C(X)$ through the Gel'fand isomorphism. One checks that

$$\widehat{(\mathcal{F}_{\mathfrak{S}} A_f \varphi)}_k(x) = (\xi_k(x); f(x)\varphi(x))_x = f(x)\ \widehat{\varphi}_k(x) \qquad k = 1, 2, \ldots, \dim\ \mathcal{H}(x). \quad (7)$$

Suppose that $\{\Phi, \mathcal{H}, \Phi^*\}$ is a Gel'fand triple for the space $\mathcal{H}$. If $\varphi \in \Phi$ then the map $\Phi \ni \varphi \mapsto \widehat{\varphi}_k(x) := (\xi_k(x); \varphi(x))_x \in \mathbb{C}$ is linear; moreover it is possible to show

that it is continuous with respect to the nuclear topology of Φ, for an appropriate choice of Φ. This means that there exists $\eta_k(x) \in \Phi^*$ such that

$$\langle \eta_k(x); \varphi \rangle := \widehat{\varphi}_k(x) = (\xi_k(x); \varphi(x))_x \qquad k = 1, 2, \ldots, \dim \mathcal{H}(x). \tag{8}$$

Suppose that $A_f : \Phi \to \Phi$ is continuous with respect to the nuclear topology for every $f \in C(X)$. Then from equations (7) and (8) one has that the extended operator $\hat{A}_f : \Phi^* \to \Phi^*$, namely $\langle \hat{A}_f \, \eta; \varphi \rangle := \langle \eta; A_{\overline{f}} \varphi \rangle$ for all $\eta \in \Phi^*$ and $\varphi \in \Phi$, satisfies

$$\begin{aligned} \langle \hat{A}_f \ \eta_k(x); \varphi \rangle &= \langle \eta_k(x); A_{\overline{f}} \varphi \rangle = \overline{f}(x) \ \widehat{\varphi}_k(x) \\ &= \langle f(x) \eta_k(x); \varphi \rangle \quad k = 1, 2, \ldots, \dim \mathcal{H}(x) \end{aligned} \tag{9}$$

for all $\varphi \in \Phi$. Hence,

$$\hat{A}_f \ \eta_k(x) = f(x) \ \eta_k(x) \qquad \text{in } \Phi^*.$$

In this sense $\eta_k(x)$ is a *generalized eigenvector* for A_f. These claims are made precise in the following statement.

Theorem 4.1 (Maurin's nuclear spectral theorem). *With the notation and the assumptions of Theorem* 3.1*, let* $\{\Phi, \mathcal{H}, \Phi^*\}$ *be a nuclear Gel'fand triple for the space* $\mathcal{H}$ *such that* Φ *is* $\mathfrak{S}$*-invariant, i.e., each* $A \in \mathfrak{S}$ *is a continuous linear map* $A : \Phi \to \Phi$*. Then:*

(i) *for all* $x \in X$ *the* $\mathfrak{S}$*-Fourier transform* $\mathcal{F}_{\mathfrak{S}}|_x : \Phi \to \mathcal{H}(x)$, $\varphi \mapsto \varphi(x) \in \mathcal{H}(x)$ *is continuous with respect to the nuclear topology for* μ*-almost every* $x \in X$*;*

(ii) *there is a family of linear functionals* $\{\eta_k(x) : k = 1, 2, \ldots, \dim \mathcal{H}(x)\} \subset \Phi^*$ *such that equations* (8) *and* (9) *hold true for* μ*-almost all* $x \in X$*;*

(iii) *with the identification* $\eta_k(x) \leftrightarrow \xi_k(x)$ *the Hilbert space* $\mathcal{H}(x)$ *is* (*isomorphic to*) *a vector subspace of* Φ^**; with this identification the* $\mathcal{F}_{\mathfrak{S}}$*-Fourier transform is defined on the dense set* Φ *by*

$$\Phi \ni \varphi \overset{\mathcal{F}_{\mathfrak{S}}|_x}{\longmapsto} \sum_{k=1}^{\dim \mathcal{H}(x)} \langle \eta_k(x); \varphi \rangle \ \eta_k(x) \in \Phi^* \tag{10}$$

and the scalar product in $\mathcal{H}(x)$ *is formally defined by posing* $(\eta_k(x); \eta_j(x))_x := \delta_{k,j}$*;*

(iv) *under the identification in* (iii) *the spaces* $\mathcal{H}(x)$ *become the* common generalized eigenspaces *of the operators in* $\mathfrak{S}$ *in the sense that if* $A_f \in \mathfrak{S}$ *then* $\hat{A}_f \ \eta_k(x) = f(x) \ \eta_k(x)$ *for* μ*-almost every* $x \in X$ *and all* $k = 1, 2, \ldots,$ $\dim \mathcal{H}(x)$*.*

For a proof we refer to [Mau68] (Chapter II). The identification at point (iii) of Theorem 4.1 depends on the choice of a fundamental family of orthonormal measurable vector fields $\{\xi_k(\cdot) : k \in I\}$ for the direct integral $\mathfrak{H}$, which is clearly not unique. If $\{\zeta_k(\cdot) : k \in I\}$ is a second fundamental family of orthonormal measurable vector fields for $\mathfrak{H}$, then there exists a decomposable unitary map $W(\cdot)$ such that $W(x)\xi_k(x) = \zeta_k(x)$ for μ-almost every $x \in X$ and every $k \in I$. The composition $U := {\mathcal{F}_{\mathfrak{S}}}^{-1} \circ W(\cdot) \circ \mathcal{F}_{\mathfrak{S}}$ is a unitary isomorphism of the Hilbert space

$\mathcal{H}$ which induces a linear isomorphism between the Gel'fand triples $\{\Phi, \mathcal{H}, \Phi^*\}$ and $\{\Psi, \mathcal{H}, \Psi^*\}$ where $\Psi := U\Phi$. One checks that Ψ is a nuclear space in $\mathcal{H}$ with respect to the topology induced from Φ by the map U (i.e., defined by the family of seminorms $p'_\alpha := p_\alpha \circ U^{-1}$). Ψ^*, the topological dual of Ψ, is $\hat{U}\Phi^*$, in view of the continuity of $U^{-1} : \Psi \to \Phi$. The isomorphism of the Gel'fand triples is compatible with the direct integral decomposition. Indeed if $\vartheta_k(x) \leftrightarrow \zeta_k(x)$ is the identification between the new orthonormal basis $\{\zeta_k(x) : k = 1, 2, \dots, \dim \mathcal{H}(x)\}$ of $\mathcal{H}(x)$ and a family of linear functionals $\{\vartheta_k(x) : k = 1, 2, \dots, \dim \mathcal{H}(x)\} \subset \Psi^*$ then equation (8) implies that for any $\varphi \in \Psi$

$$\begin{aligned} \langle \vartheta_k(x); \varphi \rangle &:= \big(\zeta_k(x); \varphi(x)\big)_x = \big(\xi_k(x); W(x)^{-1}\varphi(x)\big)_x \\ &= \langle \eta_k(x); U^{-1}\varphi \rangle = \langle \hat{U}\,\eta_k(x); \varphi \rangle. \end{aligned} \tag{11}$$

As a consequence, we get the following result.

Proposition 4.2. *Up to a canonical identification of isomorphic Gel'fand triples the realization* (10) *of the fiber spaces $\mathcal{H}(x)$ as common generalized eigenspaces is canonical in the sense that it does not depend on the choice of a fundamental family of orthonormal measurable fields.*

From Proposition 4.2 and Corollary 3.4 it follows that:

Corollary 4.3. *Up to a canonical identification of isomorphic Gel'fand triples, the realization* (10) *of the fiber spaces $\mathcal{H}(x)$ as generalized common eigenspaces is preserved by a unitary transform of the triple $\{\mathcal{H}, \mathfrak{A}, \mathfrak{S}\}$.*

Theorem 4.1 assumes the existence of a $\mathfrak{S}$-invariant nuclear space and the related Gel'fand triple. If $\mathfrak{S}$ is generated by a countable family, such a nuclear space does exist and there is an algorithmic procedure to construct it.

Theorem 4.4 (Existence of the nuclear space [Mau68]). *Let $\{A_1, A_2, \dots\}$ be a countable family of commuting bounded normal operators on the separable Hilbert space $\mathcal{H}$, generating the commutative C^*-algebra $\mathfrak{S}$. Then there exists a countable $\mathfrak{S}$-cyclic system $\{\psi_1, \psi_2, \dots\}$ which generates a nuclear space $\Phi \subset \mathcal{H}$ such that:* a) *Φ is dense in $\mathcal{H}$;* b) *the embedding $\imath : \Phi \hookrightarrow \mathcal{H}$ is continuous;* c) *the maps $A_j^m : \Phi \to \Phi$ are continuous for all $j, m \in \mathbb{N}$.*

Remark 4.5. For the proof of Theorem 4.4 see [Mau68] (Chapter II, Theorem 6). We recall that a countable (or finite) family $\{\psi_1, \psi_2, \dots\}$ of orthonormal vectors in $\mathcal{H}$ is a $\mathfrak{S}$-*cyclic system* if the set $\{A^{\dagger^b} A^a \psi_k \ : \ k \in I, \ \ a, b \in \mathbb{N}^\infty_{\text{fin}}\}$ is total in $\mathcal{H}$, where $\mathbb{N}^\infty_{\text{fin}}$ is the space of $\mathbb{N}$-valued sequences which are definitely zero (i.e., $a_n = 0$ for any $n \in \mathbb{N} \setminus I$ with $|I| < +\infty$) and $A^a := A_1^{a_1} A_2^{a_2} \dots A_N^{a_N}$ for some integer N.

Any C^*-algebra $\mathfrak{S}$ (not necessarily commutative) has many $\mathfrak{S}$-cyclic systems. Indeed one can start from any normalized vector $\psi_1 \in \mathcal{H}$ to build the closed subspace $\mathcal{H}_1$ spanned by the action of $\mathfrak{S}$ on ψ_1. If $\mathcal{H}_1 \neq \mathcal{H}$ one can choose a second normalized vector ψ_2 in the orthogonal complement of $\mathcal{H}_1$ to build the closed subspace $\mathcal{H}_2$. Since $\mathcal{H}$ is separable, this procedure produces a countable (or

finite) family $\{\psi_1, \psi_2, \ldots\}$ such that $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \cdots$. Obviously this construction is not unique. The nuclear space Φ claimed in Theorem 4.4 depends on the choice of a $\mathfrak{S}$-cyclic system and generally many inequivalent choices are possible. ⧫◊

5. The wandering property

An interesting and generally unsolved problem is the construction of the invariant subspaces of an operator or of a family of operators. Let $\mathfrak{S}$ be a C^*-algebra contained in $\mathscr{B}(\mathcal{H})$. If $\psi \in \mathcal{H}$ then the subspace $\mathfrak{S}[\psi]$ generated by the action of $\mathfrak{S}$ on the vector ψ is an invariant subspace for the C^*-algebra. The existence of a particular decomposition of the Hilbert space into invariant subspaces depends on the nature of the C^*-algebra. The problem is reasonably simple to solve for the C^*-algebras which satisfy the wandering property.

Definition 5.1 (wandering property). *Let $\mathfrak{S}$ be a commutative unital C^*-algebra generated by the countable family $\{A_1, A_2, \ldots\}$ of commuting bounded normal operators in a separable Hilbert space $\mathcal{H}$. We say that $\mathfrak{S}$ has the* wandering property *if there exists a (at most) countable family $\{\psi_1, \psi_2, \ldots\} \subset \mathcal{H}$ of orthonormal vectors which is $\mathfrak{S}$-cyclic (according to Remark 4.5) and such that*

$$(\psi_k; {A^\dagger}^b A^a \psi_h)_{\mathcal{H}} = \|A^a \psi_k\|^2_{\mathcal{H}}\ \delta_{k,h}\ \delta_{a,b} \qquad \forall\ h,k \in I,\quad \forall\ a,b \in \mathbb{N}^\infty_{\mathrm{fin}}, \tag{12}$$

where $A^a := A_1^{a_1} A_2^{a_2} \ldots A_N^{a_N}$, $\delta_{k,h}$ is the usual Kronecker delta and $\delta_{a,b}$ is the Kronecker delta for the multiindices a and b.

Let $\mathcal{H}_k := \mathfrak{S}[\psi_k]$ be the Hilbert subspace generated by the action of $\mathfrak{S}$ on the vector ψ_k. If $\mathfrak{S}$ has the wandering property then the Hilbert space decomposes as $\mathcal{H} = \bigoplus_{k\in I} \mathcal{H}_k$ and each $\mathcal{H}_k$ is an $\mathfrak{S}$-invariant subspace. We will refer to $\mathcal{H}_k$ as a *wandering subspace* and to $\{\psi_1, \psi_2, \ldots\}$ as the *wandering system*. In these subspaces each operator A_j acts as a unilateral weighted shift and this justifies the use of the adjective "wandering" (see [NF70] Chapter 1, Sections 1 and 2). The wandering property implies many interesting consequences.

Proposition 5.2. *Let $\mathfrak{S}$ be a commutative unital C^*-algebra generated by the (at most) countable family $\{A_1, A_2, \ldots\}$ of commuting bounded normal operators on a separable Hilbert space $\mathcal{H}$. Suppose that $\mathfrak{S}$ has the wandering property with respect to the family of vectors $\{\psi_1, \psi_2, \ldots\}$, then:*

(i) *the generators are not selfadjoint, and $A_j^n \neq \mathbb{1}$ for every $n \in \mathbb{N} \setminus \{0\}$;*
(ii) *every generator which is unitary has no eigenvectors;*
(iii) *if $\mathfrak{S}$ is generated by N unitary operators then $\mathfrak{S}$ is a $\mathbb{Z}^N$-algebra.*

Proof. To prove (i) observe that the condition $A_j = A_j^\dagger$ implies that $A_j \psi_k = 0$ for all ψ_k in the system and the $\mathfrak{S}$-cyclicity imposes $A_j = 0$. As for the second claim, by setting $b = 0$ and $h = k$ in equation (12) one sees that $A^a = \mathbb{1}$ implies $a = 0$.

To prove (ii) observe that if $\{U, A_1, A_2, \ldots\}$ is a set of commuting generators for $\mathfrak{S}$ with U unitary, then each vector $\varphi \in \mathcal{H}$ can be written as $\varphi = \sum_{n\in\mathbb{Z}} U^n \chi_n$

where $\chi_n = \sum_{k\in I,\, a\in\mathbb{Z}^N} \alpha_{k,a}\, A^a\psi_k$. Clearly $U\varphi = \sum_{n\in\mathbb{Z}} U^n\chi_{n-1}$ and equation (12) implies that $\|\varphi\|^2_{\mathcal{H}} = \sum_{n\in\mathbb{Z}} \|\chi_n\|^2_{\mathcal{H}}$. If $U\varphi = \lambda\varphi$, with $\lambda \in \mathbb{S}^1$, then a comparison between the components provides $\chi_{n-1} = \lambda\chi_n$, i.e., $\chi_n = \lambda^{-n}\chi_0$ for all $n \in \mathbb{Z}$. This contradicts the convergence of the series expressing the norm of φ.

To prove (iii) observe that the map $\mathbb{Z}^N \ni a := (a_1, \dots, a_N) \mapsto U^a = U_1^{a_1} \dots U_N^{a_N} \in \mathscr{U}(\mathcal{H})$ is a unitary representation of $\mathbb{Z}^N$ on $\mathcal{H}$. To show that the representation is algebraically compatible, suppose that $\sum_{a\in\mathbb{Z}^N} \alpha_a U^a = 0$; then from equation (12) it follows that $0 = (U^b\psi_k; \sum_{a\in\mathbb{Z}^N} \alpha_a U^a\psi_k)_{\mathcal{H}} = \alpha_b$ for all $b \in \mathbb{Z}^N$, and this concludes the proof. □

Proposition 5.2 shows that the wandering property forces a commutative C^*-algebra generated by a finite number of unitary operators to be a $\mathbb{Z}^N$-algebra. This is exactly what happens in the cases in which we are mostly interested.

Example 5.3 (Periodic systems, part two). The commutative unital C^*-algebra $\mathfrak{S}_T$ defined in Example 2.1 is generated by a unitary faithful representation of $\mathbb{Z}^d$ on $L^2(\mathbb{R}^d)$, given by $\mathbb{Z}^d \ni m \mapsto T^m \in \mathscr{U}(L^2(\mathbb{R}^d))$ where $m := (m_1, \dots, m_d)$ and $T^m := T_1^{m_1} \dots T_d^{m_d}$. It is easy to show that the C^*-algebra $\mathfrak{S}_T$ has the wandering property. Indeed let $\mathcal{Q}_0 := \{x = \sum_{j=1}^d x_j\gamma_j \ : \ -1/2 \leqslant x_j \leqslant 1/2, \quad j = 1, \dots, d\}$ be the *fundamental unit cell* of the lattice Γ and $\mathcal{Q}_m := \mathcal{Q}_0 + m$ its translation by the lattice vector $m := \sum_{j=1}^d m_j\gamma_j$. Let $\{\psi_k\}_{k\in\mathbb{N}} \subset L^2(\mathbb{R}^d)$ be a family of functions with support in $\mathcal{Q}_0$ providing an orthonormal basis of $L^2(\mathcal{Q}_0)$ up to the natural inclusion $L^2(\mathcal{Q}_0) \hookrightarrow L^2(\mathbb{R}^d)$. This system is $\mathfrak{S}_T$-cyclic since $L^2(\mathbb{R}^d) = \bigoplus_{m\in\mathbb{Z}^d} L^2(\mathcal{Q}_m)$. Moreover, it is wandering under the action of $\mathfrak{S}_T$ since the intersection $\mathcal{Q}_0 \cap \mathcal{Q}_m$ has zero measure for every $m \neq 0$. The cardinality of the wandering system is $\aleph_0$. Proposition 5.2 assures that $\mathfrak{S}_T$ is a $\mathbb{Z}^d$-algebra. Moreover, as a consequence of Proposition 5.5, the Gel'fand spectrum of $\mathfrak{S}_T$ is homeomorphic to the d-dimensional torus $\mathbb{T}^d$ and the normalized basic measure is the Haar measure dz on $\mathbb{T}^d$. ◀▷

Example 5.4 (Mathieu-like Hamiltonians, part two). The unital commutative C^*-algebra $\mathfrak{S}^q_{\mathrm{M}} \subset \mathscr{B}(L^2(\mathbb{T}))$ defined in Example 2.2 is generated by a unitary faithful representation of the group $\mathbb{Z}$ on the Hilbert space $L^2(\mathbb{T})$. Indeed, the map $\mathbb{Z} \ni k \mapsto \mathfrak{w}^k \in \mathscr{U}(L^2(\mathbb{T}))$ is an injective group homomorphism. The set of vectors $\{e_0, \dots, e_{q-1}\} \subset L^2(\mathbb{T})$ shows that the C^*-algebra $\mathfrak{S}^q_{\mathrm{M}}$ has the wandering property. In this case the cardinality of the wandering system is q. Proposition 5.2 assures that $\mathfrak{S}^q_{\mathrm{M}}$ is a $\mathbb{Z}$-algebra. Moreover, Proposition 5.5 will show that the Gel'fand spectrum of $\mathfrak{S}^q_{\mathrm{M}}$ is homeomorphic to the 1-dimensional torus $\mathbb{T}$ and the normalized basic measure on the spectrum coincides with the Haar measure dz on $\mathbb{T}$. The first claim agrees with the fact that the Gel'fand spectrum of $\mathfrak{S}^q_{\mathrm{M}}$ coincides with the (Hilbert space) spectrum of $\mathfrak{w}$, the generator of the C^*-algebra, and $\sigma(\mathfrak{w}) = \mathbb{T}$. The claim about the basic measure agrees with the fact that the vector e_0 is cyclic for the commutant of $\mathfrak{S}^q_{\mathrm{M}}$ (which is the von Neumann algebra generated by $\mathfrak{A}_{\mathrm{M}}^{p/q}$). Indeed, a general result (see Appendix A) assures that the spectral measure μ_{e_0,e_0}

provides the basic measure. To determine μ_{e_0,e_0} let $\mathcal{P}(\mathfrak{w}) := \sum_{k\in\mathbb{Z}} \alpha_k \mathfrak{w}^k$ be any element of $\mathfrak{S}^q_{\mathrm{M}}$. From the definition of spectral measure it follows that

$$\alpha_0 = (e_0; \mathcal{P}(\mathfrak{w})e_0) = \int_{\mathbb{T}} \mathcal{P}(z)\ d\mu_{e_0,e_0}(z) = \sum_{k\in\mathbb{Z}} \alpha_k \int_0^{2\pi} \mathrm{e}^{ikt}\ d\widetilde{\mu}_{e_0,e_0}(t). \tag{13}$$

where the measure $\widetilde{\mu}_{e_0,e_0}$ is related to μ_{e_0,e_0} by the change of variables $\mathbb{T} \ni z \mapsto t \in [0, 2\pi)$ defined by $z := \mathrm{e}^{it}$ according to Remark 2.3. Equation (13) implies that $\widetilde{\mu}_{e_0,e_0}$ agrees with $dt/2\pi$ on $C(\mathbb{T})$, namely the basic measure μ_{e_0,e_0} is the normalized Haar measure. ◀▷

In the relevant cases of commutative unital C^*-algebras generated by a finite set of unitary operators the wandering property provides a useful characterization of the Gel'fand spectrum and the basic measure. We firstly introduce some notation and terminology. Let $\mathbb{G}$ be a discrete group and $\ell^1(\mathbb{G})$ be the set of sequences $c = \{c_g\}_{g\in\mathbb{G}}$ such that $\|c\|_{\ell^1} = \sum_{g\in\mathbb{G}} |c_g| < +\infty$. Equipped with the convolution product $(c * d)_g := \sum_{h\in\mathbb{G}} c_h d_{g-h}$ and involution $c^\dagger := \{\overline{c}_{-g}\}_{g\in\mathbb{G}}$, $\ell^1(\mathbb{G})$ becomes a unital Banach $*$-algebra called the *group algebra* $\mathbb{G}$. The latter is not a C^*-algebra since the norm $\|\cdot\|_{\ell^1}$ does not verify the C^*-condition $\|c * c^*\|_{\ell^1} = \|c\|^2_{\ell^1}$. In general there exist several inequivalent ways to complete $\ell^1(\mathbb{G})$ to a C^*-algebra by introducing suitable C^*-norms. Two of these C^*-extensions are of particular interest. The first is obtained as the completion of $\ell^1(\mathbb{G})$ with respect to the *universal enveloping norm*

$$\|c\|_u := \sup\{\|\pi(c)\|_{\mathcal{H}} \ :\ \pi : \ell^1(\mathbb{G}) \to \mathscr{B}(\mathcal{H}) \text{ is a } *\text{-representation}\}.$$

The resulting abstract C^*-algebra, denoted by $C^*(\mathbb{G})$, is called the *group C^*-algebra* of $\mathbb{G}$ (or *enveloping* C^*-algebra).

The second relevant extension is obtained by means of the concrete representation of the elements $\ell^1(\mathbb{G})$ as (convolution) multiplicative operators on the Hilbert space $\ell^2(\mathbb{G})$. In other words, for any $\xi = \{\xi_g\}_{g\in\mathbb{G}} \in \ell^2(\mathbb{G})$ and $c = \{c_g\}_{g\in\mathbb{G}} \in \ell^1(\mathbb{G})$ one defines the representation $\pi_r : \ell^1(\mathbb{G}) \to \mathscr{B}(\ell^2(\mathbb{G}))$ as

$$\pi_r(c)\xi := c * \xi = \left\{ \sum_{h\in\mathbb{G}} c_h \xi_{g-h} \right\}_{g\in\mathbb{G}}.$$

The representation π_r, known as *left regular representation*, is injective. The norm $\|c\|_r := \|\pi_r(c)\|_{\mathscr{B}(\ell^2(\mathbb{G}))}$ defines a new C^*-norm on $\ell^1(\mathbb{G})$, called *reduced norm*, and a new C^*-extension denoted by $C^*_r(\mathbb{G})$ and called *reduced group C^*-algebra*. Since $\|\cdot\|_r \le \|\cdot\|_u$ it follows that $C^*_r(\mathbb{G})$ is $*$-isomorphic to a quotient C^*-algebra of $C^*(\mathbb{G})$. Nevertheless, if the group $\mathbb{G}$ is abelian, one has the relevant isomorphism $C^*_r(\mathbb{G}) = C^*(\mathbb{G}) \simeq C(\widehat{\mathbb{G}})$ where $\widehat{\mathbb{G}}$ denotes the dual (or character) group of $\mathbb{G}$. For more details the reader can refer to [Dix82] (Chapter 13) or [Dav96] (Chapter VII).

Proposition 5.5. *Let $\mathcal{H}$ be a separable Hilbert space and $\mathfrak{S} \subset \mathscr{B}(\mathcal{H})$ a unital commutative C^*-algebra generated by a finite family $\{U_1, \ldots, U_N\}$ of unitary operators. Assume the wandering property. Then:*

(i) *the Gel'fand spectrum of* $\mathfrak{S}$ *is homeomorphic to the* N*-dimensional torus* $\mathbb{T}^N$*;*
(ii) *the basic measure of* $\mathfrak{S}$ *is the normalized Haar measure* dz *on* $\mathbb{T}^N$*.*

Proof. We use the short notation $U^a = U_1^{a_1} \dots U_N^{a_N}$ for any $a = (a_1, \dots, a_N) \in \mathbb{Z}^N$.

To prove (i) one notices that the map $F : \ell^1(\mathbb{Z}^N) \to \mathscr{B}(\mathcal{H})$, defined by $F(c) := \sum_{a\in\mathbb{Z}^N} c_a\ U^a$, is a $*$-representation of $\ell^1(\mathbb{Z}^N)$ in $\mathscr{B}(\mathcal{H})$. As in the proof of Proposition 5.2, one exploits the wandering property to see that for any $c \in \ell^1(\mathbb{Z}^N)$, $\sum_a c_a U^a = 0$ implies $c = 0$. Thus F is a faithful representation. Moreover $\|F(c)\|_{\mathscr{B}(\mathcal{H})} \leqslant \|c\|_{\ell^1}$ for all $c \in \ell^1(\mathbb{C})$. Finally, the unital $*$-algebra $\mathfrak{L}^1(\mathbb{Z}^N) := F(\ell^1(\mathbb{Z}^N)) \subset \mathscr{B}(\mathcal{H})$ is dense in $\mathfrak{S}$ (with respect to the operator norm), since it does contain the polynomials in $U_1, \dots, U_N$, which are a dense subset of $\mathfrak{S}$.

In view of the fact that $\mathbb{Z}^N$ is abelian, to prove (i) it is sufficient to show that $\mathfrak{S} \simeq C_r^*(\mathbb{Z}^N)$. Since $\ell^1(\mathbb{Z}^N)$ and $\mathfrak{L}^1(\mathbb{Z}^N)$ are isomorphic Banach $*$-algebras, and $\mathfrak{L}^1(\mathbb{Z}^N)$ is dense in $\mathfrak{S}$, the latter claims follows if one proves that $\|c\|_r = \|F(c)\|_{\mathscr{B}(\mathcal{H})}$ for any $c \in \ell^1(\mathbb{Z}^N)$. Let $\{\psi_k\}_{k\in I}$ be the wandering system of vectors for $\mathfrak{S}$. The wandering property assures that the closed subspace $\mathfrak{S}[\psi_k] =: \mathcal{H}_k \subset \mathcal{H}$ is isometrically isomorphic to $\ell^2(\mathbb{Z}^N)$, with unitary isomorphism given by $\mathcal{H}_k \ni \sum_{a\in\mathbb{Z}^N} \xi_a U^a\psi_k \mapsto \{\xi_a\}_{a\in\mathbb{Z}^N} \in \ell^2(\mathbb{Z}^N)$. Then, due to the mutual orthogonality of the spaces $\mathcal{H}_k$, there exists a unitary map $\mathcal{R} : \mathcal{H} \to \bigoplus_{k\in I} \ell^2(\mathbb{Z}^N)$ which extends all the isomorphisms above. A simple computation shows that $\mathcal{R}F(c)\mathcal{R}^{-1} = \bigoplus_{k\in I} \pi_r(c)$ for any $c \in \ell^1(\mathbb{Z}^N)$. Since $\mathcal{R}$ is isometric, it follows that $\|F(c)\|_{\mathscr{B}(\mathcal{H})} = \|\bigoplus_{k\in I} \pi_r(c)\|_{\bigoplus_{k\in I} \ell^2} = \|\pi_r(c)\|_{\ell^2}$, which is exactly the definition of the norm $\|c\|_r$.

To prove (ii) let $\mu_k := \mu_{\psi_k,\psi_k}$ be the spectral measure defined by the vector of the wandering system ψ_k. The Gel'fand isomorphism identifies the generator $U_j \in \mathfrak{S}$ with $z_j \in C(\mathbb{T}^N)$. It follows that for every $a \in \mathbb{Z}^N$ one has

$$\delta_{a,0} = (\psi_k; U^a\psi_k) = \int_{\mathbb{T}^N} z^a\ d\mu_k(z) := \int_0^{2\pi} \dots \int_0^{2\pi} z_1^{a_1}(t) \dots z_N^{a_N}(t)\ d\widetilde{\mu}_k(t), \quad (14)$$

where the measure $\widetilde{\mu}_k$ is related to μ_k by the change of variables $\mathbb{T}^N \ni z \mapsto t \in [0, 2\pi)^N$ defined by $z := \mathrm{e}^{it}$ according to Remark 2.3. Equation (14) shows that for all k the spectral measure $\widetilde{\mu}_k$ agrees with $dz(t) := {}^{dt_1\dots dt_N}\!/_{(2\pi)^N}$.

Let A_f be the element of $\mathfrak{S}$ whose image via the Gel'fand isomorphism is the function $f \in C(\mathbb{T}^N)$. Then

$$(U^b\psi_j; A_f U^a\psi_k)_{\mathcal{H}} = \delta_{j,k}(\psi_k; A_f U^{a-b}\psi_k)_{\mathcal{H}} = \int_{\mathbb{T}^N} f(z)\ \delta_{j,k}\ z^{a-b}\ dz.$$

So the spectral measure $\mu_{U^b\psi_j, U^a\psi_k}$ is related to the Haar measure dz by the function $\delta_{j,k}\ z^{a-b}$. Let $\varphi := \sum_{k\in I, a\in\mathbb{N}^N} \alpha_{a,k}\ U^a\psi_k$ be any vector in $\mathcal{H}$. Notice that, in view of the wandering property, one has $\alpha_{k,a} \in \ell^2(\mathbb{N}) \otimes \ell^2(\mathbb{Z}^N)$. Then a direct computation shows that $\mu_{\varphi,\varphi}(z) = h_{\varphi,\varphi}(z)\ dz$, where $h_{\varphi,\varphi}(z) = \sum_{k\in I} |F_\varphi^{(k)}(z)|^2$ with $F_\varphi^{(k)}(z) := \sum_{a\in\mathbb{N}^N} \alpha_{k,a} z^a$. Since $F_\varphi^{(k)} \in L^2(\mathbb{T}^N)$, one has $|F_\varphi^{(k)}|^2 \in L^1(\mathbb{T}^N)$. Let $h_{\varphi,\varphi}^{(M)}(z) = \sum_{k=0}^M |F_\varphi^{(k)}(z)|^2$. Since $h_{\varphi,\varphi}^{(M+1)} \geqslant h_{\varphi,\varphi}^{(M)} \geqslant 0$ and $\int_{\mathbb{T}^N} h_{\varphi,\varphi}^{(M)}(z)\ dz =$

$\sum_{k=0}^{M}\sum_{a\in\mathbb{N}^N}|\alpha_{k,a}|^2 \leqslant \|\varphi\|^2_{\mathcal{H}}$ for all M, one concludes by the monotone convergence theorem that $h_{\varphi,\varphi}\in L^1(\mathbb{T}^N)$. □

Not every commutative C^*-algebra generated by a faithful unitary representation of $\mathbb{Z}^N$ has a wandering system. In this situation, even if the spectrum is still a torus, the basic measure can be inequivalent to the Haar measure, as illustrated by the following example.

Example 5.6. Let R_α be the unitary operator on $L^2(\mathbb{R}^2)$ which implements a rotation around the origin of the angle α, with $\alpha\notin 2\pi\mathbb{Q}$. Since $R_\alpha^N = R_{N\alpha}\neq \mathbb{1}$ for every integer N, it follows that the commutative unital C^*-algebra $\mathfrak{R}_\alpha$ generated by R_α is a $\mathbb{Z}$-algebra. The Gel'fand spectrum of $\mathfrak{R}_\alpha$, which coincides with the spectrum of R_α, is $\mathbb{T}$. Indeed, the vector $\psi_N(\rho,\phi) := \mathrm{e}^{iN\phi}f(\rho)$ (in polar coordinates) is an eigenvector corresponding to the eigenvalue $\mathrm{e}^{iN\alpha}$. The spectrum of R_α is the closure of $\{\mathrm{e}^{iN\alpha} \,:\, N\in\mathbb{Z}\}$, which is $\mathbb{T}$ in view of the irrationality of α. The existence of eigenvectors excludes the existence of a wandering system (see Proposition 5.2). Moreover, since R_α has point spectrum it follows that the basic measure is not the Haar measure. Indeed, the spectral measure μ_{ψ_N,ψ_N} corresponding to the eigenvector ψ_N is the *Dirac measure* concentrated in $\{\mathrm{e}^{iN\alpha}\}\subset\mathbb{C}$. ◀▷

6. The generalized Bloch-Floquet transform

The aim of this section is to provide a general algorithm for constructing the direct integral decomposition of a commutative C^*-algebra which appears in the von Neumann's complete spectral theorem. In this approach a relevant role will be played by the wandering property. We consider a commutative unital C^*-algebra $\mathfrak{S}$ on a separable Hilbert space $\mathcal{H}$ generated by the finite family $\{U_1,U_2,\ldots,U_N\}$ of unitary operators admitting a wandering system $\{\psi_k\}_{k\in I}\subset\mathcal{H}$. According to the results of Section 5, $\mathfrak{S}$ is a $\mathbb{Z}^N$-algebra with Gel'fand spectrum $\mathbb{T}^N$ and with the Haar measure dz as basic measure.

Construction of the wandering nuclear space

The existence of a wandering system makes possible the explicit construction of a $\mathfrak{S}$-invariant nuclear space, which we call the *wandering nuclear space*.

Consider the orthonormal basis $\{U^a\psi_k\}_{k\in I,a\in\mathbb{Z}^N}$, where $\{\psi_k\}_{k\in I}$ is the wandering system, and denote by $\mathcal{L}\subset\mathcal{H}$ the family of all finite linear combinations of the vectors of this basis. For every integer $m\geqslant 0$ denote by $\mathcal{H}_m$ the finite-dimensional Hilbert space generated by the finite set of vectors $\{U^a\psi_k \,:\, 0\leqslant k\leqslant m,\, 0\leqslant|a|\leqslant m\}$, where $|a| := |a_1|+\cdots+|a_N|$. Obviously $\mathcal{H}_m\subset\mathcal{L}$. Let D_m denote the dimension of the space $\mathcal{H}_m$. If $\varphi=\sum_{k\in I,a\in\mathbb{Z}^N}\alpha_{k,a}U^a\psi_k$ is any element of $\mathcal{H}$ then the formula

$$p_m^2(\varphi) := D_m\sum_{\substack{0\leqslant k\leqslant m\\ 0\leqslant|a|\leqslant m}}|(U^a\psi_k;\varphi)_{\mathcal{H}}|^2 = D_m\sum_{\substack{0\leqslant k\leqslant m\\ 0\leqslant|a|\leqslant m}}|\alpha_{k,a}|^2, \tag{15}$$

defines a seminorm for every $m \geqslant 0$. From (15) it follows that $p_m \leqslant p_{m+1}$ for all m. The countable family of seminorms $\{p_m\}_{m\in\mathbb{N}}$ provides a locally convex topology for the vector space $\mathcal{L}$. Let Σ denote the pair $\{\mathcal{L}, \{p_m\}_{m\in\mathbb{N}}\}$, i.e., the vector space $\mathcal{L}$ endowed with the locally convex topology induced by the seminorms (15). Σ is a complete and metrizable (i.e., Fréchet) space. However, for our purposes, we need a topology on $\mathcal{L}$ which is strictly stronger than the metrizable topology induced by the seminorms (15).

The quotient space $\Phi_m := \mathcal{L}/\mathcal{N}_m$, with $\mathcal{N}_m := \{\varphi \in \mathcal{L} \ : \ p_m(\varphi) = 0\}$, is isomorphic to the finite-dimensional vector space $\mathcal{H}_m$, hence it is nuclear and Fréchet. This follows immediately observing that the norm p_m on Φ_m coincides, up to the positive constant $\sqrt{D_m}$, with the usual Hilbert norm. Obviously $\Phi_m \subset \Phi_{m+1}$ for all $m \geqslant 0$ and the topology of Φ_m agrees with the topology inherited from Φ_{m+1}, indeed $p_{m+1}|_{\Phi_m} = \sqrt{\frac{D_{m+1}}{D_m}}\, p_m$. We define Φ to be $\bigcup_{m\in\mathbb{N}} \Phi_m$ (which is $\mathcal{L}$ as a set) endowed with the *strict inductive limit topology* which is the strongest topology which makes all injections $\imath_m : \Phi_m \hookrightarrow \Phi$ continuous. The space Φ is called a *LF-space* (according to the definition of [Tre67] Chapter 13) and it is a nuclear space since it is the strict inductive limit of nuclear spaces (see [Tre67] Proposition 50.1). We will say that Φ is the *wandering nuclear space* defined by the $\mathbb{Z}^N$-algebra $\mathfrak{S}$ on the wandering system $\{\psi_k\}_{k\in I}$.

Proposition 6.1. *The wandering nuclear space Φ defined by the previous construction satisfies all the properties stated in Theorem* 4.4.

Proof. A linear map $\jmath : \Phi \to \Psi$, with Ψ is an arbitrary locally convex topological vector space, is continuous if and only if the restriction $\jmath|_{\Phi_m}$ of $\jmath$ to Φ_m is continuous for each $m \geqslant 0$ (see [Tre67] Proposition 13.1). This implies that the canonical embedding $\imath : \Phi \hookrightarrow \mathcal{H}$ is continuous, since its restrictions are linear operators defined on finite-dimensional spaces. The linear maps $U^a : \Phi \to \Phi$ for all $a \in \mathbb{N}^N$ are also continuous for the same reason. Finally Φ is norm-dense in $\mathcal{H}$ since as a set it is the dense domain $\mathcal{L}$. □

The transform

We are now in position to define the *generalized Bloch-Floquet transform* $\mathcal{U}_{\mathfrak{S}}$ for the C^*-algebra $\mathfrak{S}$. The Gel'fand spectrum of $\mathfrak{S}$ is $\mathbb{T}^N$ and the Gel'fand isomorphism associates to the generator U_j the function $z_j \in C(\mathbb{T}^N)$, according to the notation of Remark 2.3. For all $t \in [0, 2\pi)^N$ and for all $\varphi \in \Phi$ we define (formally for the moment) the Bloch-Floquet transform of φ at point t as

$$\boxed{\Phi \ni \varphi \overset{\mathcal{U}_{\mathfrak{S}}|_t}{\longmapsto} (\mathcal{U}_{\mathfrak{S}}\varphi)(t) := \sum_{a\in\mathbb{Z}^N} z^{-a}(t)\ U^a\varphi} \tag{16}$$

where $z^a(t) := e^{ia_1t_1} \dots e^{ia_Nt_N}$ and $U^a := U_1^{a_1} \dots U_N^{a_N}$. The structure of equation (16) suggests that $(\mathcal{U}_{\mathfrak{S}}\varphi)(t)$ is a common generalized eigenvector for the elements

of $\mathfrak{S}$, indeed a formal computation shows that

$$U_j(\mathcal{U}_{\mathfrak{S}}\varphi)(t) = z_j(t) \sum_{a\in\mathbb{Z}^N} z_j^{-1}(t) z^{-a}(t) U_j\, U^a\varphi = \mathrm{e}^{it_j}\ (\mathcal{U}_{\mathfrak{S}}\varphi)(t). \tag{17}$$

This guess is clarified by the following result.

Theorem 6.2 (Generalized Bloch-Floquet transform). *Let $\mathfrak{S}$ be a $\mathbb{Z}^N$-algebra in the separable Hilbert space $\mathcal{H}$ with generators $\{U_1,\dots,U_N\}$ and wandering system $\{\psi_k\}_{k\in I}$, and let Φ be the corresponding wandering nuclear space. Then the* generalized Bloch-Floquet transform (16) *defines an injective linear map from the nuclear space Φ into its topological dual Φ^* for every $t\in[0,2\pi)^N$. More precisely, the transform $\mathcal{U}_{\mathfrak{S}}|_t$ maps Φ onto a subspace $\Phi^*(t)\subset\Phi^*$ which is a common generalized eigenspace for the commutative C^*-algebra $\mathfrak{S}$, i. e.,*

$$\hat{U}_j\,(\mathcal{U}_{\mathfrak{S}}\varphi)(t) = e^{it_j}\,(\mathcal{U}_{\mathfrak{S}}\varphi)(t) \qquad \text{in}\ \ \Phi^*.$$

The map $\mathcal{U}_{\mathfrak{S}}|_t : \Phi\to\Phi^*(t)\subset\Phi^*$ is a continuous linear isomorphism, provided Φ^* is endowed with the weak-$*$ topology.

Proof. We need to verify that the right-hand side of (16) is well defined as a linear functional on Φ. Any vector $\varphi\in\Phi$ is a finite linear combination $\varphi = \sum_{k\in I}^{\mathrm{fin}}\sum_{b\in\mathbb{Z}^N}^{\mathrm{fin}} \alpha_{k,b}\ U^b\psi_k$ (the complex numbers $\alpha_{k,b}$ are different from zero only for a finite set of the values of the index k and the multiindex b). Let $\phi = \sum_{h\in\mathbb{N}}^{\mathrm{fin}}\sum_{c\in\mathbb{N}^N}^{\mathrm{fin}} \beta_{h,c}\ U^c\psi_h$ be another element in Φ. The linearity of the dual pairing between Φ^* and Φ and the compatibility of the pairing with the Hermitian structure of $\mathcal{H}$ imply

$$\langle(\mathcal{U}_{\mathfrak{S}}\varphi)(t);\phi\rangle := \sum_{k\in I}^{\mathrm{fin}}\ \sum_{b,c\in\mathbb{Z}^N}^{\mathrm{fin}} \overline{\alpha}_{k,b}\beta_{k,c}\left(\sum_{a\in\mathbb{Z}^N} z^a(t)\ (U^{a+b}\psi_k; U^c\psi_k)_{\mathcal{H}}\right) \tag{18}$$

where in the right-hand side we used the orthogonality between the spaces generated by ψ_k and ψ_h if $k\neq h$. Without further conditions equation (18) is a finite sum in k,b,c (this is simply a consequence of the fact that φ and ϕ are "test functions") but it is an infinite sum in a which generally does not converge. However, in view of the wandering property one has that $(U^{a+b}\psi_k; U^c\psi_k)_{\mathcal{H}} = \delta_{a+b,c}$, so that (18) reads

$$\langle(\mathcal{U}_{\mathfrak{S}}\varphi)(t);\phi\rangle = \sum_{k\in I}^{\mathrm{fin}}\ \sum_{b,c\in\mathbb{Z}^N}^{\mathrm{fin}} \overline{\alpha}_{k,b}\beta_{k,c}\ z^c(t)z^{-b}(t). \tag{19}$$

Let $C_{\varphi;k} := \sum_{b\in\mathbb{Z}^N}^{\mathrm{fin}} |\alpha_{k,b}|$ and $C_\varphi := \max_{k\in I}\{C_{\varphi;k}\}$ (which is well defined since the set contains only a finite numbers of non-zero elements). An easy computation shows that

$$|\langle(\mathcal{U}_{\mathfrak{S}}\varphi)(t);\phi\rangle| \leqslant \sum_{k\in I}^{\mathrm{fin}} C_{\varphi,k}\left(\sum_{c\in\mathbb{Z}^N}^{\mathrm{fin}} |\beta_{k,c}|\right) \leqslant C_\varphi \sum_{k\in I}^{\mathrm{fin}}\ \sum_{c\in\mathbb{Z}^N}^{\mathrm{fin}} |\beta_{k,c}|\,.$$

Let $m \geqslant 0$ be the smallest integer such that $\phi \in \Phi_m$. The number of the coefficients $\beta_{k,c}$ different from zero is smaller than the dimension D_m of Φ_m. Using the Cauchy-Schwarz inequality one has

$$|\langle(\mathcal{U}_{\mathfrak{S}}\varphi)(t);\phi\rangle| \leqslant C_\varphi \sqrt{D_m} \left(\sum_{k\in I}^{\text{fin}} \sum_{c\in\mathbb{N}^N}^{\text{fin}} |\beta_{k,c}|^2 \right)^{\frac{1}{2}} = C_\varphi \; p_m(\phi). \tag{20}$$

The inequality (20) shows that the linear map $(\mathcal{U}_{\mathfrak{S}}\varphi)(t) : \Phi \to \mathbb{C}$ is continuous when it is restricted to each finite-dimensional space Φ_m. Since Φ is endowed with the strict inductive limit topology, this is enough to assure that $(\mathcal{U}_{\mathfrak{S}}\varphi)(t)$ is a continuous linear functional on Φ. So, in view of (20), $(\mathcal{U}_{\mathfrak{S}}\varphi)(t) \in \Phi^*$ for all $t \in [0, 2\pi)^N$ and for all $\varphi \in \Phi$.

The linearity of the map $\mathcal{U}_{\mathfrak{S}}|_t : \Phi \to \Phi^*$ is immediate and from equation (19) it follows that $(\mathcal{U}_{\mathfrak{S}}\varphi)(t) = 0$ (as functional) implies that $\alpha_{k,b} = 0$ for all k and b, hence $\varphi = 0$. This proves the injectivity. To prove the continuity of the map $\mathcal{U}_{\mathfrak{S}}|_t : \Phi \to \Phi^*$, in view of the strict inductive topology on Φ, we only need to check the continuity of the maps $\mathcal{U}_{\mathfrak{S}}|_t : \Phi_m \to \Phi^*$ for all $m \geqslant 0$. Since Φ_m is a finite-dimensional vector space with norm p_m, it is sufficient to prove that the norm-convergence of the sequence $\varphi_n \to 0$ in Φ_m implies the weak-$*$ convergence $(\mathcal{U}_{\mathfrak{S}}\varphi_n)(t) \to 0$ in Φ^*, i.e., $|\langle(\mathcal{U}_{\mathfrak{S}}\varphi_n)(t);\phi\rangle| \to 0$ for all $\phi \in \Phi$. As inequality (20) suggests, it is enough to show that $C_{\varphi_n} \to 0$. This is true since $\varphi_n := \sum_{0<k,|b|\leqslant m} \alpha^{(n)}_{k,b}\; U^b\psi_k \to 0$ in Φ_m implies $\alpha^{(n)}_{k,b} \to 0$.

Finally, since the map $U^{-a} = (U^a)^\dagger$ is continuous on Φ for all $a \in \mathbb{Z}^N$ then $(\hat{U^a}) : \Phi^* \to \Phi^*$ defines a continuous map which extends the operator U^a originally defined on $\mathcal{H}$. In this context the equation (17) is meaningful and shows that $\Phi^*(t) := \mathcal{U}_{\mathfrak{S}}|_t(\Phi) \subset \Phi^*$ is a space of common generalized eigenvectors for the elements of $\mathfrak{S}$. □

The decomposition

The wandering system $\{\psi_k\}_{k\in I}$ generates under the Bloch-Floquet transform a special family of elements of Φ^*, denoted by

$$\boxed{\zeta_k(t) := (\mathcal{U}_{\mathfrak{S}}\psi_k)(t) = \sum_{a\in\mathbb{Z}^N} z^{-a}(t)\; U^a\psi_k \qquad \forall\; k \in I.} \tag{21}$$

The injectivity of the map $\mathcal{U}_{\mathfrak{S}}$ implies that the functionals $\{\zeta_k(t)\}_{k\in I}$ are linearly independent for every t. If $\varphi = \sum_{k\in I}^{\text{fin}} \sum_{b\in\mathbb{Z}^N}^{\text{fin}} \alpha_{k,b}\; U^b\psi_k$ is any element in Φ then a simple computation shows that

$$(\mathcal{U}_{\mathfrak{S}}\varphi)(t) = \sum_{k\in I}^{\text{fin}} \sum_{b\in\mathbb{Z}^N}^{\text{fin}} \alpha_{k,b} \sum_{a\in\mathbb{N}^N} z^{-a}(t)\; U^{a+b}\psi_k = \sum_{k\in I}^{\text{fin}} f_{\varphi;k}(t)\; \zeta_k(t) \tag{22}$$

where $f_{\varphi;k}(t) := \sum_{b\in\mathbb{Z}^N}^{\text{fin}} \alpha_{k,b}\; z^b(t)$. The equalities in (22) should be interpreted in the sense of "distributions", *i. e.*, elements of Φ^*. The functions $f_{\varphi;k} : \mathbb{T}^N \to$

$\mathbb{C}$, for all $k \in I$, are finite linear combinations of continuous functions, hence continuous. Equation (22) shows that any subspace $\Phi^*(t)$ is generated by finite linear combinations of the functionals (21). For every $t \in [0, 2\pi)^N$ we denote by $\mathcal{K}(t)$ the space of the elements of the form $\sum_{k\in I} \alpha_k\ \zeta_k(t)$ with $\{\alpha_k\}_{k\in I} \in \ell^2(I)$. This is a Hilbert space with the inner product induced by the isomorphism with $\ell^2(I)$. In other words the inner product is induced by the "formal" conditions $(\zeta_k(t); \zeta_h(t))_t := \delta_{k,h}$. All the Hilbert spaces $\mathcal{K}(t)$ have the same dimension which is the cardinality of the system $\{\psi_k\}_{k\in I}$.

Proposition 6.3. *For all $t \in [0, 2\pi)^N$ the inclusions $\Phi^*(t) \subset \mathcal{K}(t) \subset \Phi^*$ hold true. Moreover the generalized Bloch-Floquet transform $\mathcal{U}_{\mathfrak{S}}|_t$ extends to a unitary isomorphism between the Hilbert space $\mathbb{H} \subset \mathcal{H}$ spanned by the orthonormal system $\{\psi_k\}_{k\in I}$ and the Hilbert space $\mathcal{K}(t) \subset \Phi^*$ spanned by $\{\zeta_k(t)\}_{k\in I}$ (assumed as orthonormal basis).*

Proof. The first inclusion $\Phi^*(t) \subset \mathcal{K}(t)$ follows from the definition. For the second inclusion we need to prove that $\omega(t) := \sum_{k\in I} \alpha_k\ \zeta_k(t)$ is a continuous functional if $\{\alpha_k\}_{k\in I} \in \ell^2(\mathbb{N})$. Let $\phi = \sum_{0\leqslant h,|c|\leqslant m} \beta_{h,c}\ U^c\psi_h$ be an element of $\Phi_m \subset \Phi$ then, from the sesquilinearity of the dual pairing and the Cauchy-Schwarz inequality it follows that

$$|\langle\omega(t); \phi\rangle|^2 \leqslant \Big(\sum_{k\in I} |\alpha_k|\ |\langle(\mathcal{U}_{\mathfrak{S}}\psi_k)(t); \phi\rangle|\Big)^2 \leqslant \|\alpha\|^2_{\ell^2} \sum_{k\in I} |\langle(\mathcal{U}_{\mathfrak{S}}\psi_k)(t); \phi\rangle|^2 \qquad (23)$$

where $\|\alpha\|^2_{\ell^2} = \sum_{k\in I} |\alpha_k|^2 < \infty$.

From equation (18) it is clear that $\langle(\mathcal{U}_{\mathfrak{S}}\psi_k)(t); \phi\rangle = 0$ if $\psi_k \notin \Phi_m$, then equation (20) and $C_{\psi_k} = 1$ imply $|\langle\omega(t); \phi\rangle| \leqslant \|\alpha\|_{\ell^2}\sqrt{m}\ p_m(\phi)$. This inequality shows that $\omega(t)$ is a continuous functional when it is restricted to each subspace Φ_m and, because the strict inductive limit topology, this proves that $\omega(t)$ lies in Φ^*.

As for the second claim, consider $\omega_n(t) := \sum_{0\leqslant k\leqslant n} \alpha_k\ \zeta_k(t)$. Obviously $\omega_n(t) = (\mathcal{U}_{\mathfrak{S}}\varphi_n)(t) \in \Phi^*(t)$ since $\varphi_n := \sum_{0\leqslant k\leqslant n} \alpha_k\ \psi_k \in \Phi$. Moreover the inequality (23) can be used to show that $(\mathcal{U}_{\mathfrak{S}}\varphi_n)(t) \to \omega(t)$ when $n \to \infty$ with respect to the weak-$*$ topology of Φ^*. This enables us to define $\omega(t) := (\mathcal{U}_{\mathfrak{S}}\varphi)(t)$ for all $\varphi := \sum_{k\in I} \alpha_k\ \psi_k \in \mathbb{H}$. The generalized Bloch-Floquet transform acts as a unitary isomorphism between $\mathbb{H}$ and $\mathcal{K}(t)$ with respect to the Hilbert structure induced in $\mathcal{K}(t)$ by the orthonormal basis $\{\zeta_k(t)\}_{k\in I}$. □

Theorem 6.4 (Bloch-Floquet spectral decomposition). *Let $\mathfrak{S}$ be a $\mathbb{Z}^N$-algebra in the separable Hilbert space $\mathcal{H}$ with generators $\{U_1, \ldots, U_N\}$, wandering system $\{\psi_k\}_{k\in I}$ and wandering nuclear space Φ. The generalized Bloch-Floquet transform $\mathcal{U}_{\mathfrak{S}}$, defined on Φ by equation* (16)*, induces a direct integral decomposition of the Hilbert space $\mathcal{H}$ which is equivalent* (*in the sense of Theorem* 3.3) *to the decomposition of von Neumann's theorem* (*Theorem* 3.1)*. Moreover, the spaces $\mathcal{K}(t)$ spanned in Φ^* by the functionals* (21) *provide an explicit realization for the family of common eigenspaces of $\mathfrak{S}$ appearing in Maurin's theorem* (*Theorem* 4.1).

Proof. Proposition 5.5 assures that the Gel'fand spectrum of $\mathfrak{S}$ is the N-dimensional torus $\mathbb{T}^N$ and the basic measure agrees with the normalized Haar measure dz. On the field of Hilbert spaces $\prod_{t\in\mathbb{T}^N}\mathcal{K}(t)$ we can introduce a measurable structure by the fundamental family of orthonormal vector fields $\{\zeta_k(\cdot)\}_{k\in I}$ defined by (21). For all $\varphi\in\Phi$ the generalized Bloch-Floquet transform defines a square integrable vector field $(\mathcal{U}_{\mathfrak{S}}\varphi)(\cdot)\in\mathfrak{K}:=\int_{\mathbb{T}^N}^{\oplus}\mathcal{K}(t)\,dz(t)$. Indeed equation (22) shows that $(\mathcal{U}_{\mathfrak{S}}\varphi)(t)\in\mathcal{K}(t)$ for any t and $\|(\mathcal{U}_{\mathfrak{S}}\varphi)(t)\|_t^2=\sum_{k\in I}^{\mathrm{fin}}|f_{\varphi;k}(t)|^2$ is a continuous function (finite sum of continuous functions) hence integrable on $\mathbb{T}^N$. In particular

$$\begin{aligned}\|(\mathcal{U}_{\mathfrak{S}}\varphi)(\cdot)\|_{\mathfrak{K}}^2&=\int_{\mathbb{T}^N}\|(\mathcal{U}_{\mathfrak{S}}\varphi)(t)\|_t^2\;dz(t)\\&=\sum_{k\in I}\int_{\mathbb{T}^N}\underbrace{\left(\sum_{b,c\in\mathbb{Z}^N}^{\mathrm{fin}}\overline{\alpha}_{k,b}\alpha_{k,c}\;z^{c-b}(t)\right)}_{=|f_{\varphi;k}(x)|^2}\;dz(t)=\|\varphi\|_{\mathcal{H}}^2.\end{aligned}$$

In view of the density of Φ, $\mathcal{U}_{\mathfrak{S}}$ can be extended to an isometry from $\mathcal{H}$ to $\mathfrak{K}$.

It remains to show that $\mathcal{U}_{\mathfrak{S}}$ is surjective. Any square integrable vector field $\varphi(\cdot)\in\mathfrak{K}$ is uniquely characterized by its expansion on the basis $\{\zeta_k(\cdot)\}_{k\in I}$, i.e., $\varphi(\cdot)=\sum_{k\in N}\widehat{\varphi}_k(\cdot)\;\zeta_k(\cdot)$ where $\{\widehat{\varphi}_k(t)\}_{k\in I}\in\ell^2(\mathbb{N})$ for all $t\in[0,2\pi)^N$. The condition

$$\|\varphi(\cdot)\|_{\mathfrak{K}}^2=\int_{\mathbb{T}^N}\sum_{k\in I}|\widehat{\varphi}_k(t)|^2\;dz(t)<+\infty$$

shows that $\widehat{\varphi}_k\in L^2(\mathbb{T}^N)$ for all $k\in I$. Let $\widehat{\varphi}_k(t)=\sum_{b\in\mathbb{Z}^N}\alpha_{k,b}z^b(t)$ be the Fourier expansion of $\widehat{\varphi}_k$. Since

$$\sum_{k\in I}\sum_{b\in\mathbb{Z}^N}|\alpha_{k,b}|^2=\sum_{k\in I}\|\widehat{\varphi}_k\|_{L^2(\mathbb{T}^N)}^2=\|\varphi(\cdot)\|_{\mathfrak{K}}^2<+\infty$$

it follows that $\{\alpha_{k,b}\}_{k\in I,b\in\mathbb{Z}^N}$ is an ℓ^2-sequences and the mapping

$$\varphi(\cdot)=\sum_{k\in\mathbb{N}}\sum_{b\in\mathbb{Z}^N}\alpha_{k,b}\;z^b(\cdot)\;\zeta_k(\cdot)\qquad\overset{\mathcal{U}_{\mathfrak{S}}{}^{-1}}{\longmapsto}\qquad\varphi:=\sum_{k\in I}\sum_{b\in\mathbb{Z}^N}\alpha_{k,b}\;U^b\psi_k\tag{24}$$

defines an element $\varphi\in\mathcal{H}$ starting from the vector field $\varphi(\cdot)\in\mathfrak{K}$. It is immediate to check that $\mathcal{U}_{\mathfrak{S}}$ maps φ in $\varphi(\cdot)$, hence $\mathcal{U}_{\mathfrak{S}}$ is surjective.

If $A_f\in\mathfrak{S}$ is an operator associated with the continuous function $f\in C(\mathbb{T}^N)$ via the Gel'fand isomorphism, then $\mathcal{U}_{\mathfrak{S}}A_f\mathcal{U}_{\mathfrak{S}}{}^{-1}\varphi(\cdot)=f(\cdot)\varphi(\cdot)$, i.e., $\mathcal{U}_{\mathfrak{S}}$ maps $A_f\in\mathfrak{S}$ in $M_f(\cdot)\in C(\mathfrak{K})$. This allows us to apply the Theorem 3.3 which assures that the direct integral $\mathfrak{K}$ coincides, up to a decomposable unitary transform, with the spectral decomposition of $\mathfrak{S}$ established in Theorem 3.1. □

The generalized Bloch-Floquet transform $\mathcal{U}_{\mathfrak{S}}$ can be seen as a "computable" realization of the abstract $\mathfrak{S}$-Fourier transform $\mathcal{F}_{\mathfrak{S}}$. From Proposition 6.3 and from

general results about direct integrals (see [Dix81] Part II, Chapter 1, Section 8) one obtains the following identifications:

$$\mathcal{H} \xrightarrow{\mathcal{U}_{\mathfrak{S}} \ldots \mathcal{U}_{\mathfrak{S}}{}^{-1}} \int_{\mathbb{T}^N}^{\oplus} \mathcal{K}(t)\, dz(t) \simeq \int_{\mathbb{T}^N}^{\oplus} \mathbb{H}\, dz(t) \simeq L^2(\mathbb{T}^N, \mathbb{H}). \tag{25}$$

Since the dimension of $\mathbb{H}$ is the cardinality of the wandering system chosen to define the Bloch-Floquet transform, and since Theorem 3.3 assures that the direct integral decomposition is essentially unique (in measure theoretic sense), one has the following:

Corollary 6.5. *Any two wandering systems associated with a $\mathbb{Z}^N$-algebra $\mathfrak{S}$ have the same cardinality. Any two wandering systems for $\mathfrak{S}$ are intertwined by a unitary operator which commutes with $\mathfrak{S}$.*

Example 6.6 (Periodic systems, part three). In the case of Example 2.1, the Bloch-Floquet transform is the usual one (see [Kuc93], [Pan07])

$$(\mathcal{U}_{\mathfrak{S}_T}\varphi)(t,y) := \sum_{m\in\Gamma} z^{-m}(t)\, T^m\varphi(y) = \sum_{m\in\Gamma} \mathrm{e}^{-im_1t_1} \ldots \mathrm{e}^{-im_dt_d}\varphi(y-m),$$

where $m := \sum_{j=1}^{d} m_j\gamma_j$, for all φ in the wandering nuclear space $\Phi \subset L^2(\mathbb{R}^d)$, built according to Proposition 6.1 from any orthonormal basis of $L^2(\mathcal{Q}_0)$. The fiber spaces in the direct integral decomposition are all unitarily equivalent to $L^2(\mathcal{Q}_0)$ hence the Hilbert space decomposition is

$$L^2(\mathbb{R}^d) \xrightarrow{\mathcal{U}_{\mathfrak{S}_T} \ldots \mathcal{U}_{\mathfrak{S}_T}{}^{-1}} \int_{\mathbb{T}^d}^{\oplus} L^2(\mathcal{Q}_0)\, dz(t). \qquad \blacktriangleleft\triangleright$$

Example 6.7 (Mathieu-like Hamiltonians, part three). In this case the wandering nuclear space Φ is the set of the finite linear combinations of the Fourier basis $\{e_n\}_{n\in\mathbb{Z}}$ and for all $g(\theta) = \sum_{n\in\mathbb{Z}}^{\mathrm{fin}} \alpha_n \mathrm{e}^{in\theta}$ in Φ the Bloch-Floquet transform is

$$(\mathcal{U}_{\mathfrak{S}^q_{\mathrm{M}}}\, g)(\theta,t) := \sum_{m\in\mathbb{Z}} \mathrm{e}^{-imt}\ \mathfrak{w}^m g(\theta) = \sum_{n\in\mathbb{Z}}^{\mathrm{fin}} \alpha_n \left(\sum_{m\in\mathbb{Z}} \mathrm{e}^{i[n\theta + m(q\theta - t)]} \right).$$

The collection $\zeta_k(\cdot;t) \in \Phi^*$, given by $\zeta_k(\theta;t) := \mathrm{e}^{ik\theta} \sum_{m\in\mathbb{Z}} \mathrm{e}^{im(q\theta-t)}$ with $k = 0, \ldots, q-1$, defines a fundamental family of orthonormal fields. The fiber spaces in the direct integral decomposition are all unitarily equivalent to $\mathbb{C}^q$ hence the Hilbert space decomposition is

$$L^2(\mathbb{T}) \xrightarrow{\mathcal{U}_{\mathfrak{S}^q_{\mathrm{M}}} \ldots \mathcal{U}_{\mathfrak{S}^q_{\mathrm{M}}}{}^{-1}} \int_{\mathbb{T}}^{\oplus} \mathbb{C}^q\, dz(t).$$

The images of the generators $\mathfrak{u}$ and $\mathfrak{v}$ under the map $\mathcal{U}_{\mathfrak{S}^q_{\mathrm{M}}} \dots \mathcal{U}^{-1}_{\mathfrak{S}^q_{\mathrm{M}}}$ are the two t dependent $q \times q$ matrices

$$\mathfrak{u}(t) := \begin{pmatrix} 0 & & & \mathrm{e}^{it} \\ 1 & \ddots & & \\ & \ddots & \ddots & \\ 0 & & 1 & 0 \end{pmatrix} \qquad \mathfrak{v}(t) := \begin{pmatrix} 1 & & & \\ & \mathrm{e}^{-i2\pi\frac{p}{q}} & & \\ & & \ddots & \\ & & & \mathrm{e}^{-i2\pi\frac{p}{q}(q-1)} \end{pmatrix}.$$

For every $t \in \mathbb{T}$ the matrices $\mathfrak{u}(t)$ and $\mathfrak{v}(t)$ generate a faithful irreducible representation of the C^*-algebra $\mathfrak{A}^{p/q}_{\mathrm{M}}$ on the Hilbert space $\mathbb{C}^q$ (see [Boc01] Theorem 1.9). ◀▷

7. Emergent geometry

From a geometric viewpoint, the field of Hilbert spaces $\mathfrak{F} := \prod_{x\in X} \mathcal{H}(x)$ can be regarded as a pseudo vector-bundle $\mathscr{E} \xrightarrow{\pi} X$, where

$$\mathscr{E} := \bigsqcup_{x\in X} \mathcal{H}(x) \tag{26}$$

is the disjoint union of the Hilbert spaces $\mathcal{H}(x)$. The use of the prefix "pseudo" refers to the fact that more ingredients are needed to turn $\mathscr{E} \xrightarrow{\pi} X$ into a vector bundle. First of all, the map π must be continuous, which requires a topology on $\mathscr{E}$. As a first attempt, assuming that $\mathcal{H}(x) \subset \Phi^*$ for every $x \in X$, one might consider $\mathscr{E} \xrightarrow{\pi} X$ as a sub-bundle of the trivial vector bundle $X \times \Phi^* \xrightarrow{\pi} X$, equipped with the topology induced by the inclusion, so that $\mathscr{E} \xrightarrow{\pi} X$ becomes a topological bundle whose fibers are Hilbert spaces. However, nothing ensures that the Hilbert space topology defined fiberwise is compatible with the topology of $\mathscr{E}$, a necessary condition to have a meaningful topological theory.

Geometric vs. analytic viewpoint

We begin our analysis with the definition of topological fibration of Hilbert spaces. Following [FD88] (Chapter II, Section 13) we pose the following

Definition 7.1 (Geometric viewpoint: Hilbert bundle). *A* Hilbert bundle *is the datum of a topological Hausdorff spaces $\mathscr{E}$ (the* total space*), a compact Hausdorff space X (the* base space*) and a map $\mathscr{E} \xrightarrow{\pi} X$ (the* canonical projection*) which is a continuous open surjection such that:*

a) *for all $x \in X$ the fiber $\pi^{-1}(x) \subset \mathscr{E}$ is a Hilbert space;*
b) *the map $\mathscr{E} \ni p \longmapsto \|p\| \in \mathbb{C}$ is continuous;*
c) *the operation $+$ is continuous as a function on $\mathscr{S} := \{(p, s) \in \mathscr{E} \times \mathscr{E} \ : \ \pi(p) = \pi(s)\}$ to $\mathscr{E}$;*
d) *for each $\lambda \in \mathbb{C}$ the map $\mathscr{E} \ni p \longmapsto \lambda\, p \in \mathscr{E}$ is continuous;*

e) *let* 0_x *be the null vector in the Hilbert space* $\pi^{-1}(x)$*; for each* $x \in X$*, the collection of all subsets of* $\mathscr{E}$ *of the form* $\mathscr{U}(O, x, \varepsilon) := \{p \in \mathscr{E} \ : \ \pi(p) \in O, \ \ \|p\| < \varepsilon\}$*, where* O *is a neighborhood of* x *and* $\varepsilon > 0$*, is a basis of neighborhoods of* $0_x \in \pi^{-1}(x)$ *in* $\mathscr{E}$*.*

We denote by the short symbol $\mathscr{E}_{\pi,X}$ the Hilbert bundle $\mathscr{E} \xrightarrow{\pi} X$. A *section* of $\mathscr{E}_{\pi,X}$ is a function $\psi : X \to \mathscr{E}$ such that $\pi \circ \psi = \mathrm{id}_X$. We denote by $\Gamma(\mathscr{E}_{\pi,X})$ the set of all *continuous sections* of $\mathscr{E}_{\pi,X}$. As shown in [FD88], from Definition 7.1 it follows that: (i) the scalar multiplication $\mathbb{C} \times \mathscr{E} \ni (\lambda, p) \mapsto \lambda \, p \in \mathscr{E}$ is continuous; (ii) the open sets of $\mathscr{E}$, restricted to a fiber $\pi^{-1}(x)$, generate the Hilbert space topology of $\pi^{-1}(x)$; (iii) the set $\Gamma(\mathscr{E}_{\pi,X})$ has the structure of a (left) $C(X)$-module. In other words, the definition of Hilbert bundle includes all the conditions which a "formal" fibration such as (26) needs to fulfill to be a topological fibration with a topology compatible with the Hilbert structure of the fibers. In this sense the Hilbert bundle is the "geometric object" of our interest.

However, the structure that emerges in a natural way from the Bloch-Floquet decomposition (Theorem 6.4) is more easily understood from the analytic viewpoint. Switching the focus from the total space $\mathscr{E}$ to the space of sections $\mathfrak{F}$, the relevant notion is that of *continuous field of Hilbert spaces*, according to [Dix82] (Section 10.1) or [DD63] (Section 1).

Definition 7.2 (Analytic viewpoint: continuous field of Hilbert spaces). *Let* X *be a compact Hausdorff space and* $\mathfrak{F} := \prod_{x \in X} \mathcal{H}(x)$ *a field of Hilbert spaces. A* continuous structure on $\mathfrak{F}$ *is the datum of a linear subspace* $\Gamma \subset \mathfrak{F}$ *such that:*

a) *for each* $x \in X$ *the set* $\{\sigma(x) \ : \ \sigma(\cdot) \in \Gamma\}$ *is dense in* $\mathcal{H}(x)$*;*
b) *for any* $\sigma(\cdot) \in \Gamma$ *the map* $X \ni x \mapsto \|\sigma(x)\|_x \in \mathbb{R}$ *is continuous;*
c) *if* $\psi(\cdot) \in \mathfrak{F}$ *and if for each* $\varepsilon > 0$ *and each* $x_0 \in X$*, there is some* $\sigma(\cdot) \in \Gamma$ *such that* $\|\sigma(x) - \psi(x)\|_x < \varepsilon$ *on a neighborhood of* x_0*, then* $\psi(\cdot) \in \Gamma$*.*

We denote by the short symbol $\mathfrak{F}_{\Gamma,X}$ the field of Hilbert spaces $\mathfrak{F}$ endowed with the continuous structure Γ. The elements of Γ are called *continuous vector fields*. The condition b) may be replaced by the requirement that for any $\sigma(\cdot), \varrho(\cdot) \in \Gamma$, the function $X \ni x \mapsto (\sigma(x); \varrho(x))_x \in \mathbb{C}$ is continuous. Condition c) is called *locally uniform closure* and guarantees that the linear space Γ is stable under multiplication by continuous functions on X. This condition implies that Γ is a *(left) $C(X)$-module*. A *total set* of continuous vector fields for $\mathfrak{F}_{\Gamma,X}$ is a subset $\Lambda \subset \Gamma$ such that $\Lambda(x) := \{\sigma(x) \ : \ \sigma(\cdot) \in \Lambda\}$ is dense in $\mathcal{H}(x)$ for all $x \in X$. The continuous field of Hilbert spaces is said to be *separable* if it has a countable total set of continuous vector fields.

The link between the notion of continuous field of Hilbert spaces and that of Hilbert bundle is clarified by the following result.

Proposition 7.3 (Equivalence between geometric and analytic viewpoint [DD63], [FD88]). *Let* $\mathfrak{F}_{\Gamma,X}$ *be a continuous field of Hilbert spaces over the compact Hausdorff space* X*. Let* $\mathscr{E}(\mathfrak{F}_{\Gamma,X}) := \bigsqcup_{x \in X} \mathcal{H}(x)$ *be the disjoint union of the Hilbert*

spaces $\mathcal{H}(x)$ and π the canonical surjection of $\mathscr{E}(\mathfrak{F}_{\Gamma,X})$ onto X. Then there exists a unique topology $\mathcal{T}$ on $\mathscr{E}(\mathfrak{F}_{\Gamma,X})$ making $\mathscr{E}(\mathfrak{F}_{\Gamma,X}) \xrightarrow{\pi} X$ a Hilbert bundle over X such that all the continuous vector fields in $\mathfrak{F}_{\Gamma,X}$ are continuous sections of $\mathscr{E}(\mathfrak{F}_{\Gamma,X})$. Moreover, every Hilbert bundle comes from a continuous field of Hilbert spaces.

For the proof we refer to [DD63] (Section 2) or [FD88] (Chapter II, Theorem 13.18). We say that the set $\mathscr{E}(\mathfrak{F})$ endowed with the topology $\mathcal{T}$ and the canonical surjection π is the Hilbert bundle associated with the continuous structure Γ of $\mathfrak{F}$.

Triviality, local triviality and vector bundle structure

A Hilbert bundle is a generalization of a (infinite-dimensional) vector bundle, in the sense that some other extra conditions are needed in order to turn it into a genuine vector bundle. For the axioms of vector bundle we refer to [Lan85]. The most relevant missing condition is the *local triviality property.*

Two Hilbert bundles $\mathscr{E}_{\pi,X}$ and $\mathscr{F}_{\tau,X}$ over the same base space X are said to be (isometrically) isomorphic if there exists a homeomorphism $\Theta : \mathscr{E} \to \mathscr{F}$ such that a) $\tau \circ \Theta = \pi$, b) $\Theta_x := \Theta|_{\pi^{-1}(x)}$ is a unitary map from the Hilbert space $\pi^{-1}(x)$ to the Hilbert space $\tau^{-1}(x)$. From the definition it follows that if the Hilbert bundles $\mathscr{E}_{\pi,X}$ and $\mathscr{F}_{\tau,X}$ are isomorphic then the map $\Gamma(\mathscr{E}_{\pi,X}) \ni \sigma \mapsto \Theta \circ \sigma \in \Gamma(\mathscr{F}_{\tau,X})$ is one to one. A Hilbert bundle is said to be *trivial* if it is isomorphic to the *constant* Hilbert bundle $X \times \mathbb{H} \to X$ where $\mathbb{H}$ is a fixed Hilbert space. It is called *locally trivial* if for every $x \in X$ there is a neighborhood O of x such that the *reduced Hilbert bundle* $\mathscr{E}|_O := \{p \in \mathscr{E} : \pi(p) \in O\} = \pi^{-1}(O)$ is isomorphic to the constant Hilbert bundle $O \times \mathbb{H} \to O$. Two continuous fields of Hilbert spaces $\mathfrak{F}_{\Gamma,X}$ and $\mathfrak{G}_{\Delta,X}$ over the same space X are said to be (isometrically) isomorphic if the associated Hilbert bundles $\mathscr{E}(\mathfrak{F}_{\Gamma,X})$ and $\mathscr{E}(\mathfrak{G}_{\Delta,X})$ are isomorphic. A continuous field of Hilbert spaces $\mathfrak{F}_{\Gamma,X}$ is said to be trivial (resp. locally trivial) if $\mathscr{E}(\mathfrak{F}_{\Gamma,X})$ is trivial (resp. locally trivial).

Proposition 7.4 ([FD88], [DD63]). *Let $\mathfrak{F}_{\Gamma,X}$ be a continuous field of Hilbert spaces over the compact Hausdorff space X and $\mathscr{E}(\mathfrak{F}_{\Gamma,X})$ the associated Hilbert bundle. Then:*

(i) *if $\mathfrak{F}_{\Gamma,X}$ is separable and X is second-countable (or equivalently metrizable) then the topology defined on the total space $\mathscr{E}(\mathfrak{F})$ is second-countable;*
(ii) *if $\dim \mathcal{H}(x) = \aleph_0$ for all $x \in X$ and if X is a finite-dimensional manifold then the Hilbert bundle $\mathscr{E}(\mathfrak{F}_{\Gamma,X})$ is trivial;*
(iii) *if $\dim \mathcal{H}(x) = q < +\infty$ for all $x \in X$ then the Hilbert bundle $\mathscr{E}(\mathfrak{F}_{\Gamma,X})$ is a Hermitian vector bundle with typical fiber $\mathbb{C}^q$.*

For the proof of (i) one can see [FD88] (Chapter II, Proposition 13.21). The proof of (ii) is in [DD63] (Theorem 5). As for the proof of (iii), we recall that a Hilbert bundle has the (stronger) structure of a vector bundle whenever the local triviality and the continuity of the transition functions (see [Lan85] Chapter III) hold true. However, if the fibers are finite dimensional then the continuity

of the transition functions follows from the existence of the local trivializations (see [Lan85] Chapter III, Proposition 1), hence one needs only to prove the local triviality. The latter follows from standard arguments, as in the final remark of Section 1 of [DD63].

Algebraic viewpoint

Roughly speaking, a continuous field of Hilbert spaces is an "analytic object" while a Hilbert bundle is a "geometric object". There is also a third point of view which is of algebraic nature. We introduce an "algebraic object" which encodes all the relevant properties of the set of continuous vector fields (or continuous sections).

Definition 7.5 (Algebraic viewpoint: Hilbert module). *A* (left) pre-C^*-module *over a commutative unital C^*-algebra $\mathcal{A}$ is a complex vector space Ω_0 that is also a* (*left*) *$\mathcal{A}$-module endowed with a pairing $\{\cdot;\cdot\} : \Omega_0 \times \Omega_0 \to \mathcal{A}$ satisfying, for $\sigma, \varrho, \varsigma \in \Omega_0$ and for $a \in \mathcal{A}$ the following requirements:*

a) $\{\sigma; \varrho + \varsigma\} = \{\sigma; \varrho\} + \{\sigma; \varsigma\}$;
b) $\{\sigma; a\varrho\} = a\{\sigma; \varrho\}$;
c) $\{\sigma; \varrho\}^* = \{\varrho; \sigma\}$;
d) $\{\sigma; \sigma\} > 0$ *if* $\sigma \neq 0$.

The map $|||\cdot||| : \Omega_0 \to [0, +\infty)$ defined by $|||\sigma||| := \sqrt{\|\{\sigma;\sigma\}\|_{\mathcal{A}}}$ is a norm in Ω_0. The completion Ω of Ω_0 with respect to the norm $|||\cdot|||$ is called (left) C^*-module *or* Hilbert module *over $\mathcal{A}$.*

Proposition 7.6 (Equivalence between algebraic and analytic viewpoint [DD63]). *Let $\mathfrak{F}_{\Gamma,X}$ be a continuous field of Hilbert spaces over the compact Hausdorff space X. The set of continuous vector fields Γ has the structure of a Hilbert module over $C(X)$. Conversely, any Hilbert module over $C(X)$ defines a continuous field of Hilbert spaces. This correspondence is one-to-one.*

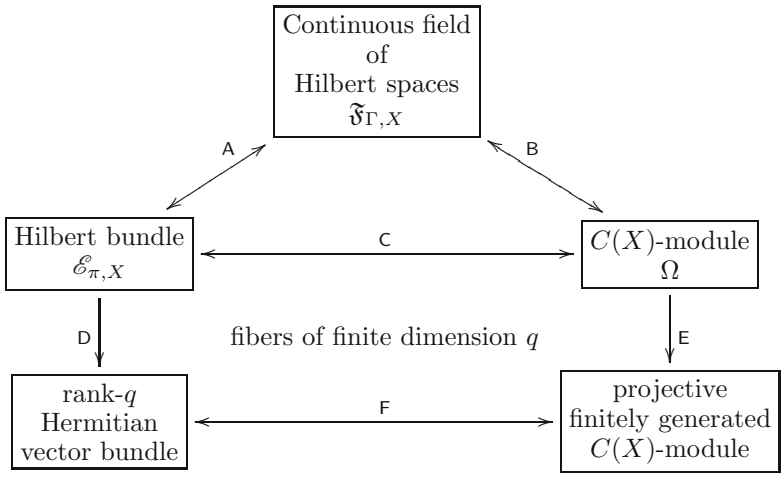
Proof. We shortly sketch the proof, see [DD63] (Section 3) for details. To prove the first part of the statement one observes that for all pairs of continuous vector fields $\sigma(\cdot), \varrho(\cdot) \in \Gamma$ the pairing $\{\cdot;\cdot\} : \Gamma \times \Gamma \to C(X)$ defined fiberwise by the inner product, i.e., by posing $\{\sigma; \varrho\}(x) := (\sigma(x); \varrho(x))_x$, satisfies Definition 7.5. The norm is defined by $|||\sigma||| := \sup_{x\in X} \|\sigma(x)\|_x$ and Γ is closed with respect to this norm in view of the property of locally uniform closure.

Conversely let Ω be a C^*-module over $C(X)$. For all $x \in X$ define a pre-Hilbert structure on Ω by $(\sigma; \varrho)_x := \{\sigma; \varrho\}(x)$. The set $\mathcal{I}_x := \{\sigma \in \Omega : \{\sigma;\sigma\}(x) = 0\}$ is a linear subspace of Ω. On the quotient space $\Omega/\mathcal{I}_x$ the inner product $(\ ;\ )_x$ is a positive definite sesqulinear form and we denote by $\mathcal{H}(x)$ the related Hilbert space. The collection $\{\mathcal{H}(x) : x \in X\}$ defines a field of Hilbert spaces $\mathfrak{F}(\Omega) = \prod_{x\in X} \mathcal{H}(x)$. For all $\sigma \in \Omega$ the canonical projection $\Omega \ni \sigma \overset{J_x}{\longmapsto} \sigma(x) \ni \Omega/\mathcal{I}_x$ defines a vector field $\sigma(\cdot) \in \mathfrak{F}(\Omega)$. It is easy to check that the map $\Omega \ni \sigma \overset{\Gamma}{\longmapsto} \sigma(\cdot) \ni \mathfrak{F}(\Omega)$ is injective. We denote by $\Gamma(\Omega)$ the image of Ω in $\mathfrak{F}(\Omega)$. The family $\Gamma(\Omega)$ defines a continuous structure on $\mathfrak{F}(\Omega)$. Indeed $\{\sigma(x) : \sigma(\cdot) \in \Gamma(\Omega)\} = \Omega/\mathcal{I}_x$ is dense in $\mathcal{H}(x)$ and $\|\sigma(x)\|_x^2 = \{\sigma;\sigma\}(x)$ is continuous. Finally locally uniform closure of $\Gamma(\Omega)$ follows

from the closure of Ω with respect to the norm $|||\sigma||| := \sup_{x\in X}\sqrt{\{\sigma;\sigma\}(x)}$ and the existence of a partition of the unit subordinate to a finite cover of X (since X is compact). □

The Hilbert bundle emerging from the Bloch-Floquet decomposition

Before proceeding with our analysis, it is useful to summarize in the following diagram the relations between the algebraic, the analytic and the geometric descriptions.



(27)

Arrows A and B summarize the content of Propositions 7.3 and 7.6 respectively, arrow D corresponds to point (iii) of Proposition 7.4, and arrow E follows by Proposition 53 in [Lan97]. Arrow F corresponds to the remarkable Serre-Swan Theorem (see [Lan97] Proposition 21), so arrow C can be interpreted as a generalization of the Serre-Swan Theorem.

Coming back to our original problem, let $\{\mathcal{H}, \mathfrak{A}, \mathfrak{S}\}$ be a physical frame with $\mathcal{H}$ a separable Hilbert space and $\mathfrak{S}$ a $\mathbb{Z}^N$-algebra with generators $\{U_1, \dots, U_N\}$ and wandering system $\{\psi_k\}_{k\in I}$. The Bloch-Floquet decomposition (Theorem 6.4) ensures the existence of a unitary map $\mathcal{U}_{\mathfrak{S}}$, which maps $\mathcal{H}$ into the direct integral $\mathfrak{K} := \int_{\mathbb{T}^N}^{\oplus} \mathcal{K}(t)\ dz(t)$. Let $\mathfrak{F} := \prod_{t\in\mathbb{T}^N} \mathcal{K}(t)$ be the corresponding field of Hilbert spaces. The space $\mathfrak{K}$ is a subset of $\mathfrak{F}$ which has the structure of a Hilbert space and whose elements can be seen as L^2-sections of a "pseudo-Hilbert bundle" $\mathscr{E}(\mathfrak{F}) := \bigsqcup_{t\in\mathbb{T}^N} \mathcal{K}(t)$. This justifies the use of the notation $\mathfrak{K} = \Gamma_{L^2}(\mathscr{E})$.

To obtain a topological decomposition, we need to know *a priori* how to select a continuous structure $\Gamma \subset \mathfrak{K}$ for the field of Hilbert spaces $\mathfrak{F}$. In view of Proposition 7.3, this procedure is equivalent to selecting *a priori* the family of the continuous section $\Gamma(\mathscr{E})$ of the Hilbert bundle $\mathscr{E}$ inside the Hilbert space of the L^2-sections $\Gamma_{L^2}(\mathscr{E})$. We can use the generalized Bloch-Floquet transform to push back this problem at the level of the original Hilbert space $\mathcal{H}$ and to adopt

the algebraic viewpoint. With this change of perspective the new, but equivalent, question which we need to answer is: does the physical frame $\{\mathcal{H}, \mathfrak{A}, \mathfrak{S}\}$ select a Hilbert module over $C(\mathbb{T}^N)$ inside the Hilbert space $\mathcal{H}$?

Generalizing an idea of [Gru01], we can use the transform $\mathcal{U}_{\mathfrak{S}}$ and the notion of wandering nuclear space Φ to provide a positive answer. The core of our analysis is the following result.

Proposition 7.7. *Let $\mathfrak{S}$ be a $\mathbb{Z}^N$-algebra in the separable Hilbert space $\mathcal{H}$ with generators $\{U_1, \ldots, U_N\}$, wandering system $\{\psi_k\}_{k\in I}$ and wandering nuclear space Φ. Let $\mathfrak{K}$ be the direct integral defined by the Bloch-Floquet transform $\mathcal{U}_{\mathfrak{S}} : \mathcal{H} \to \mathfrak{K}$. Then the Bloch-Floquet transform endowes Φ with the structure of a (left) pre-C^*-module over $C(\mathbb{T}^N)$. Let $\Omega_{\mathfrak{S}}$ be the completion of Φ with respect to the C^*-module norm. Then $\Omega_{\mathfrak{S}}$ is a Hilbert module over $C(\mathbb{T}^N)$ such that $\Omega_{\mathfrak{S}} \subset \mathcal{H}$.*

Proof. The set Φ is a complex vector space which can be endowed with the structure of a $C(\mathbb{T}^N)$-module by means of the Gel'fand isomorphism. For any $f \in C(\mathbb{T}^N)$ and $\varphi \in \Phi$ we define the (*left*) *module product* $\star$ by

$$C(\mathbb{T}^N) \times \Phi \ni (f, \varphi) \longmapsto f \star \varphi := A_f \varphi \in \Phi \tag{28}$$

where $A_f \in \mathfrak{S}$ is the operator associated with $f \in C(\mathbb{T}^N)$. The product is well defined since Φ is $\mathfrak{S}$-invariant by construction. The Bloch-Floquet transform allows us also to endow Φ with a pairing $\{\cdot;\cdot\} : \Phi \times \Phi \to C(\mathbb{T}^N)$. Indeed, for any pair $\varphi, \phi \in \Phi$ and for all $t \in \mathbb{T}^n$ we define a sesquilinear form

$$\Phi \times \Phi \ni (\varphi, \phi) \longmapsto \{\varphi, \phi\}(t) := ((\mathcal{U}_{\mathfrak{S}}\varphi)(t); (\mathcal{U}_{\mathfrak{S}}\phi)(t))_t \in \mathbb{C}. \tag{29}$$

Moreover $\{\varphi, \phi\}(t)$ is a continuous function of t. Indeed $\varphi, \phi \in \Phi$ means that φ and ϕ are finite linear combinations of the vectors $U^a\psi_k$ and from equation (24) and the orthonormality of the fundamental vector fields $\zeta_k(\cdot)$ it follows that $\{\varphi, \phi\}(t)$ consists of a finite linear combination of the exponentials $\mathrm{e}^{it_1}, \ldots, \mathrm{e}^{it_N}$.

Endowed with the operations (28) and (29), the space Φ becomes a (left) pre-C^*-module over $C(\mathbb{T}^N)$. The Hilbert module $\Omega_{\mathfrak{S}}$ is defined to be the completion of Φ with respect to the norm

$$|||\varphi|||^2 := \sup_{t\in\mathbb{T}^N} \|(\mathcal{U}_{\mathfrak{S}}\varphi)(t)\|_t^2 = \sup_{t\in\mathbb{T}^N} \left(\sum_{k\in I}^{\text{fin}} |f_{\varphi;k}(t)|^2 \right) \tag{30}$$

according to the notation in the proof of Theorem 6.4. Let $\{\varphi_n\}_{n\in\mathbb{N}}$ be a sequence in Φ which is Cauchy with respect to the norm $|||\cdot|||$. From (30), the unitarity of $\mathcal{U}_{\mathfrak{S}}$ and the normalization of the Haar measure dz on $\mathbb{T}^N$ it follows that $\|\varphi_n - \varphi_m\|_{\mathcal{H}} \leqslant |||\varphi_n - \varphi_m|||$, hence $\{\varphi_n\}_{n\in\mathbb{N}}$ is also Cauchy with respect to the norm $\|\cdot\|_{\mathcal{H}}$, so the limit $\varphi_n \to \varphi$ is an element of $\mathcal{H}$. □

Once the Hilbert module $\Omega_{\mathfrak{S}}$ is selected, we can use it to define a continuous field of Hilbert spaces as explained in Proposition 7.6. It is easy to convince oneself that the abstract construction proposed in Proposition 7.6 is concretely

implemented by the generalized Bloch-Floquet transform $\mathcal{U}_{\mathfrak{S}}$. Then the set of vector fields $\Gamma_{\mathfrak{S}} := \mathcal{U}_{\mathfrak{S}}(\Omega_{\mathfrak{S}})$ defines a continuous structure on the field of Hilbert spaces $\mathfrak{F} := \prod_{t\in\mathbb{T}^N} \mathcal{K}(t)$ and, in view of Proposition 7.3, a Hilbert bundle over the base manifold $\mathbb{T}^N$. This Hilbert bundle, which we will denote by $\mathscr{E}_{\mathfrak{S}}$, is the set $\bigsqcup_{t\in\mathbb{T}^N} \mathcal{K}(t)$ equipped by the topology prescribed by the set of the continuous sections $\Gamma_{\mathfrak{S}}$. The structure of $\mathscr{E}_{\mathfrak{S}}$ depends only on the equivalence class of the physical frame $\{\mathcal{H}, \mathfrak{A}, \mathfrak{S}\}$ and we will refer to it as the *Bloch-Floquet Hilbert bundle*.

Theorem 7.8 (Emerging geometric structure). *Let $\mathfrak{S}$ be a $\mathbb{Z}^N$-algebra in the separable Hilbert space $\mathcal{H}$ with generators $\{U_1, \dots, U_N\}$, wandering system $\{\psi_k\}_{k\in I}$ and wandering nuclear space Φ. Let $\mathfrak{K}$ be the direct integral defined by the Bloch-Floquet transform $\mathcal{U}_{\mathfrak{S}} : \mathcal{H} \to \mathfrak{K}$ and $\Omega_{\mathfrak{S}} \subset \mathcal{H}$ the Hilbert module over $C(\mathbb{T}^N)$ defined in Proposition* 7.7*. Then:*

(i) *the family of vector fields $\mathcal{U}_{\mathfrak{S}}(\Omega_{\mathfrak{S}}) =: \Gamma_{\mathfrak{S}}$ defines a continuous structure on $\mathfrak{F} = \Pi_{t\in\mathbb{T}^N}\mathcal{K}(t)$ which realizes the correspondence stated in Proposition* 7.6*;*

(ii) *the Bloch-Floquet Hilbert bundle $\mathscr{E}_{\mathfrak{S}}$, defined by $\Gamma_{\mathfrak{S}}$ according to Proposition* 7.3*, depends only on the equivalence class of the physical frame $\{\mathcal{H}, \mathfrak{A}, \mathfrak{S}\}$.*

Proof. To prove (i) let $\mathcal{I}_t := \{\varphi \in \Phi \ : \ ((\mathcal{U}_{\mathfrak{S}}\varphi)(t); (\mathcal{U}_{\mathfrak{S}}\varphi)(t))_t = 0\}$. The space $\Phi/\mathcal{I}_t$ is a pre-Hilbert space with respect to the scalar product induced by $\mathcal{U}_{\mathfrak{S}}|_t$. The map $\mathcal{U}_{\mathfrak{S}}|_t : \Phi/\mathcal{I}_t \to \mathcal{K}(t)$ is obviously isometric and so can be extended to a linear isometry from the norm-closure of $\Phi/\mathcal{I}_t$ into $\mathcal{K}(t)$. The map $\mathcal{U}_{\mathfrak{S}}|_t$ is also surjective, indeed $\mathcal{K}(t)$ is generated by the orthonormal basis $\{\zeta_k(t)\}_{k\in I}$ and ${\mathcal{U}_{\mathfrak{S}}|_t}^{-1}\zeta_k(t) = \psi_k \in \Phi/\mathcal{I}_t$. Then the fiber Hilbert spaces appearing in the proof of Proposition 7.6 coincide, up to a unitary equivalence, with the fiber Hilbert spaces $\mathcal{K}(t)$ obtained through the Bloch-Floquet decomposition. Moreover the Bloch-Floquet transform acts as the map defined in the proof of Proposition 7.6, which sends any element of the Hilbert module Φ to a continuous section of $\mathfrak{F}$.

To prove (ii) let $\{\mathcal{H}_1, \mathfrak{A}_1, \mathfrak{S}_1\}$ and $\{\mathcal{H}_2, \mathfrak{A}_2, \mathfrak{S}_2\}$ be two physical frames related by a unitary map $U : \mathcal{H}_1 \to \mathcal{H}_2$. If $\mathfrak{S}_1$ is a $\mathbb{Z}^N$-algebra in $\mathcal{H}_1$ then also $\mathfrak{S}_2 = U\mathfrak{S}_1U^{-1}$ is a $\mathbb{Z}^N$-algebra in $\mathcal{H}_2$ and if $\{\psi_k\}_{k\in I} \subset \mathcal{H}_1$ is a wandering system for $\mathfrak{S}_1$ then $\{\widetilde{\psi}_k := U\psi_k\}_{k\in I} \subset \mathcal{H}_2$ is a wandering system for $\mathfrak{S}_2$ (with the same cardinality). The two wandering nuclear spaces $\Phi_1 \subset \mathcal{H}_1$ and $\Phi_2 \subset \mathcal{H}_2$ are related by $\Phi_2 = U\Phi_1$. Let $\mathcal{U}_{\mathfrak{S}_1} : \mathcal{H}_1 \to \mathfrak{H}_1$ and $\mathcal{U}_{\mathfrak{S}_2} : \mathcal{H}_2 \to \mathfrak{H}_2$ be the two generalized Bloch-Floquet transforms defined by the two equivalent physical frames. From the explicit expression of $\mathcal{U}_{\mathfrak{S}_2}$ and ${\mathcal{U}_{\mathfrak{S}_1}}^{-1}$, and in accordance with Corollary 3.4, one argues that $\mathcal{U}_{\mathfrak{S}_2} \circ U \circ {\mathcal{U}_{\mathfrak{S}_1}}^{-1} =: W(\cdot)$ is a decomposable unitary which is well defined for all t. Let $\varphi, \phi \in \Phi_1$ then

$$\begin{aligned}\{\varphi;\phi\}_1(t) :&= ((\mathcal{U}_{\mathfrak{S}_1}\varphi)(t); (\mathcal{U}_{\mathfrak{S}_1}\phi)(t))_t = (W(t)(\mathcal{U}_{\mathfrak{S}_1}\varphi)(t); W(t)(\mathcal{U}_{\mathfrak{S}_1}\phi)(t))_t \\ &= ((\mathcal{U}_{\mathfrak{S}_2}U\varphi)(t); (\mathcal{U}_{\mathfrak{S}_2}U\phi)(t))_t = \Big((\mathcal{U}_{\mathfrak{S}_2}\widetilde{\varphi})(t); (\mathcal{U}_{\mathfrak{S}_2}\widetilde{\phi})(t)\Big)_t =: \{\widetilde{\varphi};\widetilde{\phi}\}_2(t)\end{aligned}$$

where $\widetilde{\varphi} := U\varphi$ and $\widetilde{\phi} := U\phi$ are elements of Φ_2. This equation shows that Φ_1 and Φ_2 have the same $C(\mathbb{T}^N)$-module structure and so define the same abstract Hilbert

module over $C(\mathbb{T}^N)$. The claim follows from the generalization of the Serre-Swan Theorem summarized by arrow C in (27). □

Remark 7.9. With a proof similar to that of point (ii) of Theorem 7.8, one deduces also that the Bloch-Floquet-Hilbert bundle $\mathscr{E}_{\mathfrak{S}}$ does not depend on the choice of two unitarily (or antiunitarily) equivalent commutative C^*-algebras $\mathfrak{S}_1$ and $\mathfrak{S}_2$ inside $\mathfrak{A}'$. Indeed, also in this case the abstract Hilbert module structure induced by the two Bloch-Floquet transforms $\mathcal{U}_{\mathfrak{S}_1}$ and $\mathcal{U}_{\mathfrak{S}_2}$ is the same. ⧫◊

After defining the topology of the Bloch-Floquet Hilbert bundle, it is natural to deduce more information about its structure. An interesting property arises from the cardinality of the wandering system, which depends only on the physical frame (see Corollary 6.5).

Corollary 7.10. *The Hilbert bundle $\mathscr{E}_{\mathfrak{S}}$ over the torus $\mathbb{T}^N$ defined by the continuous structure $\Gamma_{\mathfrak{S}}$ is trivial if the cardinality of the wandering system is $\aleph_0$, and is a rank-q Hermitian vector bundle if the cardinality of the wandering system is q. In the latter case the transition functions of the vector bundle can be expressed in terms of the fundamental orthonormal frame $\{\zeta_k(\cdot) := (\mathcal{U}_{\mathfrak{S}}\psi_k)\}_{k=1,\ldots,q}$.*

Decomposition of the observables and endomorphism sections

According to Theorem 6.4, the Bloch-Floquet transform (16) provides a concrete realization for the unitary map ($\mathfrak{S}$-Fourier transform) whose existence is claimed by von Neumann's complete spectral theorem. Point (ii) of Theorem 3.1 implies that under the Bloch-Floquet transform any $O \in \mathfrak{A}$ is mapped into a decomposable operator on the direct integral $\int_{\mathbb{T}^N}^{\oplus} \mathcal{K}(t)\, dz(t)$, i.e., $\mathcal{U}_{\mathfrak{S}}\, O\, \mathcal{U}_{\mathfrak{S}}{}^{-1} =: O(\cdot) : t \mapsto O(t) \in \mathscr{B}(\mathcal{K}(t))$ with $O(\cdot)$ weakly mesurable.

The natural question which arises is the following: there exists any topological structure in the C^*-algebra $\mathfrak{A}$ compatible with the Bloch-Floquet Hilbert bundle which emerges from the Bloch-Floquet transform? In order to answer this question, we first analyze the nature of the linear maps which preserve the (Hilbert module) structure of the set of the continuous sections.

Definition 7.11 (Hilbert module endomorphism). *Let Ω be a (left) Hilbert module over the commutative unital C^*-algebra $\mathcal{A}$. An* endomorphism *of Ω is an $\mathcal{A}$-linear map $O : \Omega \to \Omega$ which is* adjointable*, i.e., there exists a map $O^\dagger : \Omega \to \Omega$ such that $\{\sigma; O\rho\} = \{O^\dagger\sigma; \rho\}$ for all $\sigma, \rho \in \Omega$. We denote by $\mathrm{End}_{\mathcal{A}}(\Omega)$ the set of all endomorphisms of Ω.*

As proven in [GVF01] (Section 2.5) or [Lan97] (Appendix A), if $O \in \mathrm{End}_{\mathcal{A}}(\Omega)$, then $O^\dagger \in \mathrm{End}_{\mathcal{A}}(\Omega)$ and $\dagger$ is an involution over $\mathrm{End}_{\mathcal{A}}(\Omega)$. Moreover, $\mathrm{End}_{\mathcal{A}}(\Omega)$ endowed with the *endomorphism norm*

$$\|O\|_{\mathrm{End}(\Omega)} := \sup\{|||O(\sigma)||| \ : \ |||\sigma||| \leqslant 1\} \tag{31}$$

becomes a C^*-algebra (of bounded operators). For any $\sigma, \rho \in \Omega$ one defines the *rank*-1 *endomorphism* $|\sigma\}\{\rho| \in \mathrm{End}_{\mathcal{A}}(\Omega)$ by $|\sigma\}\{\rho|(\varsigma) := \{\rho; \varsigma\}\ \sigma$ for all $\varsigma \in \Omega$.

The adjoint of $|\sigma\}\{\rho|$ is given by $|\rho\}\{\sigma|$. The linear span of the rank-1 endomorphisms is a selfadjoint two-sided ideal of $\mathrm{End}_{\mathcal{A}}(\Omega)$ (*finite rank endomorphisms*) and its (operator) norm closure is denoted by $\mathrm{End}^0_{\mathcal{A}}(\Omega)$. The elements of the latter are called *compact endomorphisms* of Ω. Since $\mathrm{End}^0_{\mathcal{A}}(\Omega)$ is an *essential ideal* of $\mathrm{End}_{\mathcal{A}}(\Omega)$, it follows that $\mathrm{End}^0_{\mathcal{A}}(\Omega) = \mathrm{End}_{\mathcal{A}}(\Omega)$ if and only if $\mathbb{1}_\Omega \in \mathrm{End}^0_{\mathcal{A}}(\Omega)$.

A remarkable result which emerges from the above theory is the characterization of the compact endomorphisms of the $C(X)$ Hilbert module $\Gamma(\mathcal{E})$ of the continuous sections of a rank-q Hermitian vector bundle.

Proposition 7.12. *Let $\mathscr{E} \to X$ be a rank-q Hermitian vector bundle over the compact Hausdorff space X and let $\Gamma(\mathscr{E})$ be the Hilbert module over $C(X)$ of its continuous sections. Then*

$$\mathrm{End}^0_{C(X)}(\Gamma(\mathscr{E})) = \mathrm{End}_{C(X)}(\Gamma(\mathscr{E})) \simeq \Gamma(\mathrm{End}(\mathscr{E})) \tag{32}$$

where $\Gamma(\mathrm{End}(\mathscr{E}))$ denotes the continuous sections of the vector bundle $\mathrm{End}(\mathscr{E}) \to X$. The localization isomorphism *appearing in right-hand side of* (32) *preserves the composition and the structure of $C(X)$-module.*

The proof is a consequence of the Serre-Swan Theorem (see [GVF01], Theorems 2.10 and 3.8) and of Proposition 3.2 in [GVF01].

In Proposition 7.7 we proved that the Gel'fand isomorphism and the Bloch-Floquet transform equip the wandering nuclear space Φ with the structure of a (left) pre-C^*-module over $C(\mathbb{T}^N)$ by means of the (left) product $\star$ defined by (28) and the pairing $\{\ ;\ \}$ defined by (29). The closure of Φ with respect to the module norm defines a Hilbert module over $C(\mathbb{T}^N)$ denoted by $\Omega_{\mathfrak{S}} \subset \mathcal{H}$. In this description, what is the role played by $\mathfrak{A}$? Is it possible, at least under some condition, to interpret the elements of $\mathfrak{A}$ as endomorphism of the Hilbert module $\Omega_{\mathfrak{S}}$? One could try to answer these questions by observing that for any $O \in \mathfrak{A}$, any $A_f \in \mathfrak{S}$ and any $\varphi \in \Omega_{\mathfrak{S}}$ one has that $O(f \star \varphi) := OA_f\varphi = A_f O\varphi$. The latter might be interpreted as $f \star O(\varphi)$, implying the $C(\mathbb{T}^N)$-linearity of $O \in \mathfrak{A}$ as operator on $\Omega_{\mathfrak{S}}$. However it may happen that $O\varphi \notin \Omega_{\mathfrak{S}}$ which implies that O can not define an endomorphism of $\Omega_{\mathfrak{S}}$. Everything works properly if one considers only elements in the subalgebra $\mathfrak{A}^0 \subset \mathfrak{A}$ defined by

$$\mathfrak{A}^0 := \{O \in \mathfrak{A} \ :\ O : \Omega_{\mathfrak{S}} \to \Omega_{\mathfrak{S}}\}. \tag{33}$$

Proposition 7.13. *Let $\Omega_{\mathfrak{S}}$ be the Hilbert module over $C(\mathbb{T}^N)$ defined by means of the Bloch-Floquet transform according to Proposition* 7.7*. Let $\mathfrak{A}^0_{\mathrm{s.a.}}$ be the C^*-subalgebra of $\mathfrak{A}$ defined by $\mathfrak{A}^0_{\mathrm{s.a.}} := \{O \in \mathfrak{A} : O, O^\dagger \in \mathfrak{A}^0\}$ (self-adjoint part of $\mathfrak{A}^0$). Then $\mathfrak{A}^0_{\mathrm{s.a.}} \subset \mathrm{End}_{C(\mathbb{T}^N)}(\Omega_{\mathfrak{S}})$.*

Proof. Let $O \in \mathfrak{A}^0_{\mathrm{s.a.}}$. By definition O is a linear map from $\Omega_{\mathfrak{S}}$ to itself; it is also $C(\mathbb{T}^N)$-linear since $O(f \star \varphi) = OA_f\varphi = A_f O\varphi$ as mentioned. We need to prove that O is bounded with respect to the endomorphism norm (31). From the definition (30) of the module norm $|||\cdot|||$ it follows that

$$|||O\varphi||| = \sup_{t\in\mathbb{T}^N} \|(\mathcal{U}_{\mathfrak{S}} O\varphi)(t)\|_t = \sup_{t\in\mathbb{T}^N} \|\pi_t(O)(\mathcal{U}_{\mathfrak{S}}\varphi)(t)\|_t \leqslant \|O\|_{\mathscr{B}(\mathcal{H})}\ |||\varphi|||$$

where $\pi_t(O) := \mathcal{U}_{\mathfrak{S}}|_t \; O \; \mathcal{U}_{\mathfrak{S}}|_t^{-1}$ defines a representation of the C^*-algebra $\mathfrak{A}$ on the fiber Hilbert space $\mathcal{K}(t)$ and $\|\pi_t(O)\|_{\mathscr{B}(\mathcal{K}(t))} \leqslant \|O\|_{\mathscr{B}(\mathcal{H})}$ since any C^* representation decreases the norm. Thus $\|O\|_{\mathrm{End}(\Omega_{\mathfrak{S}})} \leqslant \|O\|_{\mathscr{B}(\mathcal{H})}$, therefore O defines a continuous $C(\mathbb{T}^N)$-linear map from $\Omega_{\mathfrak{S}}$ to itself. To prove that $O \in \mathrm{End}_{C(\mathbb{T}^N)}(\Omega_{\mathfrak{S}})$ we must show that O is adjointable, which follows from the definition of $\mathfrak{A}^0_{\mathrm{s.a.}}$. □

It is of particular interest to specialize the previous result to the case of a finite wandering system.

Theorem 7.14 (Bloch-Floquet endomorphism bundle). *Let $\{\mathcal{H}, \mathfrak{A}, \mathfrak{S}\}$ be a physical frame where $\mathfrak{S}$ is a $\mathbb{Z}^N$-algebra with generators $\{U_1, \dots, U_N\}$ and wandering system $\{\psi_1, \dots, \psi_q\}$ of finite cardinality. Then:*

(i) $\mathfrak{A}^0_{\mathrm{s.a.}} = \mathfrak{A}^0$;

(ii) $\mathcal{U}_{\mathfrak{S}}\ \mathfrak{A}^0\ \mathcal{U}_{\mathfrak{S}}{}^{-1} \subseteq \Gamma(\mathrm{End}(\mathscr{E}_{\mathfrak{S}}))$ *where $\mathscr{E}_{\mathfrak{S}} \to \mathbb{T}^N$ is the rank q Bloch-Floquet vector bundle defined in Corollary* 7.10.

Proof. To prove (i) let $O \in \mathfrak{A}^0$ and observe that if

$$O\psi_k = \sum_{h=1}^{q} \sum_{b \in \mathbb{Z}^N} \alpha^{(k)}_{h,b}\, U^b \psi_h \quad \text{then} \quad O^\dagger \psi_k = \sum_{h=1}^{q} \sum_{b \in \mathbb{Z}^N} \overline{\alpha}^{(h)}_{k,b}\, U^{-b} \psi_h.$$

Since $O\psi_k \in \Omega_{\mathfrak{S}}$, then $f^{(k)}_h(t) := \sum_{b \in \mathbb{Z}^N} \alpha^{(k)}_{h,b}\, z^b(t)$ is a continuous function on $\mathbb{T}^N$ and

$$|||O^\dagger \psi_k|||^2 = \sup_{t \in \mathbb{T}^N} \left(\sum_{h=1}^{q} |f^{(h)}_k(t)|^2 \right) < +\infty.$$

Then $O^\dagger \psi_k \in \Omega_{\mathfrak{S}}$ for all $k = 1, \dots, q$. Since $O^\dagger(U^b \psi_k) = U^b(O^\dagger \psi_k) \in \Omega_{\mathfrak{S}}$ for all $b \in \mathbb{Z}^N$ it follows that also $O^\dagger \in \mathfrak{A}^0$.

Point (ii) is an immediate consequence of Proposition 7.13, Corollary 7.10 and Proposition 7.12. □

Example 7.15 (Mathieu-like Hamiltonians, part four). It is immediate to check that both $\mathfrak{u}$ and $\mathfrak{v}$ preserve the wandering nuclear space Φ, so that the full C^*-algebra $\mathfrak{A}^{p/q}_{\mathrm{M}}$ consists of endomorphisms for the Hilbert module realized by means of the Bloch-Floquet transform $\mathcal{U}_{\mathfrak{S}^q_{\mathrm{M}}}$. Theorem 7.14 claims that $\mathcal{U}_{\mathfrak{S}^q_{\mathrm{M}}}$ maps $\mathfrak{A}^{p/q}_{\mathrm{M}}$ into a subalgebra of the endomorphisms of the trivial bundle $\mathbb{T} \times \mathbb{C}^q \to \mathbb{T}$. The matrices $\mathfrak{u}(t)$ and $\mathfrak{v}(t)$ in Example 6.7 define the representation of the generators as elements of $\Gamma(\mathrm{End}(\mathbb{T} \times \mathbb{C}^q)) \simeq C(\mathbb{T}) \otimes \mathrm{Mat}_q(\mathbb{C})$. ◀▷

Appendix A. Gel'fand theory, joint spectrum and basic measures

Let $\mathfrak{A}$ be a unital (not necessarily commutative) C^*-algebra and $\mathfrak{A}^\times$ the *group of the invertible elements* of $\mathfrak{A}$. The *algebraic spectrum* of $A \in \mathfrak{A}$ is defined to be $\sigma_{\mathfrak{A}}(A) := \{\lambda \in \mathbb{C} \;:\; (A - \lambda \mathbb{1}) \notin \mathfrak{A}^\times\}$. If $\mathfrak{A}_0$ is a non unital C^*-algebra and $\imath : \mathfrak{A}_0 \hookrightarrow \mathfrak{A}$ is the canonical embedding of $\mathfrak{A}_0$ in the unital C^*-algebra $\mathfrak{A}$ (see [BR87] Proposition 2.1.5) then one defines $\sigma_{\mathfrak{A}_0}(A) := \sigma_{\mathfrak{A}}(\imath(A))$ for all $A \in \mathfrak{A}_0$. If

$\mathfrak{A}$ is unital and $C^*(A) \subset \mathfrak{A}$ is the unital C^*-subalgebra generated algebraically by A, its adjoint $A^\dagger$ and $\mathbb{1}$ (=: A^0 for definition) then $\sigma_{\mathfrak{A}}(A) = \sigma_{C^*(A)}(A)$ (see [BR87] Proposition 2.2.7). As a consequence we have that if $\mathfrak{A} \subset \mathscr{B}(\mathcal{H})$ is a concrete C^*-algebra of operators on the Hilbert space $\mathcal{H}$ and $A \in \mathfrak{A}$ then the algebraic spectrum $\sigma_{\mathfrak{A}}(A)$ agrees with the *Hilbert space spectrum* $\sigma(A) := \{\lambda \in \mathbb{C} \ : \ (A - \lambda\mathbb{1}) \notin \mathrm{GL}(\mathcal{H})\}$ where $\mathrm{GL}(\mathcal{H}) := \mathscr{B}(\mathcal{H})^\times$ is the group of the invertible bounded linear operators on the Hilbert space $\mathcal{H}$.

Let us denote by $\mathfrak{S}$ a commutative C^*-algebra. A *character* of $\mathfrak{S}$ is a nonzero homomorphism $x : \mathfrak{S} \to \mathbb{C}$ (also called pure state). The *Gel'fand spectrum* of $\mathfrak{S}$, denoted by $X(\mathfrak{S})$ or simply by X, is the set of all characters of $\mathfrak{S}$. The space X, endowed with the weak-$*$ topology (topology of the pointwise convergence on $\mathfrak{S}$) becomes a topological Hausdorff space, which is compact if $\mathfrak{S}$ is unital and only locally compact otherwise (see [BR87] Theorem 2.1.11A). If $\mathfrak{S}$ is *separable* (namely it is generated algebraically by a countable family of commuting elements) then the weak-$*$ topology in X is metrizable (see [Bré87] Theorem III.25) and if, in addition, $\mathfrak{S}$ is also unital then X is compact and metrizable which implies (see [Cho66] Proposition 18.3 and Theorem 20.9) that X is second-countable (has a countable basis of open sets), separable (has a countable everywhere dense subset) and complete. Summarizing, the Gel'fand spectrum of a commutative separable unital C^*-algebra has the structure of a *Polish space* (separable complete metric space).

The *Gel'fand-Naĭmark Theorem* (see [BR87] Section 2.3.5 or [GVF01] Section 1.2 or [Lan97] Section 2.2) states that there is a canonical isomorphism between any commutative unital C^*-algebra $\mathfrak{S}$ and the commutative C^*-algebra $C(X)$ of the continuous complex-valued functions on its spectrum endowed with the norm of the uniform convergence. The *Gel'fand isomorphism* $C(X) \ni f \overset{\mathscr{G}}{\mapsto} A_f \in \mathfrak{S}$ maps any continuous f into the unique element A_f which satisfies the relation $f(x) = x(A_f)$ for all $x \in X$. Then we can use the continuous functions on X to "label" the elements of $\mathfrak{S}$. If $\mathfrak{S}_0$ is a non-unital commutative C^*-algebra then the Gel'fand-Naĭmark Theorem proves the isomorphism between $\mathfrak{S}_0$ and the commutative C^*-algebra $C_0(X_0)$ of the continuous complex-valued functions vanishing at infinity on the locally compact space X_0 which is the spectrum of $\mathfrak{S}_0$. If $\mathfrak{S}_0 \subset \mathscr{B}(\mathcal{H})$ we define the *multiplier algebra* (or *idealizer*) of $\mathfrak{S}_0$ to be $\mathfrak{S} := \{B \in \mathscr{B}(\mathcal{H}) \ : \ BA, AB \in \mathfrak{S}_0 \ \ \forall A \in \mathfrak{S}_0\}$ (see [GVF01] Definition 1.8 and Lemma 1.9). Obviously $\mathfrak{S}$ is a unital C^*-algebra and the commutativity of $\mathfrak{S}_0$ implies the commutativity of $\mathfrak{S}$. Moreover $\mathfrak{S}$ contains $\mathfrak{S}_0$ as an *essential ideal*. The Gel'fand spectrum X of $\mathfrak{S}$ corresponds to the *Stone-Čech compactification* of the spectrum X_0. Since $C(X) \simeq C_{\mathrm{b}}(X_0)$, the Gel'fand isomorphism asserts that the multiplier algebra $\mathfrak{S}$ can be described as the unital commutative C^*-algebra of the bounded continuous functions on the locally compact space X_0 (see [GVF01] Proposition 1.10). For every $A_f \in \mathfrak{S}$ one has that $\sigma_{\mathfrak{S}}(A_f) = \{f(x) \ : \ x \in X\}$ (see [Hör90] Theorem 3.1.6) then A_f is invertible if and only if $0 < |f(x)| \leqslant \|A_f\|_{\mathfrak{S}}$ for all $x \in X$.

We often consider the relevant case when the unital commutative C^*-algebra is *finitely generated*, i.e., when $\mathfrak{S}$ is generated by a finite family $\{A_1, \dots, A_N\}$

of commuting normal elements and the identity $\mathbb{1}$ (=: A_j^0 by definition). Let $f_1, \ldots, f_N$ be the continuous functions which label the elements of the generating system. The map $X \ni x \overset{\varpi}{\mapsto} (f_1(x), \ldots, f_N(x)) \in \mathbb{C}^N$ is a homeomorphism from the Gel'fand spectrum X to a compact subset of $\mathbb{C}^N$ called the *joint spectrum* of the generating system $\{A_1, \ldots, A_N\}$ (see [Hör90] Theorem 3.1.15). Then, when $\mathfrak{S}$ is finitely generated, we can identify the Gel'fand spectrum X with its homeomorphic image $\varpi(X)$ (the joint spectrum) which is a compact, generally proper, subset of $\sigma_{\mathfrak{S}}(A_1) \times \cdots \times \sigma_{\mathfrak{S}}(A_N)$. When $\{A_1, \ldots, A_N\} \subset \mathscr{B}(\mathcal{H})$ a necessary and sufficient condition for $\lambda := (\lambda_1, \ldots, \lambda_N)$ to be in $\varpi(X)$ is that there exists a sequence of normalized vectors $\{\psi_n\}_{n\in\mathbb{N}}$ such that $\|(A_j - \lambda_j)\psi_n\| \to 0$ if $n \to \infty$ for all $j = 1, \ldots, N$ (see [Sam91] Proposition 2).

Remark A.1 (Dual group). The Gel'fand theory has an interesting application to abelian locally compact groups $\mathbb{G}$. Usually the *dual group* (or character group) $\widehat{\mathbb{G}}$ is defined to be the set of all continuous characters of $\mathbb{G}$, namely the set of all continuous homomorphisms of $\mathbb{G}$ into the group $\mathbb{S}^1 := \{z \in \mathbb{C} \,:\, |z| = 1\}$. However, to endow $\widehat{\mathbb{G}}$ with a natural topology it is useful to give an equivalent definition of dual group. Since $\mathbb{G}$ is locally compact and abelian there exists a unique (up to a multiplicative constant) invariant *Haar measure* on $\mathbb{G}$ denoted by dg. The space $L^1(\mathbb{G})$ becomes a commutative Banach $*$-algebra, if multiplication is defined by convolution; it is called the *group algebra* of $\mathbb{G}$. If $\mathbb{G}$ is discrete then $L^1(\mathbb{G})$ is unital otherwise $L^1(\mathbb{G})$ has always an *approximate unit* (see [Rud62] Theorems 1.1.7 and 1.1.8). Every $\chi \in \widehat{\mathbb{G}}$ defines a linear multiplicative functional $\widehat{\chi}$ on $L^1(\mathbb{G})$ by $\widehat{\chi}(f) := \int_{\mathbb{G}} f(g)\chi(-g)\, d\mu(g)$ for all $f \in L^1(\mathbb{G})$ (the Fourier transform). This map defines a one to one correspondence between $\widehat{\mathbb{G}}$ and the Gel'fand spectrum of the algebra $L^1(\mathbb{G})$ (see [Rud62] Theorem 1.2.2). This enables us to consider $\widehat{\mathbb{G}}$ as the Gel'fand spectrum of $L^1(\mathbb{G})$. When $\widehat{\mathbb{G}}$ is endowed with the weak-$*$ topology with respect to $L^1(\mathbb{G})$ then it becomes a Hausdorff locally compact space. Moreover $\widehat{\mathbb{G}}$ is compact if $\mathbb{G}$ is discrete and it is discrete when $\mathbb{G}$ is compact (see [Rud62] Theorem 1.2.5). ⧫◇

Let X be a compact Polish space and $\mathcal{B}(X)$ the Borel σ-algebra generated by the topology of X. The pair $\{X, \mathcal{B}(X)\}$ is called *standard Borel space*. A mapping $\mu : \mathcal{B}(X) \to [0, +\infty]$ such that $\mu(\emptyset) = 0$ and $\mu(X) < \infty$, which is additive with respect to the union of countable families of pairwise disjoint subsets of X, is called a *finite Borel measure*. If $\mu(X) = 1$ then we will said that μ is a *probability* Borel measure. Any Borel measure on a standard Borel space $\{X, \mathcal{B}(X)\}$ is *regular*, i.e., for all $Y \in \mathcal{B}(X)$ one has that $\mu(Y) = \sup\{\mu(K) \,:\, K \subset Y,\ K \text{ compact}\} = \inf\{\mu(O) \,:\, Y \subset O,\ O \text{ open}\}$.

Let N be the union of all the open sets $O_\alpha \subset X$ such that $\mu(O_\alpha) = 0$. The closed set $X \setminus N$ is called the *support* of μ. If μ is a regular Borel measure then $\mu(N) = 0$ and μ is concentrated on its support.

Let $\mathfrak{S}$ be a unital commutative C^*-algebra acting on the separable Hilbert space $\mathcal{H}$ with Gel'fand spectrum X. For all pairs $\psi, \varphi \in \mathcal{H}$ the mapping $C(X) \ni$

$f \mapsto (\psi; A_f\varphi)_{\mathcal{H}} \in \mathbb{C}$ is a continuous linear functional on $C(X)$; hence the *Riesz-Markov Theorem* (see [Rud87] Theorem 2.14) implies the existence of a unique regular (complex) Borel measure $\mu_{\psi,\varphi}$, with finite total variation, such that

$$(\psi; A_f\varphi)_{\mathcal{H}} = \int_X f(x)\, d\mu_{\psi,\varphi}(x) \quad \text{for all } f \in C(X).$$

We will refer to $\mu_{\psi,\varphi}$ as a *spectral measure*. The union of the supports of the (positive) spectral measures $\mu_{\psi,\psi}$ is dense, namely for every non-void open set $O \subset X$ there exists a $\psi \in \mathcal{H}$ such that $\mu_{\psi,\psi}(O) > 0$. A positive measure μ on X is said to be *basic* for the unital C^*-algebra $\mathfrak{S}$ if: for every $Y \subset X$, $\mu(Y) = 0$ if and only if $\mu_{\psi,\psi}(Y) = 0$ for every $\psi \in \mathcal{H}$. From the definition it follows that:

(i) if there exists a basic measure μ on X, then every other basic measure is *equivalent* (has the same null sets) to μ;

(ii) for all $\psi, \varphi \in \mathcal{H}$ the spectral measure $\mu_{\psi,\varphi}$ is *absolutely continuous* with respect to μ, and there exists a unique element $h_{\psi,\varphi} \in L^1(X)$ (the *Radon-Nikodym derivative*) such that $\mu_{\psi,\varphi} = h_{\psi,\varphi}\mu$;

(iii) since the union of the supports of the measures $\mu_{\psi,\psi}$ is dense in X, then the support of a basic measure μ is all of X (see [Dix81] Part I, Chapter 7).

The existence of a basic measure for a commutative C^*-algebra $\mathfrak{S} \subset \mathscr{B}(\mathcal{H})$ follows from general arguments. Indeed the existence of a basic measure is equivalent to the existence of a cyclic vector ϕ for the commutant $\mathfrak{S}'$ and the basic measure can be chosen to be the spectral measure $\mu_{\phi,\phi}$ (see [Dix81] Part I, Chapter 7, Proposition 3). Since a vector ϕ is cyclic for $\mathfrak{S}'$ if and only if it is separating for the commutative von Neumann algebra $\mathfrak{S}'' \supset \mathfrak{S}$, and since any commutative von Neumann algebra of operators on a separable Hilbert space has a separating vector, it follows that any commutative unital C^*-algebra $\mathfrak{S}$ of operators which acts on a separable Hilbert space has a basic measure carried on its spectrum (see [Dix81] Part I, Chapter 7, Propositions 4).

Appendix B. Direct integral of Hilbert spaces

General references about the notion of a direct integral of Hilbert spaces can be found in [Dix81] (Part II, Chapters 1–5) or in [Mau68] (Chapter I, Section 6). In the following we assume that the pair $\{X, \mathcal{B}(X)\}$ is a standard Borel space and μ a (regular) Borel measure on X. For every $x \in X$ let $\mathcal{H}(x)$ be a Hilbert space with scalar product $(\ ;\ )_x$. The set $\mathfrak{F} := \prod_{x\in X} \mathcal{H}(x)$ (Cartesian product) is called a *field of Hilbert spaces* over X. A *vector field* $\varphi(\cdot)$ is an element of $\mathfrak{F}$, namely a map $X \ni x \mapsto \varphi(x) \in \mathcal{H}(x)$. A countable family $\{\xi_j(\cdot) \ :\ j \in \mathbb{N}\}$ of vector fields is called a *fundamental family of measurable vector fields* if:

a) for all $i, j \in \mathbb{N}$ the functions $X \ni x \mapsto (\xi_i(x); \xi_j(x))_x \in \mathbb{C}$ are measurable;

b) for each $x \in X$ the set $\{\xi_j(x) \ :\ j \in \mathbb{N}\}$ spans the space $\mathcal{H}(x)$.

The field $\mathfrak{F}$ has a *measurable structure* if it has a fundamental family of measurable vector fields. A vector field $\varphi(\cdot) \in \mathfrak{F}$ is said to be *measurable* if all the functions $X \ni x \mapsto (\xi_j(x); \varphi(x))_x \in \mathbb{C}$ are measurable for all $j \in \mathbb{N}$. The set of all measurable vector fields is a linear subspace of $\mathfrak{F}$. By the Gram-Schmidt orthonormalization we can always build a fundamental family of orthonormal measurable fields (see [Dix81] Part II, Chapter 1, Propositions 1 and 4). Such a family is called a *measurable field of orthonormal frames*. Two fields are said to be equivalent if they are equal μ-almost everywhere on X. The *direct integral* $\mathfrak{H}$ of the Hilbert spaces $\mathcal{H}(x)$ (subordinate to the measurable structure of $\mathfrak{F}$), is the Hilbert space of the equivalence classes of measurable vector fields $\varphi(\cdot) \in \mathfrak{F}$ satisfying

$$\|\varphi(\cdot)\|^2_{\mathfrak{H}} := \int_X \|\varphi(x)\|^2_x \, d\mu(x) < \infty. \tag{34}$$

The scalar product on $\mathfrak{H}$ is defined by

$$\langle \varphi_1(\cdot); \varphi_2(\cdot) \rangle_{\mathfrak{H}} := \int_X (\varphi_1(x); \varphi_2(x))_x \, d\mu(x) < \infty. \tag{35}$$

The Hilbert space $\mathfrak{H}$ is often denoted by the symbol $\int_X^{\oplus} \mathcal{H}(x) \, d\mu(x)$. It is separable if X is separable.

Let ν be a positive measure equivalent to μ. The Radon-Nikodym theorem ensures the existence of a positive $\rho \in L^1(X, \mu)$ with $\frac{1}{\rho} \in L^1(X, \nu)$ such that $\nu = \rho\mu$. Let $\mathfrak{H}$ be the direct integral with respect to μ, $\mathfrak{K}$ the direct integral with respect to ν and $\varphi(\cdot) \in \mathfrak{H}$. The mapping $\mathfrak{H} \ni \varphi(\cdot) \mapsto \varphi'(\cdot) \in \mathfrak{K}$ defined by $\varphi'(x) = \frac{1}{\sqrt{\rho(x)}} \varphi(x)$ for all $x \in X$ is an unitary map of $\mathfrak{H}$ onto $\mathfrak{K}$ and for fixed μ and ν. This isomorphism does not depend on the choice of the representative for ρ and it is called the *canonical rescaling isomorphism*.

A *(bounded) operator field* $A(\cdot)$ is a map $X \ni x \mapsto A(x) \in \mathscr{B}(\mathcal{H}(x))$. It is called measurable if the function $X \ni x \mapsto (\xi_i(x); A(x)\xi_j(x))_x \in \mathbb{C}$ is measurable for all $i, j \in \mathbb{N}$. A measurable operator field is called a *decomposable operator* in the Hilbert space $\mathfrak{H}$. Let $f \in L^\infty(X)$ (with respect to the measure μ); then the map $X \ni x \mapsto M_f(x) := f(x)\mathbb{1}_x \in \mathscr{B}(\mathcal{H}(x))$ (with $\mathbb{1}_x$ the identity in $\mathcal{H}(x)$) defines a simple example of decomposable operator called *diagonal operator*. When $f \in C(X)$, the diagonal operator $M_f(\cdot)$ is called a *continuously diagonal operator*. Denote by $C(\mathfrak{H})$ (resp. $L^\infty(\mathfrak{H})$) the set of the continuously diagonal operators (resp. the set of diagonal operators) on $\mathfrak{H}$. Suppose that $\mathcal{H}(x) \neq 0$ μ-almost everywhere on X, then the following facts hold true (see [Dix81] Part II, Chapter 2, Section 4): (i) $L^\infty(\mathfrak{H})$ is a commutative von Neumann algebra and the mapping $L^\infty(X) \ni f \mapsto M_f(\cdot) \in L^\infty(\mathfrak{H})$ is a (canonical) isomorphism of von Neumann algebras; (ii) the commutant $L^\infty(\mathfrak{H})'$ is the von Neumann algebra of decomposable operators on $\mathfrak{H}$; (iii) the mapping $C(X) \ni f \mapsto M_f(\cdot) \in C(\mathfrak{H})$ is a (canonical) homomorphism of C^*-algebras which becomes an isomorphism if the support of μ is all X; in this case X is the Gel'fand spectrum of $C(\mathfrak{H})$ and μ is a basic measure.

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Discrete Schrödinger Operators with Random Alloy-type Potential

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Abstract. We review recent results on localization for discrete alloy-type models based on the multiscale analysis and the fractional moment method, respectively. The discrete alloy-type model is a family of Schrödinger operators $H_\omega = -\Delta + V_\omega$ on $\ell^2(\mathbb{Z}^d)$ where Δ is the discrete Laplacian and V_ω the multiplication by the function $V_\omega(x) = \sum_{k\in\mathbb{Z}^d} \omega_k u(x-k)$. Here ω_k, $k \in \mathbb{Z}^d$, are i.i.d. random variables and $u \in \ell^1(\mathbb{Z}^d;\mathbb{R})$ is a so-called single-site potential. Since u may change sign, certain properties of H_ω depend in a non-monotone way on the random parameters ω_k. This requires new methods at certain stages of the localization proof.

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1. Introduction

The paradigmatic model for the study of localization properties of quantum states of single electrons in disordered solids is the Anderson Hamiltonian on the lattice $\mathbb{Z}^d$. It consists of the sum of the finite difference Laplacian and a multiplication operator by a sequence of independent identically distributed random variables. There are two independent (though related in sprit) frequently used methods to prove rigorously in appropriate energy and disorder regimes localization statements: the multiscale analysis and the fractional moment method. Both of them rely strongly on the independence property of the random variables. If this property is removed much less is known. Specific cases of random fields with correlations which have been studied so far include the Gaussian field (cf. Section 4 of

[DK91] and Section 4 of [AM93]) and potentials whose distribution is given by a completely analytic Gibbs measure (cf. Section 5 of [DK91] and [DS87]).

A particularly problematic aspect of dependence are negative correlations between values of the potential at different lattice sites. This is intuitively clear when having in mind the role played by the local variation of eigenvalues in localization proofs. An example of a random potential which exhibits negative correlations is an Anderson or alloy-type potential with single-site potentials of changing sign: if one increases a single coupling constant there are regions in space where the potential increases and others where it decreases. Such models have been studied in a number of works devoted to the continuum setting, i.e., for operators on $\mathbb{R}^d$. In this paper we want to summarize and discuss a number of results which have been obtained more recently for their lattice counterparts.

The study of Anderson-type models with sign-indefinite single-site potentials can be seen as part of the interest attracted recently by several classes of random operators with a non-monotone dependence on the random variables. They exhibit a variety of intriguing features not encountered in the standard alloy-type model: already when considering the very basic features of the spectrum as a subset of the real line, one sees that it makes an essential difference whether the operator depends in a monotone or non-monotone way on the random variables entering the model. For operators with monotone parameter dependence the spectral bottom of the operator family corresponds to the configuration where all random variables are set to one of the extremal values. Furthermore, in the monotone situation the band structure of the spectrum can be analyzed using rather basic bracketing arguments, see, e.g., [KSS98b]. It is consistent with these elementary examples of the advantages of monotonicity that there is a rather good understanding of typical energy/disorder regimes where monotone models exhibit localization of waves, see the monographs and survey articles [Sto01, KM07, Ves07, Kir08].

If the dependence of the operator, respectively the quadratic form, on the random variables is not monotone, already the identification of the spectral minimum is a highly non-trivial question, see, e.g., [BLS08, KN09]. For more intricate properties, like the regularity of the density of states or the analysis of spectral fluctuation boundaries, the difference between monotone and non-monotone models is even more striking.

Nevertheless there has been a continuous effort to bring the understanding of models with non-monotone dependence on the randomness to a similar level as the one for monotone models. This includes alloy-type Schrödinger operators with single-site potentials of changing sign, see, e.g., [Klo95, Sto00, Klo02, Ves02, HK02, KV06, KN09], and their lattice counterparts cf., e.g., [Ves10b, ETV10, Ves10a, TV10, ETV11, Krü12]. Electromagnetic Schrödinger operators with random magnetic field [Uek94, Uek00, HK02, KNNN03, Uek08, Bou09, EHc, EHa, EHb], Laplace-Beltrami operators with random metrics [LPV04, LPPV08, LPPV09], randomly curved waveguides [BV11], as well as the random displacement model, cf., e.g., [Klo93, BLS08, KLNS], are other examples with non-monotonous parameter dependence.

Another relevant model without obvious monotonicity is a random potential given by a Gaussian stochastic field with sign-changing covariance function, cf. [HLMW01, Uek04, Ves11].

The methods which have been developed for the discrete alloy-type potentials with sign-indefinite single-site potentials presented here could be applied to other non-monotone models, as well. In fact the results of [Krü12] apply to a much larger class of lattice Schrödinger operator with non-monotone, correlated random potential.

2. Discrete Anderson models with general alloy-type potential

To define the random operators we will be looking at, we first introduce the corresponding Hilbert and probability spaces. Let $d \geq 1$. For $x \in \mathbb{Z}^d$ we denote by $|x|_1 = \sum_{i=1}^d |x_i|$ and $|x|_\infty = \max\{|x_1|, \ldots, |x_d|\}$ the ℓ^1 and ℓ^∞ norms on $\mathbb{Z}^d$. For $\Gamma \subset \mathbb{Z}^d$ we introduce the Hilbert space $\ell^2(\Gamma) = \{\psi : \Gamma \to \mathbb{C} : \sum_{k\in\Gamma} |\psi(k)|^2 < \infty\}$ with inner product $\langle \phi, \psi \rangle = \sum_{k\in\Gamma} \overline{\phi(k)}\psi(k)$.

For each $\Gamma \subset \mathbb{Z}^d$ we introduce a probability space $(\Omega_\Gamma, \mathcal{A}_\Gamma, \mathbb{P}_\Gamma)$. Here Ω_Γ is the product $\Omega_\Gamma := \times_{k\in\Gamma} \mathbb{R}$, $\mathcal{A}_\Gamma$ is the associated product sigma algebra generated by cylinder sets, and $\mathbb{P}_\Gamma(\mathrm{d}\omega) := \prod_{k\in\Gamma} \mu(\mathrm{d}\omega_k)$ the product measure, with μ a probability measure on $\mathbb{R}$ with bounded support. The mathematical expectation with respect to $\mathbb{P}_\Gamma$ is denoted by $\mathbb{E}_\Gamma$. Note that the projections $\Omega \ni \omega = \{\omega_k\}_{k\in\Gamma} \mapsto \omega_j$, $j \in \Gamma$, give rise to a collection of independent identically distributed (i.i.d.) bounded real random variables. If $\Gamma = \mathbb{Z}^d$ we will suppress the subscript Γ in $\Omega_\Gamma, \mathbb{P}_\Gamma$ and $\mathbb{E}_\Gamma$.

On $\ell^2(\mathbb{Z}^d)$ we consider the discrete random Schrödinger operator

$$H_\omega := -\Delta + \lambda V_\omega, \quad \omega \in \Omega, \quad \lambda > 0. \tag{1}$$

Here $\Delta, V_\omega : \ell^2\left(\mathbb{Z}^d\right) \to \ell^2\left(\mathbb{Z}^d\right)$ denote the discrete Laplace and a random multiplication operator defined by

$$\left(\Delta\psi\right)(x) := \sum_{|e|_1=1} \psi(x+e) \quad \text{and} \quad \left(V_\omega\psi\right)(x) := V_\omega(x)\psi(x).$$

The parameter λ models the strength of the disorder and ω denotes the randomness. It enters the potential in the following way. Let the *single-site potential* $u : \mathbb{Z}^d \to \mathbb{R}$ be a function in $\ell^1(\mathbb{Z}^d; \mathbb{R})$. We assume that the random potential V_ω has an *alloy-type structure*, i.e., the potential value

$$V_\omega(x) := \sum_{k\in\mathbb{Z}^d} \omega_k u(x-k)$$

at a lattice site $x \in \mathbb{Z}^d$ is a linear combination of the i.i.d. random variables ω_k, $k \in \mathbb{Z}^d$, with coefficients provided by the single-site potential. We assume (without loss of generality) that $0 \in \operatorname{supp} u$. The family of operators H_ω, $\omega \in \Omega$, in Eq. (1) is called *discrete alloy-type model*.

Notice that the single-site potential u may change its sign. As a consequence the quadratic form associated to H_ω does not necessarily depend in a monotone way on the random parameters ω_k, $k \in \mathbb{Z}^d$. This is in sharp contrast to the properties of the *standard Anderson model* which corresponds to the choice of the single-site potential $u = \delta_0$. Here

$$\delta_k(j) = \begin{cases} 1 \text{ if } k = j, \\ 0 \text{ else,} \end{cases}$$

denotes the Dirac function.

3. Localization properties

We present several properties related to localization. They concern on the one hand several mathematical signatures of localization, and on the other estimates on the average of resolvents and number of eigenvalues in intervals of finite volume systems, which are instrumental in the arguments leading to localization. They are well established for the standard Anderson model on $\mathbb{Z}^d$, see, e.g., [Sto01, GK04, Kir08] and the references therein.

Definition 3.1 (Dynamical localization). A selfadjoint operator H on $\ell^2(\mathbb{Z}^d)$ is said to exhibit *dynamical localization* in the interval $I \subset \mathbb{R}$, if for every $x \in \mathbb{Z}^d$ and $p \geq 1$ we have

$$\sup_{t\in\mathbb{R}} \Big(\sum_{n\in\mathbb{Z}^d} \big(1 + |n|_\infty\big)^p \big| \langle \delta_n, \mathrm{e}^{-\mathrm{i}tH} \chi_I(H) \delta_x \rangle \big|^2 \Big) < \infty.$$

Definition 3.2 (Exponential localization). Let $I \subset \mathbb{R}$. A selfadjoint operator $H : \ell^2(\mathbb{Z}^d) \to \ell^2(\mathbb{Z}^d)$ is said to exhibit *exponential localization in* I, if the spectrum of H in I is exclusively of pure point type, i.e., $\sigma_{\mathrm{c}}(H) \cap I = \emptyset$, and the eigenfunctions of H corresponding to the eigenvalues in I decay exponentially. If $I = \mathbb{R}$, we say that H exhibits *exponential localization.*

A family of operators $(H_\omega)_\omega$ indexed by elements of a probability space $(\Omega, \mathbb{P})$ is said to exhibit dynamical/exponential localization in the interval $I \subset \mathbb{R}$ if the corresponding property holds for H_ω for almost all $\omega \in \Omega$.

Several important properties of random Hamiltonians are defined in terms of restrictions to a finite system size. We review them next. Let $\Gamma \subset \mathbb{Z}^d$. We define $P_\Gamma : \ell^2(\mathbb{Z}^d) \to \ell^2(\Gamma)$ by

$$P_\Gamma \psi := \sum_{k\in\Gamma} \psi(k) \delta_k,$$

where here δ_k is the Dirac function in $\ell^2(\Gamma)$.

The restricted operators $\Delta_\Gamma, V_{\omega,\Gamma}, H_{\omega,\Gamma} : \ell^2(\Gamma) \to \ell^2(\Gamma)$ are defined by

$$\Delta_\Gamma := P_\Gamma \Delta P_\Gamma^*, \quad V_{\omega,\Gamma} := P_\Gamma V_\omega P_\Gamma^*, \quad H_{\omega,\Gamma} := P_\Gamma H_\omega P_\Gamma^* = -\Delta_\Gamma + V_{\omega,\Gamma}.$$

For $z \in \mathbb{C} \setminus \sigma(H_{\omega,\Gamma})$ we define the corresponding *resolvent* $G_{\omega,\Gamma}(z) := (H_{\omega,\Gamma} - z)^{-1}$ and the *Green function*

$$G_{\omega,\Gamma}(z; x, y) := \left\langle \delta_x, (H_{\omega,\Gamma} - z)^{-1} \delta_y \right\rangle, \quad x, y \in \mathbb{Z}^d.$$

If $\Gamma = \mathbb{Z}^d$ we drop the subscript Γ in $H_{\omega,\Gamma}, G_{\omega,\Gamma}(z)$ and $G_{\omega,\Gamma}(z; x, y)$. If $\Lambda \subset \mathbb{Z}^d$ is finite, $|\Lambda|$ denotes the number of elements of Λ. We will use the notation $\mathbb{R}^+ := \{x \in \mathbb{R} : x > 0\}$.

Definition 3.3 (Decay of fractional moments of the Green function). There exist constants $s \in (0,1)$ and $A, \gamma \in \mathbb{R}^+$ such that for all $\Gamma \subset \mathbb{Z}^d$, $z \in \mathbb{C} \setminus \mathbb{R}$ and $x, y \in \Gamma$ we have

$$\mathbb{E}\left\{ |G_{\omega,\Gamma}(z; x, y)|^s \right\} \leq A \mathrm{e}^{-\gamma |x-y|_\infty}.$$

For $x \in \mathbb{Z}^d$ and $L > 0$, we denote by $\Lambda_{L,x} = \{k \in \mathbb{Z}^d : |x - k|_\infty \leq L\}$ the cube of side length $2L$ centered at x. For the cube centered at zero we use the notation $\Lambda_L = \Lambda_{L,0}$. We also we write $H_{\omega,L}$ instead of H_{ω,Λ_L} and $G_{\omega,L}(z)$ and $G_{\omega,L}(z; x, y)$ instead of $G_{\omega,\Lambda_L}(z)$ and $G_{\omega,\Lambda_L}(z; x, y)$. For $\Lambda \subset \mathbb{Z}^d$ we denote by $\partial^{\mathrm{i}}\Lambda = \{k \in \Lambda : |\{j \in \Lambda : |k - j|_1 = 1\} < 2d\}|$ the interior boundary of Λ and by $\partial^{\mathrm{o}}\Lambda = \partial^{\mathrm{i}}\Lambda^{\mathrm{c}}$ the exterior boundary of Λ. Here $\Lambda^{\mathrm{c}} = \mathbb{Z}^d \setminus \Lambda$ denotes the complement of Λ.

Definition 3.4 (Wegner estimate). There are constants $C_{\mathrm{W}}, L_0 \in \mathbb{R}^+$, $b \geq 1$, and a function $f : \mathbb{R}^+ \to \mathbb{R}^+$ satisfying $\lim_{\varepsilon \searrow 0} f(\varepsilon) = 0$ such that we have for any $L \geq L_0$, $E \in \mathbb{R}$ and $\varepsilon \in (0,1)$

$$\begin{aligned} \mathbb{P}\left\{ [E - \varepsilon, E + \varepsilon] \cap \sigma(H_{\omega,L}) \neq \emptyset \right\} &\leq \mathbb{E}\left\{ \mathrm{Tr}\left[\chi_{[E-\varepsilon, E+\varepsilon]}(H_{\omega,L}) \right] \right\} \\ &\leq C_{\mathrm{W}} f(\varepsilon) (2L+1)^{bd}. \end{aligned} \tag{2}$$

In specific applications of a Wegner estimate (for example as an ingredient for the multiscale analysis) one needs a specific rate of decay on the function f near zero. The original estimate of Wegner [Weg81] corresponds to $f(\varepsilon) = \varepsilon$ and $b = 1$ and implies the Lipschitz-continuity of the integrated density of states. In many situations one can establish (2) with $b = 1$ or $b = 2$ and $f(\varepsilon) = \varepsilon^a$ for $a \in (0,1)$. In certain situations variants of the Wegner estimate which do not control only the global property $d(E, \sigma(H_{\omega,L}) \leq \varepsilon$ but also specific coefficients of the resolvent, as well, need to be used, cf. Section 8.2 or [Bou09, Krü12].

Definition 3.5. Let $m, L > 0$, $x \in \mathbb{Z}^d$ and $E \in \mathbb{R}$. A cube $\Lambda_{L,x}$ is called (m, E)-*regular* (for a fixed potential), if $E \notin \sigma(H_{\Lambda_{L,x}})$ and

$$\sup_{w \in \partial^{\mathrm{i}}\Lambda_{L,x}} |G_{\Lambda_{L,x}}(E; x, w)| \leq \mathrm{e}^{-mL}.$$

Otherwise we say that $\Lambda_{L,x}$ is (m, E)-*singular*.

Rather than looking at the fractional moments of the Green function one can consider the probability of a box to be regular. The decay of these probabilities is closely related to the localization phenomenon. For simplicity we define one variant

of this decay property and restrict ourselves to the case of finitely supported single-site potentials u.

Definition 3.6 (Probabilistic decay of Green's function). Let $\Theta := \operatorname{supp} u$ be finite, $I \subset \mathbb{R}$ be an interval and let $p > d$, $L_0 > 1$, $\alpha \in (1, 2p/d)$ and $m > 0$. Set $L_k = L_{k-1}^{\alpha}$, for $k \in \mathbb{N}$. For any $k \in \mathbb{N}_0$

$$\mathbb{P}\{\forall\, E \in I \text{ either } \Lambda_{L_k,x} \text{ or } \Lambda_{L_k,y} \text{ is } (m,E)\text{-regular}\} \geq 1 - L_k^{-2p}$$

for any $x, y \in \mathbb{Z}^d$ with $|x - y|_\infty \geq 2L_k + \operatorname{diam}\Theta + 1$.

Here we denote for finite $\Gamma \subset \mathbb{Z}^d$ by $\operatorname{diam}\Gamma$ the diameter of Γ with respect to the supremum norm, i.e., $\operatorname{diam}\Gamma = \sup_{x,y\in\Gamma}|x - y|_\infty$. In the subsequent sections we describe which of these localization properties have been proven for the non-monotone model we are interested in.

The most general result concerning (large disorder) localization for the discrete alloy-type model is [Krü12]. Krüger proves for exponentially decaying single-site potentials dynamical localization in the case of sufficiently large disorder. Indeed, this result applies for a class of models including the discrete alloy-type model with exponentially decaying singe-site potential as a special case. Notice that dynamical localization implies spectral localization via the RAGE-Theorem, see, e.g., [Sto10], but not vice versa as examples in [dRJLS96] show. The proof of Krüger's result uses the multiscale analysis and is discussed in Section 8.

There are also localization results not using the multiscale analysis but the fractional moment method. In [ETV10] the authors prove exponential localization in the case of space dimension $d = 1$, compactly supported single-site potentials and sufficiently large disorder. This result was extended in [ETV11] to arbitrary space dimension assuming that the single-site potential has fixed sign at the boundary of its support, a property which can be assumed without loss of generality in $d = 1$. This result is discussed in Section 7.

In Section 5 we present certain estimates concerning averages of polynomials and resolvents which are fundamental for the results presented in Sections 7 and 8.

In Section 6 we discuss certain results on Wegner estimates for the discrete alloy-type model [Ves10a, PTV11]. With the help of such Wegner-estimates one can implement a proof of localization via the multiscale analysis in the regime where an appropriate initial length scale estimate is available.

In the following Section 4 we show that the almost sure spectrum of the discrete alloy-type model is an interval.

4. The spectrum

Before studying the properties of the spectral measure under the Lebesgue decomposition, one wants to understand basic features of the set $\Sigma \subset \mathbb{R}$ which coincides with the spectrum of H_ω almost surely. This concerns in particular the infimum

and supremum of the spectrum and internal spectral edges (if any). For the standard Anderson model there is a nice formula for the spectrum:

$$\Sigma = [-2d, 2d] + \operatorname{supp} \mu$$

where $[-2d, 2d]$ is the spectrum of the free Laplacian Δ and $\operatorname{supp} \mu$ the spectrum of the multiplication operator given by the random potential. Related descriptions of Σ for the (continuum) alloy-type model have been studied in [KM82]. In particular, a description of Σ in terms of admissible potentials was given. In many cases this class consists of an appropriate family of periodic potentials. Let us quote a specific result from [KSS98b]: if $S := \operatorname{supp} \mu$ is a bounded interval and the single-site potential u is non-negative, then

$$\Sigma = \overline{\bigcup_{\kappa \in S} \sigma\Big(-\Delta + \kappa \sum_{n \in \mathbb{Z}^d} u(\cdot - n)\Big)}.$$

The proof of this equality uses that u has fixed sign and is thus not applicable in our case. Our result about the set Σ is

Theorem 4.1. *Let H_ω be a discrete random Schrödinger operators as in* (1)*. If $S := \operatorname{supp} \mu$ is bounded and connected, then the spectrum of H_ω is almost surely an interval.*

Proof. Denote by Σ the almost sure spectrum of H_ω. It is well known that

$$\Sigma = \overline{\bigcup_{\omega \in S^{\mathbb{Z}^d}} \sigma(H_\omega)}$$

cf. the discussion in Section 6 of [Kir89]. Now we assume $0 \in S$ without loss of generality. For $\omega \in S^{\mathbb{Z}^d}$ and $t \in [0,1]$ denote $t \cdot \omega = (t\omega_x)_{x \in \mathbb{Z}^d}$ the scaled configuration. We then have that $\sigma(H_{0 \cdot \omega}) = [-2d, 2d]$. Fix now $\omega \in S^{\mathbb{Z}^d}$. We show that

$$\Sigma_\omega := \bigcup_{t \in [0,1]} \sigma(H_{t \cdot \omega})$$

is an interval. For this purpose we use that $\sigma(H_{0 \cdot \omega}) = [-2d, 2d]$ and that the spectral maximum and spectral minimum

$$[0,1] \ni t \mapsto \max \sigma(H_{t \cdot \omega}), \quad [0,1] \ni t \mapsto \min \sigma(H_{t \cdot \omega})$$

are continuous functions of t. This follows by the min-max-principle. Thus

$$\Sigma_\omega = \Big[\min_{t \in [0,1]} \min \sigma(H_{t \cdot \omega}), \max_{t \in [0,1]} \max \sigma(H_{t \cdot \omega})\Big] \supset [-2d, 2d].$$

Choose now $\lambda \in \bigcup_{\omega \in S^{\mathbb{Z}^d}} \sigma(H_\omega)$. Then there exists $\tilde{\omega} \in S^{\mathbb{Z}^d}$ such that $\lambda \in \sigma(H_{\tilde{\omega}}) \subset \Sigma_{\tilde{\omega}}$. Since the latter set is an interval containing $[-2d, 2d]$, it follows that Σ is an interval. □

5. Averaging of determinants and resolvents

In the energy regime where localization holds, eigenvalues are sensitive to fluctuations of the random potential. In particular, the mathematical expectation leads to a regularization of the finite volume eigenvalue counting function. Likewise, (appropriate) averages of the resolvent enjoy boundedness properties which are impossible to hold for resolvents associated to individual realizations of the random potential. In this section we discuss bounds of the type indicated above and in the following sections their relation to localization proofs.

We start with a well-known weak L^1-bound formulated in Lemma 5.1 (see, e.g., [AEN$^+$06, Lemma 3.1] for a more general result), which can be used to obtain bounds on certain averages of resolvents in the monotone case, i.e., where the single-site potential u is non-negative. Recall, a densely defined operator T on some Hilbert space $\mathcal{H}$ with inner product $\langle\cdot,\cdot\rangle_{\mathcal{H}}$ is called *dissipative* if $\mathrm{Im}\langle x, Tx\rangle_{\mathcal{H}} \geq 0$ for all $x \in D(T)$.

Lemma 5.1. *Let $A \in \mathbb{C}^{n\times n}$ be a dissipative matrix, $V \in \mathbb{R}^{n\times n}$ diagonal and strictly positive definite and $M_1, M_2 \in \mathbb{C}^{n\times n}$ be arbitrary matrices. Then there exists a constant C_{W} (independent of A, V, M_1, M_2 and n), such that*

$$\mathcal{L}\big\{r \in \mathbb{R} : \|M_1(A+rV)^{-1}M_2\|_{\mathrm{HS}} > t\big\} \leq C_{\mathrm{W}}\|M_1V^{-1/2}\|_{\mathrm{HS}}\|M_2V^{-1/2}\|_{\mathrm{HS}}\frac{1}{t}.$$

Here, $\mathcal{L}$ denotes the Lebesgue-measure and $\|\cdot\|_{\mathrm{HS}}$ the Hilbert Schmidt norm.

If the single-site potential u has fixed sign (and compact support) Lemma 5.1 is applicable and yields (together with a decoupling argument) the decay of fractional moments of the Green function. A generalization of Lemma 5.1 also applies to the continuous alloy-type model on $L^2(\mathbb{R}^d)$ to obtain bounds on fractional moments of the Green function, see [AEN$^+$06].

Since we allow the single-site potential to change its sign, we want to get rid of the positivity assumption on the operator V. The first observation is, that if one considers averages of determinants, then the definiteness of V plays no longer a role.

5.1. Estimates on polynomials and resolvents

In this section, we discuss estimates as used by Elgart, Tautenhahn, and Veselić in [ETV10] and [ETV11].

Lemma 5.2 ([ETV10]). *Let $n \in \mathbb{N}$, $P(x) = x^n + \cdots$ a monic polynomial of degree n, $0 \leq \rho \in L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$ and $s \in (0,1)$. Then we have*

$$\int_{\mathbb{R}} \frac{1}{|P(x)|^{s/n}}\rho(x)dx \leq \|\rho\|_{L^1}^{1-s}\|\rho\|_\infty^s \frac{2^s s^{-s}}{1-s}. \tag{3}$$

In [ETV10], this result is stated as

$$\int_{\mathbb{R}} |\det(A+rV)|^{-s/n}\,\rho(r)\mathrm{d}r \le |\det V|^{-s/n}\,\|\rho\|_{L^1}^{1-s}\|\rho\|_\infty^s \frac{2^s s^{-s}}{1-s}$$
$$\le |\det V|^{-s/n}\left(\lambda^{-s}\|\rho\|_{L^1} + \frac{2\lambda^{1-s}}{1-s}\|\rho\|_\infty\right)$$

for $\lambda > 0$, $A \in \mathbb{C}^{n\times n}$, and $V \in \mathbb{C}^{n\times n}$ invertible. Since $r \mapsto \frac{1}{\det(V)}\det(A+rV)$ is a monic polynomial of degree n, (3) implies this statement. For the converse, use that $P(x) = x^n + \sum_{j=0}^{n-1}\alpha_j x^j$ can be rewritten in terms of the companion matrix as

$$P(x) = \det(x+A), \quad A = \begin{pmatrix} 0 & 0 & \dots & 0 & -\alpha_0 \\ 1 & 0 & \dots & 0 & -\alpha_1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & -\alpha_{n-1} \\ 0 & 0 & \dots & 1 & -\alpha_n \end{pmatrix}.$$

The given form of Lemma 5.2 has the advantage that its relation to Pólya's inequality becomes more apparent. Namely, that for any monic polynomial $P(x) = x^n + \cdots$ of degree n, we have

$$|\{x \in \mathbb{R} : \quad |P(x)| \le \alpha\}| \le 4\left(\frac{\alpha}{2}\right)^{\frac{1}{n}} \tag{4}$$

for $\alpha > 0$.

In $d = 1$ the bound from Lemma 5.2 is precisely what is needed to show the boundedness of averaged fractional powers of the Green function, since certain matrix elements of the Green function can be represented as an inverse of a determinant of the above type. More precisely, if $d = 1$ and $\operatorname{supp} u = \{0, 1, \dots, n-1\}$ then we have for all $x \in \mathbb{Z}$ and $z \in \mathbb{C} \setminus \mathbb{R}$

$$|G_\omega(z; x, x+n-1)| = \frac{1}{|\det(A + \omega_x \lambda V)|},$$

where $V \in \mathbb{R}^{n\times n}$ is diagonal with diagonal elements $u(k-x)$, $k = x, \dots, x+n-1$, and where $A \in \mathbb{C}^{n\times n}$ is independent of ω_x. By Lemma 5.2 one obtains a bound on the expectation of an averaged fractional power on certain Green's function elements, which is sufficient to start the proof of localization via the fractional moment method. See [ETV10] for details.

Let us turn to the higher-dimensional case. For $B \in \mathbb{C}^{n\times n}$ we have

$$\|B^{-1}\| \le \frac{\|B\|^{n-1}}{|\det(B)|}.$$

Thus one can use (3) to obtain bounds on the inverse of $A + rV$. More precisely, we have for $s \in (0,1)$, $R > 0$ and A, V as above the estimate

$$\int_{-R}^{R} \left\|(A+rV)^{-1}\right\|^{s/n}\mathrm{d}r \le \frac{2R^{1-s}(\|A\| + R\|V\|)^{s(n-1)/n}}{s^s(1-s)\,|\det V|^{s/n}}. \tag{5}$$

In $d > 1$ Lemma 5.2 is no longer applicable, but estimate (5) is. However, the problem with estimate (5) is that the upper bound depends on the background operator A. Note that A arises by a Schur-complement formula and has a complicated dependence on the randomness. For this reason we have to assume additional properties on the single-site potential u (i.e., that u has fixed sign on the boundary of its (bounded) support) to show bounds on averaged fractional powers of the Green function, see Section 7 or [ETV11] for details.

5.2. Cartan estimates

We have now discussed the facts from complex analysis on which [ETV10] and [ETV11] are based. Let us now discuss the ones used in [Krü12] and Bourgain [Bou09], which are based on ideas from quasi-periodic Schrödinger operators see Bourgain, Goldstein and Schlag [BGS02, Bou04, Bou07]

Like the estimates discussed in the first part of this section, they control the size of the set where an analytic function is small. The main difference is that instead of requiring as an input that the analytic function is a polynomial of small degree, one assumes that the analytic function is not small at a single point. Here is the simplest form of such an estimate.

Theorem 5.3. *Let f be an analytic function on the disc of radius* 2e *satisfying*

$$\sup_{|z|<2\mathrm{e}} |f(z)| \leq 1, \quad |f(0)| \geq \varepsilon.$$

Then for $s > 0$, we have

$$|\{x \in [-1,1] : \quad |f(x)| \leq \mathrm{e}^{-s}\}| \leq 30\mathrm{e}^3 \exp\left(-\frac{s}{\log(\varepsilon^{-1})}\right).$$

Proof. For a proof see Theorem 11.3.4 in [Lev96]. See also Theorem 10.2 in [Krü12] for the deduction of this statement. □

This form of the Cartan estimate is not sufficient for the application to random Schrödinger operators as done in [Bou09] and [Krü12]. For these results, one needs to apply the Cartan estimate to functions depending on many variables, and thus needs an estimate that is well behaved in the number of variables. Such an estimate was first proven by Nazarov, Sodin, and Volberg [NSV03]. Unfortunately, they work on balls and not on poly-disks as necessary for our applications. The result for poly-disks was proven by Bourgain in [Bou09]. We will state here a formulation which was given in [Krü12].

Theorem 5.4 (Theorem 10.1, [Krü12]). *Denote by $\mathbb{D}_r$ the disc of radius r in $\mathbb{C}$. Let $f : (\mathbb{D}_{2\mathrm{e}})^n \to \mathbb{C}$ be an analytic function satisfying*

$$\|f\|_{L^\infty((\mathbb{D}_{2\mathrm{e}})^n)} \leq 1, \quad |f(0)| \geq \varepsilon.$$

Then for $s > 0$, we have

$$\frac{|\{x \in [-1,1]^n : \quad |f(x)| \leq \mathrm{e}^{-s}\}|}{2^n} \leq 30\mathrm{e}^3 n \exp\left(-\frac{s}{\log(\varepsilon^{-1})}\right).$$

Note that the dimension dependence is n. The proof is based on a clever change to spherical coordinates. We give an exposition on how to apply this to Schrödinger operators in Section 8.2.

6. Wegner estimates

This section is concerned with averaging of spectral projections. For any $\omega \in \Omega$ and $L \in \mathbb{N}$ the restriction $H_{\omega,L}$ is a selfadjoint finite rank operator. In particular its spectrum consists entirely of real eigenvalues $E(\omega, L, 1) \leq E(\omega, L, 2) \leq \cdots \leq E(\omega, L, |\Lambda_L|)$ counted including multiplicities. Wegner estimates [Weg81] are bounds on the expected number of eigenvalues of the finite box Hamiltonians $H_{\omega,L}$ in a compact energy interval $I = [E-\varepsilon, E+\varepsilon]$. They can be used as an ingredient for a localization proof via the multiscale analysis. The symbol $\chi_I(H_{\omega,L})$ denotes the spectral projection onto I with respect to the operator $H_{\omega,L}$.

Theorem 6.1 ([Ves10a], [PTV11]). *Assume that μ has a density ρ of finite total variation and u is not identically zero.*

(a) *Assume that the single-site potential u has support in $[0,n]^d \cap \mathbb{Z}^d$. Then there exists a constant c_u depending only on u such that for any $L \in \mathbb{N}$, $E \in \mathbb{R}$ and $\varepsilon > 0$ we have*

$$\mathbb{E}\left\{\operatorname{Tr} \chi_{[E-\varepsilon,E+\varepsilon]}(H_{\omega,L})\right\} \leq c_u \, |\operatorname{supp} u| \, \|\rho\|_{\mathrm{BV}} \, \varepsilon \, (2L+n)^{d\cdot(n+1)}.$$

(b) *Assume $\bar{u} = \sum_{k\in\mathbb{Z}^d} u(k) \neq 0$ and that ρ has compact support. Then we have for any $L \in \mathbb{N}$, $E \in \mathbb{R}$ and $\varepsilon > 0$*

$$\mathbb{E}\left\{\operatorname{Tr} \chi_{[E-\varepsilon,E+\varepsilon]}(H_{\omega,L})\right\} \leq \frac{8}{\bar{u}} \, \min\big((2L)^d, |\operatorname{supp} u|\big) \, \|\rho\|_{\mathrm{BV}} \, \varepsilon \, (2L+m)^d,$$

where $m \in \mathbb{N}$ is such that $\sum_{\|k\|\geq m} |u(k)| \leq |\bar{u}/2|$.

(c) *Assume there are constants $C, \alpha \in \mathbb{R}^+$ such that $|u(k)| \leq Ce^{-\alpha\|k\|_1}$ for all $k \in \mathbb{Z}^d$, and that ρ has bounded support. Then there exists $c_u > 0$ and $I_0 \in \mathbb{N}_0^d$ both depending only on u such that for any $L \in \mathbb{N}$, $E \in \mathbb{R}$ and $\varepsilon > 0$ we have*

$$\mathbb{E}\big\{\operatorname{Tr} \chi_{[E-\varepsilon,E+\varepsilon]}(H_{\omega,L})\big\} \leq c_u \|\rho\|_{\mathrm{BV}} \, \varepsilon \, (2L+1)^{2d+|I_0|}.$$

In the case where the support of u is compact, part (b) of Theorem 6.1 has an important corollary.

Corollary 6.2 ([Ves10a]). *Assume $\bar{u} \neq 0$ and $\operatorname{supp} u \subset [0,n] \cap \mathbb{Z}^d$. Then we have for any $L \in \mathbb{N}$, $E \in \mathbb{R}$ and $\varepsilon > 0$*

$$\mathbb{E}\left\{\operatorname{Tr} \chi_{[E-\varepsilon,E+\varepsilon]}(H_{\omega,L})\right\} \leq \frac{4}{\bar{u}} \operatorname{rank} u \, \|\rho\|_{BV} \, \varepsilon \, (2L+n)^d.$$

In particular, the function $\mathbb{R} \ni E \to \mathbb{E}\left\{\operatorname{Tr}\left[\chi_{(-\infty,E]}(H_{\omega,L})\right]\right\}$ is Lipschitz continuous.

Remark 6.3.

(i) Note, that apart of the exponential decay condition on u, Theorem 6.1 (c) gives a Wegner estimate for the discrete alloy-type model without any further

assumption on the single-site potential. In particular, u may change its sign arbitrarily.

(ii) The proof of Theorem 6.1 is (roughly speaking) based on a transformation of the probability space to recover monotonicity. With other words, once you find a finite linear combination of translated single-site potentials which is positive, then monotone spectral averaging leads to a Wegner estimate, see [KV06, Ves10b, Ves10a, PTV11] where this approach is used.

Remark 6.4 (Continuous alloy-type model). The *alloy-type model* is the Schrödinger operator $H_\omega = -\Delta + V_0 + V_\omega$ on $L^2(\mathbb{R}^d)$, where Δ is the Laplacian on $\mathbb{R}^d$, V_0 is a $\mathbb{Z}^d$ periodic potential, and V_ω is given by

$$V_\omega(x) = \sum\nolimits_{k\in\mathbb{Z}^d} \omega_k U(x-k)$$

with $U : \mathbb{R}^d \to \mathbb{R}$ a single-site potential. It is assumed that V_0 and V_ω are infinitesimally bounded with respect to Δ, with constants uniformly bounded in $\omega \in \Omega$. We will be concerned with the case that the distribution μ has a density ρ of finite total variation and U is a *generalized step-function*, i.e.,

$$U(x) = \sum\nolimits_{k\in\mathbb{Z}^d} u(k) w(x-k).$$

Here $L^p_{\mathrm{c}}(\mathbb{R}^d) \ni w \geq \kappa\chi_{(-1/2,1/2)^d}$ with $\kappa > 0$, $p = 2$ for $d \leq 3$ and $p > d/2$ for $d \geq 4$, and $u \in \ell^1(\mathbb{Z}^d;\mathbb{R})$ the discrete single-site potential.

In [PTV11] a Wegner estimate similar to part (c) in Theorem 6.1 is proven for the (continuous) alloy-type model. More precisely, assume that U is a generalized step-function and there are constants $C, \alpha \in \mathbb{R}^+$ such that $|u(k)| \leq C\mathrm{e}^{-\alpha\|k\|_1}$. Then there exists $c_U > 0$ and $I_0 \in \mathbb{N}_0^d$ both depending only on U such that for any $L \in \mathbb{N}$ and any bounded interval $I := [E_1, E_2] \subset \mathbb{R}$ we have

$$\mathbb{E}\big\{\operatorname{Tr}\chi_I(H_{\omega,L})\big\} \leq \mathrm{e}^{E_2} c_U \|\rho\|_{\mathrm{Var}} |I| (2l+1)^{2d+|I_0|}.$$

Here $H_{\omega,L}$ denotes the restriction of H_ω to the cube $(-L,L)^d \subset \mathbb{R}^d$ with either Dirichlet or periodic boundary conditions. The stated Wegner estimate is valid for both types of boundary conditions.

A drawback of this results is that they fail if U is not a generalized step function. Contrary to this, the papers [Klo95, HK02] obtain Wegner estimates for energies in a neighborhood of the infimum of the spectrum which are valid for arbitrary non-vanishing single-site potentials $u \in C_{\mathrm{c}}(\mathbb{R}^d)$ and coupling constants whose distribution has a piecewise absolutely continuous density.

Remark 6.5 (Localization). Notice that the Wegner estimates from Theorem 6.1 are valid on the whole energy axis. Therefore, one can prove localization via multiscale analysis [FS83, DK89] in any energy region where an initial length scale estimate holds. If the single-site potential does not have compact support one has to use a modified version of the multiscale analysis [KSS98a].

7. Localization via fractional moment method

7.1. Boundedness of fractional moments

The lemmata from Section 5 can be used to obtain bounds on averaged fractional powers of the Green function. One possible approach to overcome the problems arising because of the lack of monotonicity is to use a special transformation of the probability space to recover some monotonicity which makes Lemma 5.1 applicable. This was done in [ETV11, Appendix] to obtain the following Theorem.

Theorem 7.1 ([ETV11]). *Assume*

(i) *The measure μ has a density ρ in the Sobolev space $W^{1,1}(\mathbb{R})$.*
(ii) *The single-site potential u has compact support and satisfies $\overline{u} := \sum_{k\in\mathbb{Z}^d} u(k) \neq 0$.*

Let further $\Lambda \subset \mathbb{Z}^d$ finite and $s \in (0,1)$. Then we have for all $x, y \in \Lambda$ and $z \in \mathbb{C}\backslash\mathbb{R}$

$$\mathbb{E}\Big\{\big|G_{\omega,\Lambda}(z;x,y)\big|^s\Big\} \leq \frac{1}{1-s}\left(\frac{2\|\rho'\|_{L^1}C}{\overline{u}}\right)^s \frac{1}{\lambda^s}$$

where C is a constant depending only on u.

The disadvantage of Theorem 7.1 is that it is non-local in the sense that we have to average with respect of the entire disorder present in the model. At the moment we do not know how to conclude the decay of fractional moments of the Green function (cf. Definition 3.3) from the non-local a priori bound in Theorem 7.1. A somewhat stronger condition, however, is sufficient to ensure decay of fractional moments. We will review this result next.

Assumption (A). Assume that

1. the measure μ has a bounded, compactly supported density $\rho \in L^\infty(\mathbb{R})$.
2. $\Theta := \operatorname{supp} u$ is finite and $u(k) > 0$ for $k \in \partial^{\mathrm{i}}\Theta$.

Under Assumption (A) and with the help of Ineq. (5) it is possible to prove a local a priori bound, which is applicable to conclude the decay of fractional moments of the Green function, see Section 7.2. Let us first introduce some more notation. For $x \in \mathbb{Z}^d$ we denote by $\mathcal{N}(x) = \{k \in \mathbb{Z}^d : |x-k|_1 = 1\}$ the neighborhood of x. For $\Lambda \subset \mathbb{Z}^d$ we also define $\Lambda_x = \Lambda + x = \{k \in \mathbb{Z}^d : k - x \in \Lambda\}$.

Lemma 7.2 ([ETV11]). *Let Assumption* (A) *be satisfied, $\Gamma \subset \mathbb{Z}^d$, $m > 0$ and $s \in (0,1)$.*

(a) *Then there is a constant C_s, depending only on d, ρ, u, m and s, such that for all $z \in \mathbb{C}\setminus\mathbb{R}$ with $|z| \leq m$, all $x, y \in \Gamma$ and all $b_x, b_y \in \mathbb{Z}^d$ with $x \in \Theta_{b_x}$ and $y \in \Theta_{b_y}$*

$$\mathbb{E}_N\Big\{\big|G_{\omega,\Gamma}(z;x,y)\big|^{s/(2|\Theta|)}\Big\} \leq C_s \Xi_s(\lambda),$$

where $\Xi_s(\lambda) = \max\{\lambda^{-s/(2|\Theta|)}, \lambda^{-2s}\}$ and $N = \{b_x, b_y\} \cup \mathcal{N}(b_x) \cup \mathcal{N}(b_y)$.

(b) *Then there is a constant D_s, depending only on d, ρ, u and s, such that for all $z \in \mathbb{C} \setminus \mathbb{R}$, all $x, y \in \Gamma$ and all $b_x, b_y \in \mathbb{Z}^d$ with*

$$x \in \Theta_{b_x} \cap \Gamma \subset \partial^{\mathrm{i}}\Theta_{b_x} \quad \text{and} \quad y \in \Theta_{b_y} \cap \Gamma \subset \partial^{\mathrm{i}}\Theta_{b_y}$$

we have

$$\mathbb{E}_{\{b_x, b_y\}}\Big\{ \big|G_{\omega,\Gamma}(z;x,y)\big|^s \Big\} \leq D_s \lambda^{-s}.$$

7.2. Decay of fractional moments

Now we explain how the so-called finite volume criterion implies exponential decay of the Green function. Together with the a-priori bound from Lemma 7.2 this gives us Theorem 7.5. For proofs we refer the reader to [ETV11].

To formulate the results of this section we will need the following notation: let $\Gamma \subset \mathbb{Z}^d$, fix $L \geq \operatorname{diam}\Theta + 2$, let

$$B = \partial^{\mathrm{i}}\Lambda_L,$$

and define the sets

$$\hat{\Lambda}_x = \{k \in \Gamma : k \in \Theta_b \text{ for some } b \in \Lambda_{L,x}\}$$

and

$$\hat{W}_x = \{k \in \Gamma : k \in \Theta_b \text{ for some } b \in B_x\}.$$

Recall that for $\Gamma \subset \mathbb{Z}^d$ we denote by $\Gamma_x = \Gamma + x = \{k \in \mathbb{Z}^d : k - x \in \Gamma\}$ the translate of Γ. Hence $(\Lambda_L)_x = \Lambda_{L,x}$ and $\hat{W}_x$ is the union of translates of Θ along the sides of B_x, restricted to the set Γ. For $\Gamma \subset \mathbb{Z}^d$ we can now introduce the sets

$$\Lambda_x := \hat{\Lambda}_x^+ \cap \Gamma \quad \text{and} \quad W_x = \hat{W}_x^+ \cap \Gamma$$

which will play a role in the assertions below.

Theorem 7.3 ([ETV11], Finite volume criterion). *Suppose that Assumption* (A) *is satisfied. Let $\Gamma \subset \mathbb{Z}^d$, $z \in \mathbb{C} \setminus \mathbb{R}$ with $|z| \leq m$ and $s \in (0, 1/3)$. Then there exists a constant B_s which depends only on d, ρ, u, m, s, such that if the condition*

$$b_s(\lambda, L, \Lambda) := \frac{B_s L^{3(d-1)} \Xi_s(\lambda)}{\lambda^{2s/(2|\Theta|)}} \sum_{w \in \partial^{\mathrm{o}} W_x} \mathbb{E}\big\{ |G_{\omega,\Lambda\setminus W_x}(z;x,w)|^{s/(2|\Theta|)} \big\} < b \qquad (6)$$

is satisfied for some $b \in (0,1)$, arbitrary $\Lambda \subset \Gamma$, and all $x \in \Lambda$, then for all $x, y \in \Gamma$

$$\mathbb{E}\big\{ |G_{\omega,\Gamma}(z;x,y)|^{s/(2|\Theta|)} \big\} \leq A \mathrm{e}^{-\mu|x-y|_\infty}.$$

Here

$$A = \frac{C_s \Xi_s(\lambda)}{b} \quad \text{and} \quad \mu = \frac{|\ln b|}{L + \operatorname{diam}\Theta + 2},$$

with C_s as in Lemma 7.2.

Note that condition (6) can be achieved by choosing λ sufficiently big and applying Lemma 7.2. The core of the proof of the theorem is Lemma 7.4.

Lemma 7.4 ([ETV11]). *Let Assumption* (A) *be satisfied. Let* $\Gamma \subset \mathbb{Z}^d$, $s \in (0, 1/3)$, $m > 0$ *and* $b_s(\lambda, L, \Lambda)$ *be the constant from Theorem* 7.3. *Then we have for all* $x, y \in \Gamma$ *with* $y \notin \Lambda_x$ *and all* $z \in \mathbb{C} \setminus \mathbb{R}$ *with* $|z| \leq m$ *the bound*

$$\mathbb{E}\big\{|G_{\omega,\Gamma}(z;x,y)|^{\frac{s}{2|\Theta|}}\big\} \leq \frac{b_s(\lambda, L, \Gamma)}{|\partial^{\mathrm{o}}\Lambda_x|} \sum_{r \in \partial^{\mathrm{o}}\Lambda_x} \mathbb{E}\big\{|G_{\omega,\Gamma\setminus\Lambda_x}(z;r,y)|^{\frac{s}{2|\Theta|}}\big\}.$$

The combination of Theorem 7.3 and Lemma 7.2 yield the following result on exponential decay of a fractional moment of the Green function under a strong disorder assumption.

Theorem 7.5 ([ETV11]). *Let* $\Gamma \subset \mathbb{Z}^d$, $s \in (0, 1/3)$ *and suppose that Assumption* (A) *is satisfied. Then for a sufficiently large* λ *there are constants* $\mu, A \in \mathbb{R}^+$, *depending only on* d, ρ, u, s *and* λ, *such that for all* $z \in \mathbb{C} \setminus \mathbb{R}$ *and all* $x, y \in \Gamma$

$$\mathbb{E}\big\{|G_{\omega,\Gamma}(z;x,y)|^{s/(2|\Theta|)}\big\} \leq A\mathrm{e}^{-\mu|x-y|_\infty}.$$

7.3. Localization

The existing proofs of localization via the fractional moment method use either the Simon Wolff criterion, see, e.g., [SW86, AM93, ASFH01], or the RAGE-Theorem, see, e.g., [Aiz94, Gra94, AEN$^+$06]. Neither dynamical nor spectral localization can be directly inferred from the behavior of the Green function using the existent methods for the model in Section 2. The reason is that the random variables $V_\omega(x)$, $x \in \mathbb{Z}^d$, are not independent, while the dependence of H_ω on the i.i.d. random variables ω_k, $k \in \mathbb{Z}^d$, is not monotone.

We outline a new variant for concluding exponential localization from bounds on averaged fractional powers of Green's function (cf. Section 7.2) without using the multiscale analysis, see [ETV10, ETV11] for details. This is done by showing that fractional moment bounds imply the "typical output" of the multiscale analysis, i.e., the hypothesis of Theorem 2.3 in [DK89]. Then one can conclude localization using existent methods.

The next proposition states that certain bounds on averaged fractional moments of Green's function imply the hypothesis of Theorem 2.3 in [DK89] (without applying the induction step of the multiscale analysis).

Proposition 7.6 ([ETV11]). *Let* $I \subset \mathbb{R}$ *be a bounded interval and* $s \in (0, 1)$. *Assume the following two statements:*

(i) *There are constants* $C, \mu \in \mathbb{R}^+$ *and* $L_0 \in \mathbb{N}_0$ *such that*

$$\mathbb{E}\big\{|G_{\omega,\Lambda_{L,k}}(E;x,y)|^s\big\} \leq C\mathrm{e}^{-\mu|x-y|_\infty}$$

for all $k \in \mathbb{Z}^d$, $L \in \mathbb{N}$, $x, y \in \Lambda_{L,k}$ *with* $|x - y|_\infty \geq L_0$, *and all* $E \in I$.

(ii) *There is a constant* $C' \in \mathbb{R}^+$ *such that*

$$\mathbb{E}\big\{|G_{\omega,\Lambda_{L,k}}(E + \mathrm{i}\varepsilon;x,x)|^s\big\} \leq C'$$

for all $k \in \mathbb{Z}^d$, $L \in \mathbb{N}$, $x \in \Lambda_{L,k}$, $E \in I$ *and all* $\varepsilon \in (0, 1]$.

Then we have for all $L \geq \max\{8\ln(8)/\mu, L_0, -(8/5\mu)\ln(|I|/2)\}$ *and all* $x, y \in \mathbb{Z}^d$ *with* $|x-y|_\infty \geq 2L + \operatorname{diam}\Theta + 1$ *that*

$$\mathbb{P}\{\forall\, E \in I \text{ either } \Lambda_{L,x} \text{ or } \Lambda_{L,y} \text{ is } (\mu/8, E)\text{-regular}\} \geq 1 - 8|\Lambda_{L,x}|(C|I| + 4C'|\Lambda_{L,x}|/\pi)\mathrm{e}^{-\mu s L/8}.$$

In the proof of Proposition 7.6 Hypothesis (ii) is only used to obtain a Wegner estimate. In particular, there is a relation between a Wegner estimate and the a priori bound in the fractional moment method. The following proposition states that the boundedness of averaged fractional powers of the diagonal Green function elements implies a Wegner estimate.

Proposition 7.7 ([ETV11]). *Let* $I \subset \mathbb{R}$ *be an interval,* $s \in (0,1)$ *and* $c > 0$. *Assume there is a constant* $C \in \mathbb{R}^+$ *such that*

$$\mathbb{E}\big\{|G_{\omega,L}(E + \mathrm{i}\varepsilon; x, x)|^s\big\} \leq C$$

for all $L \in \mathbb{N}$, $x \in \Lambda_L$, $E \in I$ *and all* $\varepsilon \in (0, c]$. *Then we have for all* $[a,b] \subset I$ *with* $0 < b - a \leq c$ *that*

$$\mathbb{E}\big\{\operatorname{Tr}\chi_{[a,b]}(H_{\omega,L})\big\} \leq \frac{4C}{\pi}|b-a|^s|\Lambda_L|.$$

Proof. Let $[a,b] \subset I$ with $0 < b - a \leq c$. Since we have for any $\lambda \in \mathbb{R}$ and $0 < \varepsilon \leq b - a$

$$\arctan\left(\frac{\lambda - a}{\varepsilon}\right) - \arctan\left(\frac{\lambda - b}{\varepsilon}\right) \geq \frac{\pi}{4}\,\chi_{[a,b]}(\lambda),$$

one obtains an inequality version of Stones formula:

$$\langle \delta_x, \chi_{[a,b]}(H_{\omega,L})\delta_x\rangle \leq \frac{4}{\pi}\int_{[a,b]} \operatorname{Im}\{G_{\omega,L}(E + \mathrm{i}\varepsilon; x, x)\}\,\mathrm{d}E \quad \forall\, \varepsilon \in (0, b-a].$$

Using triangle inequality, $|\operatorname{Im} z| \leq |z|$ for $z \in \mathbb{C}$, Fubini's theorem, $|G_{\omega,L}(E + \mathrm{i}\varepsilon; x, x)|^{1-s} \leq \operatorname{dist}(\sigma(H_{\omega,L}), E + i\varepsilon)^{s-1} \leq \varepsilon^{s-1}$ and hypothesis (ii) we obtain for all $\varepsilon \in (0, b-a]$

$$\begin{aligned}
\mathbb{E}\big\{\operatorname{Tr}\chi_{[a,b]}(H_{\omega,L})\big\} &\leq \mathbb{E}\Big\{\sum_{x\in\Lambda_L}\frac{4}{\pi}\int_{[a,b]}\operatorname{Im}\{G_{\omega,L}(E+\mathrm{i}\varepsilon;x,x)\}\,\mathrm{d}E\Big\} \\
&\leq \frac{\varepsilon^{s-1}}{\pi/4}\sum_{x\in\Lambda_L}\int_{[a,b]}\mathbb{E}\Big\{\big|G_{\omega,L}(E+\mathrm{i}\varepsilon;x,x)\big|^s\Big\}\mathrm{d}E \\
&\leq 4\pi^{-1}\varepsilon^{s-1}|\Lambda_L|\,|b-a|C.
\end{aligned}$$

We minimize the right-hand side by choosing $\varepsilon = b - a$ and obtain the statement of the proposition. □

Let us note that a Wegner estimate implies the boundedness of an averaged fractional power of the (finite-volume) Green function. At the moment we only know a proof where the bound depends polynomially on the volume of the cube.

From the discussion so far it follows that Hypothesis (ii) of Proposition 7.6 can be replaced by a Wegner estimate. Specifically, the following assertion holds true.

Proposition 7.8 ([ETV11]). *Let $I \subset \mathbb{R}$ be a bounded interval and $s \in (0,1)$. Assume the following two statements:*

(i) *There are constants $C, \mu \in \mathbb{R}^+$ and $L_0 \in \mathbb{N}_0$ such that*

$$\mathbb{E}\big\{|G_{\omega,\Lambda_{L,k}}(E;x,y)|^s\big\} \leq C\mathrm{e}^{-\mu|x-y|_\infty}$$

for all $k \in \mathbb{Z}^d$, $L \in \mathbb{N}$, $x, y \in \Lambda_{L,k}$ with $|x-y|_\infty \geq L_0$, and all $E \in I$.

(ii) *There are constants $C_{\mathrm{W}} \in \mathbb{R}^+$, $\beta \in (0,1]$, and $D \in \mathbb{N}$ such that*

$$\mathbb{P}\big\{\sigma(H_{\omega,\Lambda_L}) \cap [a,b] \neq \emptyset\big\} \leq C_{\mathrm{W}}|b-a|^\beta L^D$$

for all $L \in \mathbb{N}$ and all $[a,b] \subset I$.

Then we have for all $L \geq \max\{8\ln(2)/\mu, L_0, -(8/5\mu)\ln(|I|/2)\}$ and all $x, y \in \mathbb{Z}$ with $|x-y|_\infty \geq 2L + \operatorname{diam}\Theta + 1$ that

$$\mathbb{P}\{\forall\, E \in I \text{ either } \Lambda_{L,x} \text{ or } \Lambda_{L,y} \text{ is } (\mu/8, E)\text{-regular}\} \geq 1 - 8(2L+1)^d|(C\,|I| + C_{\mathrm{W}}L^D)\mathrm{e}^{-\mu\beta L/8}.$$

To conclude exponential localization from the estimates provided in Propositions 7.6 or 7.8 we will use Theorem 2.3 in [DK89]. More precisely we need a slight extension of the result, which can be proven with the same arguments as the original result. What matters for the proof of Theorem 7.9 is that there is an $l_0 \in \mathbb{N}$ such that potential values at different lattice sites are independent if their distance is larger or equal l_0.

Theorem 7.9 ([DK89]). *Let $I \subset \mathbb{R}$ be an interval and let $p > d$, $L_0 > 1$, $\alpha \in (1, 2p/d)$ and $m > 0$. Set $L_k = L_{k-1}^\alpha$, for $k \in \mathbb{N}$. Suppose that for any $k \in \mathbb{N}_0$*

$$\mathbb{P}\{\forall\, E \in I \text{ either } \Lambda_{L_k,x} \text{ or } \Lambda_{L_k,y} \text{ is } (m,E)\text{-regular}\} \geq 1 - L_k^{-2p}$$

for any $x, y \in \mathbb{Z}^d$ with $|x-y|_\infty \geq 2L_k + \operatorname{diam}\Theta + 1$. Then H_ω exhibits exponential localization in I for almost all $\omega \in \Omega$.

From Proposition 7.6 and Theorem 7.9 we conclude that the decay of fractional moments of the Green function implies exponential localization.

Theorem 7.10 ([ETV11]). *Let $s \in (0,1)$, $C, \mu, \in \mathbb{R}^+$, and $I \subset \mathbb{R}$ be a interval. Assume that*

$$\mathbb{E}\big\{|G_{\omega,\Lambda_{L,k}}(E + \mathrm{i}\varepsilon; x, y)|^s\big\} \leq C\mathrm{e}^{-\mu|x-y|_\infty}$$

for all $k \in \mathbb{Z}^d$, $L \in \mathbb{N}$, $x, y \in \Lambda_{L,k}$, $E \in I$ and all $\varepsilon \in (0,1]$. Then H_ω exhibits exponential localization in I for almost all $\omega \in \Omega$.

Putting together Theorem 7.5 and Theorem 7.10, one can prove without the use of MSA exponential localization in the case of sufficiently large disorder.

Theorem 7.11 ([ETV11], Exponential localization via fractional moments). *Let Assumption* (A) *be satisfied and λ sufficiently large. Then H_ω exhibits exponential localization for almost all $\omega \in \Omega$.*

8. Localization via multiscale analysis

The goal of this section is to explain how to obtain localization for the discrete alloy-type model using multiscale analysis under the assumptions

- $u(0) \neq 0$, $|u(k)| \leq \mathrm{e}^{-c|k|_\infty}$ for some positive constant c, and
- the measure μ has a bounded density ρ with $\operatorname{supp} \rho \subset [-1, 1]$.

For background on multiscale analysis, we refer for example to [Kir08] and [Sto01]. The main idea behind the multiscale analysis is that the decay of the Green function on some scale implies its decay on a larger scale as well. In order to quantify decay of the Green's function, we introduce

Definition 8.1. Let $\gamma > 0$. A box $\Lambda_{r,n} \subseteq \mathbb{Z}^d$ is called γ-suitable for $H_\omega - E$ if

(i) $\|(H_{\omega,\Lambda_{r,n}} - E)^{-1}\| \leq \mathrm{e}^{\sqrt{r}}$.
(ii) For $x, y \in \Lambda_{r,n}$ with $|x - y| \geq \frac{r}{10}$, we have

$$|G_{\omega,\Lambda_{r,n}}(E; x, y)| \leq \frac{1}{|\Lambda_{r,n}|} \mathrm{e}^{-\gamma|x-y|}.$$

Only condition (ii) is needed for multiscale analysis when a Wegner estimate is available. However, our goal is to do without it and then (i) takes the role of the Wegner estimate.

The essential step in [Krü12] to conclude exponential and dynamical localization is

Theorem 8.2. *Given $\gamma > 0$ and $E \in \mathbb{R}$, there is $R = R(\gamma, u, \mu) \geq 1$ such that if*

$$\mathbb{P}\{\Lambda_r \text{ is not } \gamma\text{-suitable for } H_\omega - E\} \leq \frac{1}{r^{4d}} \tag{7}$$

holds for $1 \leq r \leq R$ then it holds for all $r > 0$ with γ replaced by $\gamma/2$.

This theorem implies localization at large coupling:

- For large coupling, the Combes–Thomas estimate and a probabilistic computation imply the assumptions of Theorem 8.2. This can be found in Appendix A of [Krü12].
- The conclusions of this theorem imply localization. Exponential localization is proven in Section 7 of [BK05] and dynamical localization in Sections 16 to 18 of [Krü12].

Theorem 8.3 ([Krü12]). *Let $\lambda > 0$ be large enough. Then, for almost all $\omega \in \Omega$, H_ω exhibits dynamical (and spectral) localization.*

We will now discuss how to prove Theorem 8.2. The main difficulty is to conclude from a probabilistic estimate on some scale, i.e., (7) for some $r \geq 1$, the estimate on the resolvent with a better probability on a larger scale, i.e.,

$$\mathbb{P}\{\|(H_{\omega,R} - E)^{-1}\| > \mathrm{e}^{\sqrt{R}}\} < \frac{1}{R^{4d}}. \tag{8}$$

It turns out, that we do not know how to do this. Instead we assume that (7) holds for all values of r in a range $[r_1, r_2]$ with $r_2 = (r_1)^3$ and use this to conclude (8).

Just using a single value of r one can conclude that there exists an event $\mathcal{B}$ with $\mathbb{P}\{\mathcal{B}\} \leq 1/(2R^{4d})$, such that for $\omega \notin \mathcal{B}$, there are $m_1, \ldots, m_L$ with L uniformly bounded in R such that for

$$\Xi = \Lambda_R \setminus \bigcup_{\ell=1}^{L} \Lambda_{r,m_\ell}$$

we have

$$\|(H_{\omega,\Xi} - E)^{-1}\| \leq \mathrm{e}^{3\sqrt{r}}. \tag{9}$$

This follows from the probabilistic estimates in Section 5 and the estimates on the resolvent in Section 9 of [Krü12].

Then one uses the assumption on the whole range $[r_1, r_2]$ to conclude that there exists a choice $\tilde{\omega}$ which agrees with ω except near the m_ℓ such that

$$\|(H_{\tilde{\omega},R} - E)^{-1}\| \leq \mathrm{e}^{10\sqrt{r_2}}.$$

We illustrate this in the next subsection. See Section 12 of [Krü12] or Section 2 in [Bou09] for the entire implementation.

In Subsection 8.2, we illustrate how to use Cartan's lemma to conclude from this information that the estimate (8) holds. For the entire analysis, see Sections 13 to 15 in [Krü12].

Then one can conclude the decay of the Green function as in the usual multiscale analysis finishing the proof of Theorem 8.2.

8.1. Probabilistic estimates

In this section, we illustrate a new form of probabilistic estimate not necessary in the usual versions of multiscale analysis. We will assume for $r_\ell = r \cdot \ell$ with $\ell = 1, \ldots, L$ that

$$\mathbb{P}\{\|(H_{\omega,r_\ell} - E)^{-1}\| > A\} \leq \varepsilon$$

and that $\mathrm{supp}(u) \subseteq \Lambda_{r-1}$. The main conclusion will be

Lemma 8.4. *There exists an event $\mathcal{B}$ with*

$$\mathbb{P}\{\mathcal{B}\} \leq \varepsilon^L$$

such that for $\omega \notin \mathcal{B}$, there exists ℓ such that there exists $\tilde{\omega}$ with

$$\omega_n = \tilde{\omega}_n, \quad n \notin \Lambda_{r_{\ell-1}}$$

such that

$$\|(H_{\tilde{\omega},r_\ell} - E)^{-1}\| \leq A.$$

Proof. Denote by X_ℓ the set of all ω such that for all $\tilde{\omega}$ with

$$\omega_n = \tilde{\omega}_n, \quad n \notin \Lambda_{r_{\ell-1}}$$

we have

$$\|(H_{\tilde{\omega},r_\ell} - E)^{-1}\| > A.$$

By assumption, we have that $\mathbb{P}\{X_\ell\} \leq \varepsilon$ and one can check that X_ℓ and X_j are independent events for $j \neq \ell$.

Take $\mathcal{B} = \bigcap_{\ell=1}^{L} X_\ell$. Independence implies $\mathbb{P}\{\mathcal{B}\} \leq \varepsilon^L$. The claim follows by construction. □

This lemma implies that given $m \in \Lambda_R$, one can always find some $\tilde{r} \leq r^2$ and $\tilde{\omega}$ such that the resolvent estimate holds for the cube $\Lambda_{\tilde{r},m}$. Using Theorem 9.4. in [Krü12], one can then extend (9) to the estimate

$$\|(H_{\tilde{\omega},R} - E)^{-1}\| \leq \mathrm{e}^r$$

for some $\tilde{\omega}$ for which $\tilde{\omega}_n = \omega_n$ whenever $|n - m_\ell| \geq r^2$.

8.2. An application of Cartan's lemma

In this section, we give a simple application of Cartan's Lemma to random Schrödinger operators. The main goal is to give a simplified account of what happens in Sections 11 to 14 of [Krü12].

Suppose we want to establish a bound on $\|(H_{\omega,L} - E)^{-1}\|$ and that we already know:

(α) For each ω, there exists $n \in \Lambda_L$ such that

$$\|(H_{\omega,\Lambda_L \setminus \Lambda_{r,n}} - E)^{-1}\| \leq A.$$

(β) For each n and ω, there exists $\tilde{\omega}$ with

$$\omega_m = \tilde{\omega}_m, \quad m \in \Lambda_L \setminus \{n\}$$

and

$$\|(H_{\tilde{\omega},L} - E)^{-1}\| \leq A.$$

This is a simplification. First, one must allow for more exceptional sites. Second, such a statement can only hold in probabilistic terms in a multi-scale scheme. [Bou09] was the first paper to propose a scheme to check (β).

For simplicity, we will also assume that

(γ) $\mathrm{supp}(u)$ is contained in Λ_r.

The analysis of u exponential decaying requires a perturbative analysis, which we avoid here for the sake of exposition.

Proposition 8.5. *Assume (α), (β), and (γ). Then*

$$\mathbb{P}\{\|(H_{\omega,L} - E)^{-1}\| \geq \mathrm{e}^s\} \leq \mathrm{e}^{-\frac{\delta s}{\log(A) \cdot r^d}}$$

for some small constant $\delta > 0$.

The proof of this proposition will be split into two parts. First, we consider the case when the single-site potential u is equal to δ_0. Second, we discuss what needs to be modified for general u. We can fix n. Then the claim follows by summing over the possible number of choices of n (less than $(3L)^d$ many).

Assume now that $u = \delta_0$, then we can write $H_{\omega,L} - E$ as

$$H_{\omega,L} - E = \begin{pmatrix} \omega_n - E & \Gamma \\ \Gamma^* & H_{\omega,\Lambda_L \setminus \{n\}} - E \end{pmatrix}.$$

An application of the Schur-complement formula shows that

$$\|(H_{\omega,L} - E)^{-1}\| \leq C \cdot A^2 |\omega_n - E - \Gamma(H_{\omega,\Lambda_L \setminus \{n\}} - E)^{-1}\Gamma^*|^{-1},$$

for some constant C. Since the dependence in ω_n is linear, it is easy to see that the set of ω_n, where the right-hand side is large, is small. Hence, we are done.

It is noteworthy that this argument did not use (β). Of course, (β) and even (α) is not necessary since the standard proof of Wegner's estimate works.

Let us now discuss what happens when u is not δ_0, but is supported on finitely many points. One could apply the Schur-complement formula as before, but the object one then obtains has a too non-trivial dependence on ω_n to be useful. Define

$$\tilde{\Xi} = \Lambda_{r,n} \cap \Lambda_L, \quad \tilde{\Theta} = \Lambda_L \setminus \tilde{\Xi}.$$

Then $H_\omega^{\tilde{\Theta}} - E$ is independent of ω_n. So an application of the Schur-complement formula shows that

$$\|(H_{\omega,L} - E)^{-1}\| \leq CA^2 \|(H_{\omega,\tilde{\Xi}} - E - \Gamma(H_{\omega,\tilde{\Theta}} - E)^{-1}\Gamma^*)^{-1}\|.$$

Fix $\{\omega_m\}_{m \neq n}$ and define a function of single-variable ω_n by

$$f(\omega_n) = \det(H_{\omega,\tilde{\Xi}} - E - \Gamma(H_{\omega,\tilde{\Theta}} - E)^{-1}\Gamma^*).$$

Define $R = |\tilde{\Xi}|$. By (α), we obtain for z with $|z| < 6$ that

$$|f(z)| \leq CA^R,$$

and by (β) that

$$|f(\tilde{\omega}_n)| \geq \frac{1}{A^R}.$$

Hence, we can apply Cartan's Lemma to obtain

$$|\{\omega_n : \quad |f(\omega_n)| \leq \mathrm{e}^{-s}\}| \leq C \exp\left(-\frac{s}{R\log(A)}\right).$$

The claim follows by $R \leq (3r)^d$.

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Operator Domains and SUSY Breaking in a Model of SUSYQM with a Singular Potential

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Abstract. The self-adjoint extension of the symmetric supercharges and Hamiltonian of a model of Supersymmetric Quantum Mechanics on the half-line, for the case of a singular superpotential, is analyzed. The compatibility of the domains of definition of the different operators and the possibility of effectively implement the graded superalgebra in a dense subspace of the Hilbert space is considered. As a consequence, conditions for SUSY breaking in this model are established.

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1. Introduction

Supersymmetry (SUSY) [1, 2, 3, 4, 5, 6, 8, 9, 10, 11] gives desirable features to quantum field theories, like an improved ultraviolet behavior, but also predicts superpartner states with degenerate mass which are not observed experimentally. Therefore, this symmetry is expected to be *spontaneously broken*.

Let us mention that a symmetry of the Hamiltonian is said to be spontaneously broken if the ground state does not exhibit this symmetry. For a continuous symmetry, this occurs when the ground state is not annihilated by the generators of these transformations.

Several schemes have been developed to try to solve the SUSY breaking problem, including the idea of non-perturbative breaking by instantons. In this context, the simplest model is the *Supersymmetric Quantum Mechanics* (SUSYQM), introduced by Witten [8] and Cooper and Freedman [10]. This is a toy model of

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a one-dimensional quantum-mechanical system whose *formal* Hamiltonian can be written as

$$H = \{\mathcal{Q}, \widetilde{\mathcal{Q}}\}_+ = \mathcal{Q}\widetilde{\mathcal{Q}} + \widetilde{\mathcal{Q}}\mathcal{Q}\,, \tag{1.1}$$

where the supercharges

$$\mathcal{Q} = \begin{pmatrix} 0 & 0 \\ A & 0 \end{pmatrix} \quad \text{and} \quad \widetilde{\mathcal{Q}} = \begin{pmatrix} 0 & \widetilde{A} \\ 0 & 0 \end{pmatrix} \tag{1.2}$$

are nilpotent operators,

$$\mathcal{Q}^2 = \widetilde{\mathcal{Q}}^2 = 0\,, \tag{1.3}$$

which commute with the Hamiltonian,

$$[H, \mathcal{Q}] = 0 = \left[H, \widetilde{\mathcal{Q}}\right]\,. \tag{1.4}$$

These conserved supercharges are the generators of the SUSY transformations.

Here, A and $\widetilde{A}$ are differential operators defined on a suitable dense subspace of functions where the necessary operator compositions in these equations are well defined,

$$A = \frac{1}{\sqrt{2}}\left(-\frac{d}{dx} + W(x)\right), \quad \widetilde{A} = \frac{1}{\sqrt{2}}\left(\frac{d}{dx} + W(x)\right), \tag{1.5}$$

where $W(x)$ is called the superpotential.

Notice that, for A closed and $\widetilde{A} = A^\dagger$ (the adjoint of A), the Hamiltonian is non-negative,

$$\langle\phi|H|\phi\rangle = \|\mathcal{Q}\,|\phi\rangle\|^2 + \left\|\widetilde{\mathcal{Q}}\,|\phi\rangle\right\|^2 \geq 0\,, \tag{1.6}$$

and then the ground state $|\phi_0\rangle$ is invariant under SUSY transformations if and only if it has a vanishing energy eigenvalue

$$\mathcal{Q}\,|\phi_0\rangle = 0 = \widetilde{\mathcal{Q}}\,|\phi_0\rangle \quad \Leftrightarrow \quad \langle\phi_0|H|\phi_0\rangle = 0\,. \tag{1.7}$$

When considering these models, several authors have suggested that singular potentials could break SUSY through nonstandard mechanisms, leading to non-degenerate energy levels and even to negative energy eigenstates [12, 13, 14, 15, 16, 17].

In particular, Jevicki and Rodrigues [12] have considered the singular superpotential $W(x) = g/x - x$, with real g. Based on the square integrable solutions of the differential operator related to the Hamiltonian of this system, previously obtained by Lathouwers [18], they concluded that, for a certain range of the parameter g, SUSY is broken with a negative energy ground state. However, they have not established that all the functions they considered correspond to eigenvectors of the same self-adjoint Hamiltonian.

Later, Das and Pernice [19] have reconsidered this problem in the framework of a SUSY preserving regularization of the singular superpotential, finding that SUSY is recovered exactly at the end, when the regularization is removed. They conclude that SUSY is robust at short distances (high energies), and the singularities that occur in quantum mechanical models are unlike to break SUSY.

We addressed this subject [20] by studying the *self-adjoint extensions* (SAE) [21] of the Hamiltonian defined by the superpotential $W(x) = g/x - x$ in the half-line $\mathbf{R}^+$. In so doing, we have considered the SAE of the symmetric supercharges and the possibility of effectively implement the algebra of SUSY in a dense subspace of the Hilbert space.

We have shown that there is a range of values of g for which the supercharges admit a one-parameter family of SAE, corresponding to a one-parameter family of SAE of the Hamiltonian.

We found that only for two particular SAE, whose domains are scale invariant, the algebra of $N = 2$ SUSY can be realized, one with exact SUSY and the other with spontaneously broken SUSY. For other values of this continuous parameter, only the $N = 1$ SUSY algebra is obtained, with spontaneously broken SUSY and non degenerate energy spectrum.

We should mention that SAE of supercharges and Hamiltonian for the SUSYQM of the free particle with a point singularity in the line and the circle have been considered in [22, 23, 24, 25], where $N = 1, 2$ realization of SUSY are described. They have also been considered in the framework of the Landau Hamiltonian for two-dimensional particles in nontrivial topologies in [26] (see also [27]).

Moreover, a *hidden* supersymmetric structure similar to that described in the following also appears when considering the quantum-mechanical behavior of particles in a plane in the presence of a singular Aharonov-Bohm magnetic flux [28, 29].

2. The model and its supercharges

We consider a quantum mechanical system living in the half-line $\mathbf{R}^+$ and subject to a superpotential given by

$$W(x) = \frac{g}{x} - x \tag{2.1}$$

for $x > 0$ and real g. Then, the two differential operators in the expression of the supercharges take the form

$$\begin{aligned} A &= \frac{1}{\sqrt{2}} \left(-\frac{d}{dx} + \frac{g}{x} - x \right), \\ \widetilde{A} &= \frac{1}{\sqrt{2}} \left(\frac{d}{dx} + \frac{g}{x} - x \right). \end{aligned} \tag{2.2}$$

Let us now introduce an operator $Q_+ = \widetilde{\mathcal{Q}} + \mathcal{Q}$, defined on the dense subspace $\mathcal{D}(Q_+) = \mathcal{C}_0^\infty(\mathbf{R}^+ \backslash \{\mathbf{0}\})$, over which its action is given by

$$Q_+ \Psi = \begin{pmatrix} 0 & \widetilde{A} \\ A & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}. \tag{2.3}$$

Its square, which is well defined within this domain, satisfies

$$Q_+{}^2 = \{\mathcal{Q}, \widetilde{\mathcal{Q}}\}_+ = H = \begin{pmatrix} H_+ & 0 \\ 0 & H_- \end{pmatrix}, \tag{2.4}$$

where H is the Hamiltonian of the system, and $H_+ = \widetilde{A}A$ and $H_- = A\widetilde{A}$ are the partner Hamiltonians. It can be easily verified that Q_+ is a symmetric operator, but it is neither self-adjoint nor even closed.

Remark. Given a SAE of Q_+, its *square* gives a SAE of the Hamiltonian H, by virtue of a theorem due to von Neumann [30].

The first step in getting the SAE of Q_+ consists in the construction of its adjoint, $Q_+^\dagger$, and the determination of the *deficiency subspaces*

$$\mathcal{K}_\pm := \mathrm{Ker}(Q_+^\dagger \mp i).$$

Notice that, within the same domain $\mathcal{C}_0^\infty(\mathbf{R}^+\backslash\{\mathbf{0}\})$, a linearly independent combination of supercharges leads to the operator

$$Q_- = i(\widetilde{\mathcal{Q}} - \mathcal{Q}) = \imath Q_+ \sigma_3\,, \tag{2.5}$$

which is also symmetric, anticommutes with Q_+, $\{Q_+, Q_-\}_+ = 0$, and satisfies $Q_-{}^2 = H$. Here, the Pauli matrix $\sigma_3 = \mathrm{diag}\,(1,-1)$ is the *grading operator*, which distinguishes *fermionic* from *bosonic* states.

Since Q_- can also be obtained from Q_+ through a unitary transformation given by

$$Q_- = e^{i\sigma_3\pi/4} Q_+ e^{-i\sigma_3\pi/4}\,, \tag{2.6}$$

the following analysis will be carried out only for Q_+, and it will extend immediately to Q_-.

The Domain of $Q_+^\dagger$

It can be seen that the domain of $Q_+^\dagger$ is

$$\mathcal{D}(Q_+^\dagger) = \{\Phi \in AC(\mathbf{R}^+\backslash\{0\}) \cap \mathbf{L_2}(\mathbf{R}^+) : A\,\phi_1,\, \widetilde{A}\,\phi_2 \in \mathbf{L_2}(\mathbf{R}^+)\}\,, \tag{2.7}$$

where the action of $Q_+^\dagger$ on $\Phi \in \mathcal{D}(Q_+^\dagger)$ reduces also to the application of the differential operator

$$Q_+^\dagger \Phi = \begin{pmatrix} 0 & \widetilde{A} \\ A & 0 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}. \tag{2.8}$$

The Spectrum of $Q_+^\dagger$

The eigenvalue problem for the adjoint, $Q_+^\dagger \Phi_\lambda = \lambda \Phi_\lambda$, reduces to the system of ordinary differential equations

$$A\,\phi_{\lambda,1} = \lambda\,\phi_{\lambda,2}, \quad \widetilde{A}\,\phi_{\lambda,2} = \lambda\,\phi_{\lambda,1}\,, \tag{2.9}$$

with $\Phi_\lambda \in \mathcal{D}(Q_+^\dagger)$ and $\lambda \in \mathbf{C}$.

The substitution $\phi_{\lambda,1}(x) = x^g\, e^{-x^2/2}\, F(x^2)$ leads to the Kummer's (Confluent Hypergeometric) equation [31] for $F(z)$,

$$z\, F''(z) + (b - z)\, F'(z) - a\, F(z) = 0\,, \tag{2.10}$$

with $a = -\frac{\lambda^2}{2}$ and $b = g + \frac{1}{2}$.

This equation has two linearly independent solutions given by the Kummer's function

$$y_1(z) = U(a,b,z) = \frac{\pi}{\sin \pi b} \left\{ \frac{M(a,b,z)}{\Gamma(1+a-b)\Gamma(b)} - z^{1-b}\, \frac{M(1+a-b, 2-b, z)}{\Gamma(a)\Gamma(2-b)} \right\}, \tag{2.11}$$

and

$$y_2(z) = e^z\, U(b-a, b, -z)\,, \tag{2.12}$$

where $M(a,b,z) = {}_1F_1(a;b;z)$.

Since, for large values of the argument,

$$U(a,b,z) = z^{-a} \left\{ 1 + \mathcal{O}(|z|^{-1}) \right\}, \tag{2.13}$$

only $y_1(x^2)$ leads to a function $\phi_{\lambda,1}(x) \in \mathbf{L_2}(1,\infty)$, while $y_2(x^2)$ should be discarded.

Therefore, for any $\lambda \in \mathbf{C}$ we get

$$\phi_{\lambda,1}(x) = x^g\, e^{-x^2/2}\, U\left(-\frac{\lambda^2}{2}, g + \frac{1}{2}, x^2 \right) \tag{2.14}$$

and

$$\phi_{\lambda,2}(x) = -\frac{\lambda}{\sqrt{2}}\, x^{g+1}\, e^{-x^2/2}\, U\left(1 - \frac{\lambda^2}{2}, g + \frac{3}{2}, x^2 \right), \tag{2.15}$$

which is also in $\mathbf{L_2}(1,\infty)$.

In order to determine the spectrum of $Q_+^\dagger$, we must now consider the behavior of $\Phi_\lambda(x)$ near the origin. From the small argument expansion of Kummer's functions [31] one can straightforwardly show that three cases should be distinguished, according to the values of the coupling g.

- If $g \geq 1/2$, it can be seen that $\Phi_\lambda(x) \notin \mathbf{L_2}(0,1)$ unless $\lambda^2 = 2n$, with $n = 0, 1, 2, \ldots$. In this case, the Kummer's function reduces to a Laguerre polynomial, $U(-n, b, z) = (-1)^n\, n!\, L_n^{(b-1)}(z)$ (of degree n in z), and we have $\phi_{\lambda,1}(x) \sim x^g$ and $\phi_{\lambda,2}(x) \sim x^{g+1}$ for $0 < x \ll 1$. Therefore, in this region $Q_+^\dagger$ has a discrete real spectrum, symmetric with respect to the origin, given by the (degeneracy one) eigenvalues

$$\lambda_0 = 0\,, \quad \lambda_{\pm,n} = \pm\sqrt{2n}\,, \quad n = 1, 2, 3, \ldots, \tag{2.16}$$

corresponding to the eigenfunctions $\Phi_0 = x^g\, e^{-x^2/2} \begin{pmatrix} 1 & 0 \end{pmatrix}^t$ and

$$\Phi_{\pm,n} = (-1)^n\, n!\, x^g\, e^{-x^2/2} \begin{pmatrix} L_n^{(g-\frac{1}{2})}(x^2) \\ \mp \dfrac{x}{\sqrt{n}}\, L_{n-1}^{(g+\frac{1}{2})}(x^2) \end{pmatrix}. \tag{2.17}$$

- For $g \leq -1/2$, it can be seen that $\Phi_\lambda(x) \notin \mathbf{L_2}(0,1)$ unless $\lambda^2 = 2(n - g + \frac{1}{2})$, with $n = 0, 1, 2, \ldots$. In this case, we have $\phi_{\lambda,1}(x) \sim x^{1-g}$ and $\phi_{\lambda,2}(x) \sim x^{-g}$ for $0 < x \ll 1$. Therefore, in this region $Q_+^\dagger$ has a discrete real spectrum, symmetric with respect to the origin, given by the (degeneracy one) eigenvalues

$$\lambda_{\pm,n} = \pm\sqrt{2n + 1 - 2g}\,, \quad n = 0, 1, 2, \ldots \tag{2.18}$$

corresponding to the eigenfunctions

$$\Phi_{\pm,n} = (-1)^n\, n! x^{-g}\, e^{-x^2/2} \begin{pmatrix} x\, L_n^{(\frac{1}{2}-g)}(x^2) \\ \mp\sqrt{n + \frac{1}{2} - g}\, L_n^{(-g-\frac{1}{2})}(x^2) \end{pmatrix}. \tag{2.19}$$

Notice that no eigenvalue vanishes for these values of the coupling.

- For $-1/2 < g < 1/2$, it can be seen that $\Phi_\lambda(x) \in \mathbf{L_2}(0,1)$, $\forall \lambda \in \mathbf{C}$. This means that, for these values of g, every complex number is an eigenvalue of $Q_+^\dagger$ with degeneracy one. In particular, the eigenfunction of $Q_+^\dagger$ corresponding to $\lambda = +i$ is given by

$$\Phi_{+\imath}(x) = \begin{pmatrix} \phi_{+\imath,1} \\ \phi_{+\imath,2} \end{pmatrix} = x^g\, e^{-x^2/2} \begin{pmatrix} U\left(\frac{1}{2}, g + \frac{1}{2}, x^2\right) \\ -\frac{i}{\sqrt{2}}\, x\, U\left(\frac{3}{2}, g + \frac{3}{2}, x^2\right) \end{pmatrix}, \tag{2.20}$$

while the eigenfunction corresponding to $\lambda = -i$ is given by its complex conjugate,

$$\Phi_{-\imath}(x) = \Phi_{+\imath}(x)^* = \begin{pmatrix} \phi_{+\imath,1} \\ -\phi_{+\imath,2} \end{pmatrix}. \tag{2.21}$$

For $|g| \geq 1/2$ the operator Q_+ is essentially self-adjoint

As previously seen, the *deficiency indices* of Q_+, defined as the dimensions of the deficiency subspaces

$$n_\pm := \dim \mathrm{Ker}(Q_+^\dagger \mp i)\,, \tag{2.22}$$

vanish for $|g| \geq 1/2$.

According to von Neumann's theory, this means that Q_+ is *essentially self-adjoint* for these values of the coupling, admitting then a unique self-adjoint extension given by $Q_+^\dagger$ (which, in this case, is itself a self-adjoint operator).

The corresponding self-adjoint extension of the Hamiltonian for $|g| \geq 1/2$ is given by

$$\bar{H} = (Q_+^\dagger)^2, \tag{2.23}$$

where the operator composition in the right-hand side is possible in the dense domain

$$\mathcal{D}(\bar{H}) = \left\{\psi \in \mathcal{D}(Q_+^\dagger) : Q_+^\dagger \psi \in \mathcal{D}(Q_+^\dagger)\right\}. \tag{2.24}$$

In particular, every eigenfunctions of $Q_+^\dagger$ belongs to $\mathcal{D}\left(\bar{H}\right)$. Therefore, it is also an eigenfunction of $\bar{H}$ with eigenvalue $E = \lambda^2$.

Therefore, we have for the spectrum of $\bar{H}$

- For $g \geq 1/2$, there is a unique zero mode, while the positive eigenvalues of $\bar{H}$, $E_n = 2\,n\,,\ n = 1, 2, 3, \ldots$, have degeneracy two (since the eigenvalues of $Q_+^\dagger$ are $\lambda_{\pm,n} = \pm\sqrt{2n}$). One can combine $\Phi_{\pm,n}$ to get energy eigenfunctions with only the upper (bosonic) or the lower (fermionic) component non vanishing. In this case the SUSY is exact.
- For $g \leq -1/2$, there is no zero mode, the eigenvalues of $\bar{H}$ are positive, $E_n = 2\,n + 1 - 2\,g \geq 2\,,\ n = 0, 1, 2, \ldots$, and have degeneracy two (since of $Q_+^\dagger$ are $\lambda_{\pm,n} = \pm\sqrt{2n + 1 - 2g}$). Once again, the eigenfunctions $\Phi_{\pm,n}$ can be combined to get energy eigenfunctions with only one non-vanishing component, *i.e.*, also eigenfunctions of the grading operator. In this case the SUSY is spontaneously broken.

For $|g| < 1/2$ the operator Q_+ is not essentially self-adjoint

As we have seen, for $|g| < 1/2$ the deficiency indices are $n_\pm = 1$. According to von Neumann's theory, in this region Q_+ admits a one parameter family of SAE, Q_+^γ, which are in a one-to-one correspondence with the isometries from $\mathcal{K}_+$ onto $\mathcal{K}_-$, characterized by

$$\mathcal{U}(\gamma)\Phi_{+\imath}(x) := e^{2i\gamma}\Phi_{-\imath}\,, \quad \gamma \in [0, \pi)\,, \tag{2.25}$$

with $\Phi_{+\imath}$ and $\Phi_{-\imath}$ eigenvectors of $Q_+^\dagger$ with eigenvalues $+\imath$ and $-\imath$ respectively.

Let us call $\bar{Q}_+$ the *closure* of Q_+, which is given by $\bar{Q}_+ := Q_+^{\dagger\dagger}$. Its domain contains those functions $\overline{\Phi}$ for which $\left(\overline{\Phi}, Q_+^\dagger\Phi\right)$ is a continuous linear functional of $\Phi \in \mathcal{D}\left(Q_+^\dagger\right)$. In particular, since Q_+ is symmetric, $\mathcal{D}\left(Q_+\right) \subset \mathcal{D}\left(\bar{Q}_+\right) \subset \mathcal{D}\left(Q_+^\dagger\right)$.

The *self-adjoint operator* Q_+^γ is defined as the *restriction* of $Q_+^\dagger$ to the dense subspace $\mathcal{D}(Q_+^\gamma) \subset \mathcal{D}(Q_+^\dagger)$ composed by those functions which can be written as

$$\Phi = \overline{\Phi} + c\left(\Phi_{+\imath} + e^{2i\gamma}\Phi_{-\imath}\right)\,, \tag{2.26}$$

with $\overline{\Phi} \in \mathcal{D}(\bar{Q}_+)$, and $c \in \mathbf{C}$. The action of Q_+^γ is given by

$$Q_+^\gamma\Phi = Q_+^\dagger\overline{\Phi} + ic\left(\Phi_{+\imath} - e^{2i\gamma}\Phi_{-\imath}\right)\,. \tag{2.27}$$

This structure of the functions in $\mathcal{D}\left(Q_+^\gamma\right)$ completely characterizes its behavior near the origin and allows to determine the spectrum of Q_+^γ. Indeed, it can be shown [20] that the functions in the domain of the closure of Q_+, $\mathcal{D}(\bar{Q}_+)$, behave as

$$\overline{\phi}_1(x) = o(x^g)\,, \quad \overline{\phi}_2(x) = o(x^{-g})\,, \tag{2.28}$$

for $x \to 0^+$.

On the other side, from the expression of the eigenfunctions Φ_λ of $Q_+^\dagger$ in terms of $U(a,b,z)$ one can easily see that its components behave as

$$\begin{aligned}\phi_{\lambda,1}(x) &= \frac{\Gamma\left(\frac{1}{2}-g\right)}{\Gamma\left(\frac{1-\lambda^2}{2}-g\right)}\, x^g + O(x^{1-g})\,,\\ \phi_{\lambda,2}(x) &= \frac{\sqrt{2}}{\lambda}\,\frac{\Gamma\left(\frac{1}{2}+g\right)}{\Gamma\left(-\frac{\lambda^2}{2}\right)}\, x^{-g} + O(x^{1+g})\,,\end{aligned} \tag{2.29}$$

and then they are dominant near the origin.

Therefore, no eigenfunction of $Q_+^\dagger$ belongs to $\mathcal{D}(\bar{Q}_+)$, and it is the contributions of $\Phi_\pm$ in $\Phi_\lambda = \overline{\Phi} + c\big(\Phi_+ + e^{2i\gamma}\Phi_-\big)$ which determine the spectrum of Q_+^γ. Indeed, for a non vanishing c, the limit

$$\lim_{x\to 0+}\frac{x^{-g}\,\phi_{\lambda,1}(x)}{x^g\,\phi_{\lambda,2}(x)} = \frac{\lambda}{\sqrt{2}}\,\frac{\Gamma\left(-\frac{\lambda^2}{2}\right)}{\Gamma\left(\frac{1-\lambda^2}{2}-g\right)}\,\frac{\Gamma\left(\frac{1}{2}-g\right)}{\Gamma\left(\frac{1}{2}+g\right)} \tag{2.30}$$

must coincide with

$$\lim_{x\to 0+}\frac{\Re\left\{e^{-i\gamma}\,x^{-g}\,\phi_{+\imath,1}(x)\right\}}{\Re\left\{e^{-i\gamma}\,x^{g}\,\phi_{+\imath,2}(x)\right\}} = -\sqrt{\frac{\pi}{2}}\,\frac{\cot(\gamma)}{\Gamma\,(1-g)}\,\frac{\Gamma\left(\frac{1}{2}-g\right)}{\Gamma\left(\frac{1}{2}+g\right)}\,. \tag{2.31}$$

Consequently, the eigenvalues of Q_+^γ (which are real) are the solutions of the transcendental equation

$$f(\lambda) := \frac{\lambda\,\Gamma\left(-\frac{\lambda^2}{2}\right)}{\Gamma\left(\frac{1-\lambda^2}{2}-g\right)} = -\frac{\sqrt{\pi}\,\cot(\gamma)}{\Gamma\,(1-g)} =: \beta(\gamma)\,. \tag{2.32}$$

Notice that $f(\lambda)$ is an odd function of λ, and $-\infty \le \beta(\gamma) < \infty$ for $0 \le \gamma < \pi$. These eigenvalues of Q_+^γ are determined by the intersections of the graphic of $f(\lambda)$ with the horizontal line corresponding to the constant $\beta(\gamma)$. The eigenvalues are non degenerate, as shown in the figure 1.

Notice that these spectra are, in general, non symmetric with respect to the origin. The exceptions are the self-adjoint extensions corresponding to $\gamma = 0$ ($\beta = -\infty$) and $\gamma = \pi/2$ ($\beta = 0$). Indeed, the condition $f(-\lambda) = f(\lambda)$ for a non vanishing λ requires that

$$\frac{1}{\Gamma\left(-\frac{\lambda^2}{2}\right)\Gamma\left(\frac{1-\lambda^2}{2}-g\right)} = 0\,, \tag{2.33}$$

whose solutions correspond to the intersections with the constant $\beta = -\infty$ ($\gamma = 0$),

$$-\frac{\lambda^2}{2} = -n \Rightarrow \lambda_{\pm,n} = \pm\sqrt{2n}, \quad n = 1,2,3,\ldots \tag{2.34}$$

or the constant $\beta = 0$ ($\gamma = \pi/2$),

$$\frac{1-\lambda^2}{2} - g = -n \Rightarrow \lambda_{\pm,n} = \pm\sqrt{2n+1-2g}, \quad n = 0,1,2,\ldots. \tag{2.35}$$

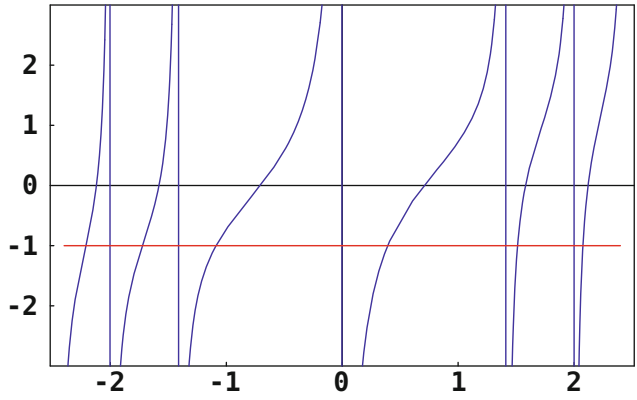

FIGURE 1. $f(\lambda) := \dfrac{\lambda\,\Gamma\left(-\frac{\lambda^2}{2}\right)}{\Gamma\left(\frac{1-\lambda^2}{2}-g\right)}$ for $g = 1/4$, and $\beta(\gamma) \equiv -1$.

Notice also that $Q_+^{\gamma=0}$ is the only self-adjoint extension having a zero mode, and for $0 < \gamma < \pi$ the eigenvalues are contained between contiguous asymptotes of the function $\Gamma\left(-\frac{\lambda^2}{2}\right)$,

$$\sqrt{2n} < |\lambda_{\pm,n}| < \sqrt{2(n+1)}\,. \tag{2.36}$$

3. The Hamiltonian

As previously stated, for each SAE Q_+^γ, with $\gamma \in [0, \pi)$, we get a self-adjoint extension of the Hamiltonian defined by

$$H_\gamma = (Q_+^\gamma)^2 \equiv (Q_+^\dagger)^2\Big|_{\mathcal{D}(H_\gamma)}\,, \tag{3.1}$$

where the operator composition on the right-hand side is defined as the restriction of $(Q_+^\dagger)^2$ to the dense subspace

$$\mathcal{D}\left(H_\gamma\right) = \left\{\psi \in \mathcal{D}\left(Q_+^\gamma\right) : Q_+^\dagger \psi \in \mathcal{D}\left(Q_+^\gamma\right)\right\}. \tag{3.2}$$

This domain includes, in particular, all the eigenfunctions of Q_+^γ, which are then also eigenvectors of H_γ:

$$Q_+^\gamma \Phi_\lambda = \lambda \Phi_\lambda \Rightarrow H_\gamma \Phi_\lambda = \lambda^2 \Phi_\lambda\,. \tag{3.3}$$

Notice that, except for the special values $\gamma = 0, \pi/2$, the spectrum of H_γ is non degenerate.

Three cases can be distinguished for $|g| < 1/2$:

- For $\gamma = 0$ ($\beta = -\infty$) we get the only self-adjoint extension of H having a non degenerate zero mode and doubly degenerate positive eigenvalues $E_{\pm,n} = (\lambda_{\pm,n})^2 = 2n,\ n = 1, 2, 3, \ldots$. The corresponding eigenvectors can be chosen to have a definite character with respecto to the grading σ_3. This SAE of the Hamiltonian corresponds to an exactly realized SUSY.
- For $\gamma = \pi/2$ ($\beta = 0$) we get a SAE of H with no zero modes and a doubly degenerate non-vanishing eigenvalues, $E_{\pm,n} = (\lambda_{\pm,n})^2 = 2n + 1 - 2g$, with $n \geq 0$. They are all positive, since $1 - 2g > 0$. The eigenvectors can also be chosen with a definite σ_3 eigenvalue. In the present case, the condition imposed on the functions in $\mathcal{D}(Q_+^{\gamma=\pi/2})$ breaks the SUSY preserving the doubly degeneracy of the spectrum. This case corresponds to a SAE of H with spontaneously broken SUSY.
- Finally, for $\gamma \neq 0, \pi/2$ we get SAE of H with no zero modes and non degenerate positive eigenvalues (the square of the solutions of $f(\lambda) = \beta(\gamma)$). The eigenfunctions of H_γ (those of Q_+^γ) have both components non-vanishing (they are not eigenvectors of the grading). Then, they have not bosonic or fermionic character. In this case, the condition imposed on the functions belonging to $\mathcal{D}\left(Q_+^\gamma\right)$ breaks not only the SUSY, but also the degeneracy of the spectrum.

4. On the existence of a second supercharge

As previously mentioned, the differential operators Q_+ and Q_- are related by a unitary transformation, $Q_- = e^{i\sigma_3\pi/4} Q_+ e^{-i\sigma_3\pi/4}$. Then, each SAE of the first, Q_+^γ, determines a SAE of the second, Q_-^γ, whose domain is obtained from $\mathcal{D}(Q_+^\gamma)$ through this unitary transformation,

$$\mathcal{D}(Q_-^\gamma) = \left\{ \Psi : e^{-i\pi\sigma_3/4}\Psi \in \mathcal{D}(Q_+^\gamma) \right\} = e^{i\pi\sigma_3/4} \left(\mathcal{D}(Q_+^\gamma) \right) . \tag{4.1}$$

Consequently, Q_-^γ is an equivalent representation of the self-adjoint supercharge Q_+^γ, sharing both operators the same spectrum.

Similarly, its square $(Q_-^\gamma)^2$, defined on the dense subspace

$$\mathcal{D}\left((Q_-^\gamma)^2\right) = \left\{ \Psi \in \mathcal{D}(Q_-^\gamma) : Q_-^\gamma \Psi \in \mathcal{D}(Q_-^\gamma) \right\} = e^{i\pi\sigma_3/4} \left(\mathcal{D}(H_\gamma) \right) , \tag{4.2}$$

is an equivalent representation of the SAE $H_\gamma = (Q_+^\gamma)^2$ of the Hamiltonian H, initially defined on $\mathcal{C}_0^\infty(\mathbf{R}^+ \backslash \{0\})$.

These equivalent representations of the Hamiltonian coincide only if the domain $\mathcal{D}(Q_+^\gamma)$ is left invariant by the grading operator σ_3 and, consequently, by the unitary transformation $e^{i\pi\sigma_3/4}$. And this occurs only for the particular self-adjoint

extensions corresponding to $\gamma = 0$ and $\gamma = \pi/2$ since

$$e^{i\pi\sigma_3/4}\left(\Phi_{+\imath}(x) + e^{2i\gamma}\Phi_{-\imath}(x)\right) = \begin{pmatrix} e^{i\frac{\pi}{4}}\left(1 + e^{2i\gamma}\right)\phi_{+\imath,1}(x) \\ \\ e^{-i\frac{\pi}{4}}\left(1 - e^{2i\gamma}\right)\phi_{+\imath,2}(x) \end{pmatrix} . \tag{4.3}$$

Consequently, the operator compositions

$$(Q_+^\gamma)^2, \quad (Q_-^\gamma)^2, \quad Q_+^\gamma Q_-^\gamma \qquad \text{and} \qquad Q_-^\gamma Q_+^\gamma \tag{4.4}$$

make sense in the same (dense) domain $\mathcal{D}(H_\gamma)$ only for $\gamma = 0, \pi/2$, values of the parameter characterizing self-adjoint extensions for which the $N = 2$ SUSY algebra is realized,

$$\{Q_+^\gamma, Q_-^\gamma\} = 0\,, \qquad H_\gamma = (Q_+^\gamma)^2 = (Q_-^\gamma)^2\,. \tag{4.5}$$

For other values of the parameter γ, $\mathcal{D}(Q_+^\gamma)$ is not left invariant by $e^{i\pi\sigma_3/4}$, and there is no dense domain in the Hilbert space where the $N = 2$ SUSY algebra could be realized in terms of self-adjoint operator compositions.

Therefore, for $\gamma \neq 0, \pi/2$ only one self-adjoint supercharge can be defined in the domain of the Hamiltonian, and the SUSY algebra reduces to the $N = 1$ case,

$$H_\gamma = (Q_+^\gamma)^2 \tag{4.6}$$

(or, equivalently, $H_\gamma = (Q_-^\gamma)^2$).

It is worthwhile to remark that the double degeneracy of the non vanishing eigenvalues of H_γ with $\gamma = 0, \pi/2$ is a consequence of the existence of a second supercharge. Indeed, if

$$Q_+^\gamma \Phi_\lambda = \lambda \Phi_\lambda\,, \tag{4.7}$$

with $\Phi_\lambda \in \mathcal{D}(H_\gamma)$ and $\lambda \neq 0$, then $\{Q_+^\gamma, Q_-^\gamma\} = 0$ imply that

$$Q_+^\gamma (Q_-^\gamma \Phi_\lambda) = -Q_-^\gamma (Q_+^\gamma \Phi_\lambda) = -\lambda (Q_-^\gamma \Phi_\lambda)\,. \tag{4.8}$$

Therefore, $Q_-^\gamma \Phi_\lambda$ $\left(\in \mathcal{D}(Q_-^\gamma) \equiv \mathcal{D}(Q_+^\gamma)\right)$ is a linearly independent eigenvector of Q_+^γ corresponding to the eigenvalue $-\lambda$, since $Q_-^\gamma \Phi_\lambda \perp \Phi_\lambda$ and

$$\| Q_-^\gamma \Phi_\lambda \|^2 = (\Phi_\lambda, (Q_-^\gamma)^2 \Phi_\lambda) = (\Phi_\lambda, H_\gamma \Phi_\lambda) = \lambda^2 \ \| \Phi_\lambda \|^2 \neq 0\,. \tag{4.9}$$

This explains why it is not possible to construct a second supercharge when the spectrum of the first one is not symmetric with respect to the origin.

5. Conclusions

Then, we have the following situation:

- For a general SAE Q_+^γ, the conditions the functions in $\mathcal{D}(H_\gamma)$ satisfy near the origin prevent the $N = 2$ SUSY. Only the $N = 1$ SUSY algebra is realized, with a non symmetric spectrum for Q_+^γ and a non degenerate spectrum for H_γ. This SUSY is spontaneously broken, since there are no zero modes.

- The only exceptions are the $\gamma = 0$ and $\gamma = \pi/2$ SAE, for which the $N = 2$ SUSY algebra can be realized. In these two cases the supercharges have a common symmetric spectrum and the positive eigenvalues of the Hamiltonian are doubly degenerate.
- For $\gamma = 0$, the (non degenerate) ground state of H_0 has a vanishing energy and the SUSY is exact, while for $\gamma = \pi/2$ the (doubly degenerate) ground state of $H_{\pi/2}$ has positive energy and the SUSY is spontaneously broken.

It is interesting to remark that a similar supersymmetric structure is found in the case of particles living in a plane and subject to the presence of an Aharonov-Bohm singular magnetic flux [28, 29].

Finally, it is worthwhile to point out that the $N = 2$ SUSY can be realized only when the supercharge domain $\mathcal{D}(Q_+^\gamma)$ is scale invariant. Indeed, given a function $\Phi(x) \in \mathcal{D}(Q_+^\gamma)$, under the scaling isometry

$$T_a\Phi(x) := a^{1/2}\Phi(ax) \tag{5.1}$$

with $a > 0$, we get

$$\lim_{x\to 0+} \frac{x^{-g}\,(T_a\Phi)_1(x)}{x^g\,(T_a\Phi)_2(x)} = -\sqrt{\frac{\pi}{2}}\,\frac{a^{2g}\cot(\gamma)}{\Gamma\,(1-g)}\,\frac{\Gamma\left(\frac{1}{2}-g\right)}{\Gamma\left(\frac{1}{2}+g\right)}\,, \tag{5.2}$$

which means that $T_a\Phi(x) \in \mathcal{D}(Q_+^{\gamma_a})$ with γ_a defined by

$$\cot(\gamma_a) = a^{2g}\cot(\gamma)\,. \tag{5.3}$$

Then, $\gamma_a = \gamma$ only for $\gamma = 0, \pi/2$. For other values of γ the domain $\mathcal{D}(Q_+^\gamma)$ is not scale invariant.

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Generalized Euclidean Bosonic String Equations

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Abstract. We consider nonlinear equations of the form $p(\Delta)u = U(x, u(x))$, in which p is a real-valued function satisfying some suitable technical conditions, and Δ stands for the Laplacian operator. We formulate a functional calculus appropriate for the study of such equations, and we establish results on the existence and regularity of solutions to the Euclidean bosonic string equation $\Delta \exp(-c\,\Delta)\, u = U(x, u(x))$, and we introduce a functional calculus appropriate for the study of very general nonlinear equations depending on functions of the Laplace operator. We also prove that under some further technical conditions, these "nonlocal" equations admit smooth, and even real-analytic, solutions. Our motivation comes from recent developments in string theory and nonlocal cosmology.

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1. Introduction

Equations with an infinite number of derivatives have appeared recently in string theory and cosmology, see for instance [2, 3, 4, 5, 6, 7, 16, 25, 32, 34] and references therein. For example, see [7], bosonic string theory in Euclidean space $\mathbb{R}^n$ is described by a special case of the nonlocal Lagrangian density

$$\mathcal{L}(\phi) = \phi\, \Delta e^{-c\,\Delta} \phi - \mathcal{U}(x, \phi)\ , \quad c > 0\ . \tag{1}$$

Applying formally the variational principle we obtain the equation of motion

$$\Delta e^{-c\,\Delta} \phi - U(x, \phi) = 0\ , \quad c > 0\ , \tag{2}$$

where $U = \partial \mathcal{U}/\partial \phi$. Our goal in this chapter is to explain how to study (global) existence and uniqueness of solutions to equations such as (2).

We will say that an operator such as $e^{-c\,\Delta}$ is *nonlocal* in the sense that the action of $e^{-c\,\Delta}$ on suitable functions is defined via a power series expansion,

$$e^{-c\,\Delta}\,\phi = \sum_{k=0}^{\infty} \frac{(-c\Delta)^k}{k!}\,\phi\,. \tag{3}$$

Thus, $e^{-c\,\Delta}$ depends (at least at a formal level) on an infinite number of derivatives of ϕ. This is precisely how this kind of equations is understood in the physical literature [2, 3, 4, 5].

It is very interesting that nonlocal equations appeared in mathematics already in the 1930s, as mentioned in [4]. It appears to us, however, that a truly fundamental stimulus for their study has been the realization that *nonlinear* nonlocal equations play a crucial role in contemporary physical theories. We specially mention the seminal paper [34], in which E. Witten presents an action defined on a non-commutative space which yields an infinite system of equations for infinitely many variables (besides [34], the reader may also wish to look at the classical paper [9] by Eliazder and Woodard, and Rastelli's recent review [27]). From this action principle, physicists have extracted nonlocal actions such as (1), see for example [6, 7]. In particular, as explained in [7], Equation (2) posed on Lorentzian manifolds is a general type of equation encompassing the bosonic string [23] and a simplified case of the supersymmetric string [7].

As we have already stated above, in this work we study analytic properties of nonlocal equations. It seems important to remark that we do not base our work on either pseudo-differential operators or generalized functions. Building on intuitions familiar from the physics approach to these equations [2, 3, 4, 5], and recalling the expansion (3), we attach a meaning to the nonlocal operator appearing in the Euclidean equation (2) by using the theory of entire vectors (see [14] and the recent [13]), and the fact that the Laplacian operator Δ in $L^2(\mathbb{R}^n)$ is the generator of an analytic semigroup with angle $\pi/2$, see [1]. This approach allows us to solve Equation (2) in a Hilbert space $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$ – to be defined precisely below – of *real-analytic* functions on which the operator $\Delta\, e^{-c\,\Delta} - I$ acts naturally.

We organize our work as follows. In Section 2 we introduce the spaces on which we can define rigorously operators of the form $\Delta e^{-c\,\Delta}$ or, more generally, $p(\Delta)$ for some function p. In Section 3 we attach a meaning to the nonlocal operator $e^{-c\Delta}$ by using analytic vectors [26] and Fourier transform arguments, and we use this construction as a motivation for defining $p(\Delta)$ in general. In Section 4 we consider nonlocal equations. We show the existence and analyticity of solutions to Equation (1) if U is a radial function on $\mathbb{R}^n$. We also explain how to generalize these results to nonlinear equations of the form

$$p(\Delta)\phi = U(\cdot, \phi)\,.$$

Finally, in Section 5 we study nonlocal equations on compact Riemannian manifolds. In this general context we do not have Fourier transforms at our disposal. However, taking advantage of Hodge's theorem, [29], we can solve nonlinear

nonlocal equations using the spectral decomposition of Δ_g. We finish in Section 6 with some concluding remarks.

This chapter contains most of the functional analytic details which were missing in our announcement [15], and it also includes a review of some of the work appearing in [17].

2. An appropriate setting for nonlocal equations

We begin by setting up our notation. The space $L^1(\mathbb{R}^n)$ is the space of all the functions $f : \mathbb{R}^n \to \mathbb{R}$ which are integrable. We set

$$\|f\|_1 = \int_{\mathbb{R}^n} |f(x)|dx$$

Sometimes we write simply L^1 instead of $L^1(\mathbb{R}^n)$. The $L^p(\mathbb{R}^n)$ spaces, $1 \leq p < \infty$, are

$$L^p(\mathbb{R}^n) = \{f : \mathbb{R}^n \to \mathbb{R} \,:\, f \text{ measurable and } |f|^p \in L^1(\mathbb{R}^n)\} \,.$$

They are Banach spaces with norm

$$\|f\|_p = \left[\int_{\mathbb{R}^n} |f(x)|^p dx\right]^{1/p} \,.$$

We also define

$$L^\infty(\mathbb{R}^n) = \{f : \mathbb{R}^n \to \mathbb{R} \,:\, f \text{ measurable and there is } C \text{ such that } |f(x)| \leq C \text{ almost everywhere}\} \,,$$

and we equip it with the norm

$$\|f\|_\infty = \inf\{C : |f(x)| \leq C \text{ almost everywhere}\} \,.$$

We also need to consider Sobolev spaces over $\mathbb{R}^n$. We recall that if $f \in L^2(\mathbb{R}^n)$, the Fourier transform of f is

$$\hat{f}(\xi) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-ix\cdot\xi} f(x)dx \,,$$

in which $\xi \in \mathbb{R}^n$. The function $\hat{f}$ will be also denoted by $\mathcal{F}(f)$ below if deemed appropriate. The Sobolev space $H^s(\mathbb{R}^n)$ is

$$H^s(\mathbb{R}^n) = \left\{ f \in L^2(\mathbb{R}^n) : \int_{\mathbb{R}^n} (1 + |\xi|^2)^s |\hat{f}(\xi)|^2 d\xi < \infty \right\} \,.$$

We recall that a function f is *radial*, or *spherically symmetric*, if $f(x) = f(|x|)$ for all $x \in \mathbb{R}^n$. The spaces of radial functions $L^2_r(\mathbb{R}^n)$ and $H^s_r(\mathbb{R}^n)$ are

$$L^2_r(\mathbb{R}^n) = \overline{C^\infty_{0,r}(\mathbb{R}^n)}^{L^2(\mathbb{R}^n)}, \quad H^s_r(\mathbb{R}^n) = \overline{C^\infty_{0,r}(\mathbb{R}^n)}^{H^s(\mathbb{R}^n)},$$

in which $C^\infty_{0,r}(\mathbb{R}^n)$ denotes the space of smooth radial functions with compact support on $\mathbb{R}^n$. The following embedding and compactness results hold:

Proposition 2.1.

1. *If $s > n/2$ then each $u \in H^s(\mathbb{R}^n)$ is bounded and continuous.*
2. *If $s > n/2 + k$ then $H^s(\mathbb{R}^n) \subset C^k(\mathbb{R}^n)$.*
3. *Let $n \geq 2$, $s > 0$, and let $2^* = 2n/(n-2s)$ if $2s < n$ or $2^* = \infty$ if $2s \geq n$. Then, the restriction to the space of radial functions of the Sobolev inclusion from $H^s(\mathbb{R}^n)$ into $L^q(\mathbb{R}^n)$ is compact whenever $2 < q < 2^*$.*

The first two results are classical and appear for example in [31]. The last result is due to P.-L. Lions, see [24].

Now we consider Gevrey spaces, as we will need them in order to discuss analyticity of solutions. We follow the paper [10] by C. Foias and R. Temam (see also [11]). First of all, we define the family of normed spaces $\mathcal{D}(\sigma, s)$ for $\sigma > 0$ and $s \in \mathbb{R}$, as

$$\mathcal{D}(\sigma, s) = \left\{ f \in L^2(\mathbb{R}^n) : \|f\|^2_{G^{\sigma,s}} = \int_{\mathbb{R}^n} (1 + |\xi|)^{2s} e^{2\sigma(1+|\xi|)} |\mathcal{F}(f)(\xi)|^2 d\xi < \infty \right\} . \tag{4}$$

Then, the Gevrey space G^σ, $\sigma > 0$, can be characterized as a bundle of Banach spaces,

$$G^\sigma = \bigcup_{s>0} \mathcal{D}(\sigma, s) . \tag{5}$$

The main property of Gevrey spaces which we will use is contained the following lemma:

Lemma 2.1. *If f is in the space G^σ, then f is the restriction to $\mathbb{R}^n$ of an holomorphic function on the domain $\{z = x + i\, y \in \mathbb{C}^n : |y| < \sigma\}$.*

Proof. If f is in the space G^σ, then f and $\widehat{f}$ are in $L^2(\mathbb{R}^n)$. Furthermore, since $\|f\|_{G^{\sigma,s}} < \infty$ for some $s > 0$, we conclude that

$$e^{b|\xi|}\, \widehat{f} \in L^2(\mathbb{R}^n)$$

for all $b < \sigma$. Theorem IX.13 from [28] (a Paley-Wiener type theorem) allows us to conclude that f has analytic continuation on the strip $\{z \in \mathbb{C}^n : |\mathrm{Im}\,(z)| < \sigma\}$. □

Now we can introduce the spaces $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$. As we mentioned in Section 1, we will use them to make sense of the formal operator

$$L_c = \Delta e^{-c\Delta} - Id\, , \quad c > 0\, , \tag{6}$$

in which $\Delta = \sum_{i=1}^n \partial^2/\partial x_i^2$.

Definition 2.1. *The space $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$, $c > 0$, is given by*

$$\mathcal{H}^{c,\infty}(\mathbb{R}^n) = \left\{ f \in L^2(\mathbb{R}^n) : \int_{\mathbb{R}^n} \left(1 + |\,\xi|^2 e^{c|\,\xi|^2}\right)^2 |\mathcal{F}(f)(\xi)|^2\, d\xi < \infty \right\} .$$

We note that Yu.A. Dubinskii defined in [8] a space of test functions in order to develop a calculus of pseudo-differential operators with analytic symbols. However, for our goals Dubinskii's space appears to be a little restrictive: our space strictly contains his class of functions. We also note that we have recently found spaces similar to our $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$ in the classical paper [33] by F. Treves.

The space $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$ is isometric to $L^2(\mathbb{R}^n)$. Indeed, let us consider the function

$$\widehat{K}(\xi) = \frac{1}{1 + |\,\xi|^2 e^{c|\,\xi|^2}} \ .$$

This function belongs to the Schwarz space $\mathcal{S}(\mathbb{R}^n)$, and therefore [30] there exists a unique function $K \in \mathcal{S}(\mathbb{R}^n)$ whose Fourier transform $\mathcal{F}(K)$ is precisely $\widehat{K}$. We have:

Proposition 2.2. *A function $h \in L^2(\mathbb{R}^n)$ belongs to the space $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$ if and only if $h = K * f$ for some $f \in L^2(\mathbb{R}^n)$. Furthermore, if we endow $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$ with the inner product*

$$\langle f, g\rangle = \int_{\mathbb{R}^n} \left(1 + |\,\xi|^2 e^{c|\,\xi|^2}\right)^2 \mathcal{F}(f)(\xi)\overline{\mathcal{F}(g)(\xi)}\, d\xi \ ,$$

then $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$ is a Hilbert space and the transformation $\mathcal{K} : L^2(\mathbb{R}^n) \to \mathcal{H}^{c,\infty}(\mathbb{R}^n)$ given by

$$\mathcal{K}(f) = K * f$$

is an isometric isomorphism.

Proof. Let us take $h \in \mathcal{H}^{c,\infty}(\mathbb{R}^n)$, so that $(1+ |\,\xi\,|^2\ e^{c|\xi|^2})\mathcal{F}(h)$ belongs to $L^2(\mathbb{R}^n)$. Since the Fourier transform is an unitary operator on $L^2(\mathbb{R}^n)$, there exists a unique $f \in L^2(\mathbb{R}^n)$ such that $\mathcal{F}(f) = (1+ |\,\xi\,|^2\ e^{c|\xi|^2})\mathcal{F}(h)$. But then, using elementary properties of Fourier transform, see for instance [30], we have

$$\mathcal{F}(h) = \frac{\mathcal{F}(f)}{1+ |\,\xi\,|^2\ e^{c|\xi|^2}} = \mathcal{F}(f)\mathcal{F}(K) = \mathcal{F}(f * K) \ , \tag{7}$$

and we conclude that $h = K * f$. Conversely, if $h = K * f$ for some $f \in L^2(\mathbb{R}^n)$, then $\mathcal{F}(h) = \mathcal{F}(K)\mathcal{F}(f)$, and therefore

$$\mathcal{F}(h)/\mathcal{F}(K) = (1+ |\,\xi\,|^2\ e^{c|\xi|^2})\mathcal{F}(h) = \mathcal{F}(f) \in L^2(\mathbb{R}^n) \ ,$$

so that indeed $h \in \mathcal{H}^{c,\infty}(\mathbb{R}^n)$. The proof of the second assertion is now clear. □

An easy consequence of this result is the fact that if D is a dense subset of $L^2(\mathbb{R}^n)$, then the set of functions

$$\Big\{u_f = K * f : \quad f \in D\Big\}$$

is dense in $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$. We will use this observation to determine the action of the operator L_c defined in (6) on $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$.

Lemma 2.2.

1. *For each non-negative* $s \in \mathbb{R}$ *the embedding* $\mathcal{H}^{c,\infty}(\mathbb{R}^n) \hookrightarrow H^s(\mathbb{R}^n)$ *holds. In other words,* $\|f\|_{H^s(\mathbb{R}^n)} \leq C(s)\|f\|_{\mathcal{H}^{c,\infty}(\mathbb{R}^n)}$ *for some constant* $C(s) > 0$.
2. *For each* $m \geq 0$ *the embedding* $\mathcal{H}^{c,\infty}(\mathbb{R}^n) \hookrightarrow C^m(\mathbb{R}^n)$ *holds.*

Proof. Claim (1) follows immediately from the elementary properties of the map $x \mapsto e^x$. The second claim follows from (1) and the Sobolev embedding theorem as it appears for example in [31]. □

Thus, we conclude that the elements of $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$ are smooth functions. Even more, we can show that if a function belongs to $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$ then it is real-analytic and in fact, it satisfies a "super-analyticity" regularity condition. We provide a full proof of this important fact:

Theorem 2.1. *The space* $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$ *is contained in the Gevrey space* $G^{1/2}$. *It is also continuously embedded into the Gevrey spaces* $G^{\sigma,s}$, $\sigma > 0$ *and* $s \in \mathbb{R}$. *In particular, the inclusion* $\mathcal{H}^{c,\infty}(\mathbb{R}^n) \subset C^\omega(\mathbb{R}^n)$ *holds.*

Proof. We fix $\sigma = 1/2$ and we take $f \in \mathcal{H}^{c,\infty}(\mathbb{R}^n)$. It follows that

$$\int |\xi|^2 e^{c|\xi|^2} |\mathcal{F}(f)(\xi)|^2 \, d\xi < \infty \,, \quad \text{and also that} \quad \int e^{c|\xi|^2} |\mathcal{F}(f)(\xi)|^2 \, d\xi < \infty \,.$$

Adding these two inequalities we obtain that f belongs to $\mathcal{D}(1/2, c/2)$ and therefore to the Gevrey class $G^{1/2}$.

We now show that for each $\sigma, s > 0$ the embedding $\mathcal{H}^{c,\infty}(\mathbb{R}^n) \hookrightarrow G^{\sigma,s}$ holds, or equivalently, that $\|f\|_{G^{\sigma,s}} \leq C\|f\|_{\mathcal{H}^{c,\infty}(\mathbb{R}^n)}$ for some constant number $C > 0$. Indeed, clearly there exists $R > 0$ such that

$$(1 + |\xi|)^{2s} e^{2\sigma|\xi|} \leq M \left(1 + |\xi|^2 e^{c|\xi|^2}\right)^2$$

for $|\xi| > R$, in which M is a constant depending on s and σ. Then we have, for any $f \in \mathcal{H}^{c,\infty}(\mathbb{R}^n)$,

$$\begin{aligned} & e^{-2\sigma} \, \|f\|^2_{G^{\sigma,s}} \\ & \quad \leq \int_{\|\xi\| \leq R} (1 + |\xi|)^{2s} e^{2\sigma|\xi|} |\mathcal{F}(f)(\xi)|^2 d\xi + M \int_{\|\xi\| > R} (1 + |\xi|^2 e^{c|\xi|^2})^2 |\mathcal{F}(f)(\xi)|^2 \, d\xi \\ & \quad \leq D \int_{\|\xi\| \leq R} |\mathcal{F}(f)(\xi)|^2 d\xi + M \, \|f\|^2_{\mathcal{H}^{c,\infty}(\mathbb{R}^n)} \,, \end{aligned}$$

in which $D = \sup_{\|\xi\| \leq R} (1 + |\xi|)^{2s} e^{2\sigma|\xi|}$. The embedding $\mathcal{H}^{c,\infty}(\mathbb{R}^n) \hookrightarrow G^{\sigma,s}$ is now clear. The last part of the theorem is a direct application of Lemma 2.1. □

Finally, following [17], we generalize the spaces $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$ in order to include nonlocal equations more general than the Euclidean generalized bosonic string equation

$$\Delta e^{-c\,\Delta} \phi - U(x, \phi) = 0 \,, \quad c > 0 \,. \tag{8}$$

Specifically, our goal now is to introduce spaces so as to make sense of the formal operator

$$L = p(\Delta) + Id \,, \tag{9}$$

as an operator defined on (a subspace of) $L^2(\mathbb{R}^n)$. We assume that p is simply a measurable function, and that the following two conditions hold [17]:

(P) The function $s \mapsto p(-s^2)$ is non-negative.
(E_β) There exist real numbers $\beta, R, M > 0$ such that

$$M(\,1 + |\xi|^2\,)^{\frac{\beta}{2}} \leq p\left(-|\xi|^2\right) \text{ for all } \xi \text{ with } |\xi| > R \,.$$

The class of measurable functions p satisfying these two conditions will be denoted by $\mathcal{G}^\beta$. A function $p \in \mathcal{G}^\beta$ is not, in general, a symbol of a pseudo-differential operator in the sense of Hörmander [21, p. 65], but Condition (E_β) is precisely the condition for ellipticity of symbols of pseudo-differential operators, see for instance [35].

Definition 2.2. *Fix $p \in \mathcal{G}^\beta$. The space $\mathcal{H}^\beta(p)$ is given by all real-valued functions g on $\mathbb{R}^n$ such that g is measurable, the Fourier transform $\mathcal{F}(g)$ exists, and*

$$\int_{\mathbb{R}^n} \left[1 + p(-|\,\xi|^2)\right]^2 |\mathcal{F}(g)(\xi)|^2 \, d\xi < \infty \,.$$

Interestingly, we mention that similar spaces have been considered in the context of pseudo-differential operators and Feller semi-groups, see for instance [22]. It follows from the Parseval identity that $\mathcal{H}^\beta(f) \subseteq L^2(\mathbb{R}^n)$. As explained in detail in [17], this space can be motivated via a formal computation with the operator $p(\Delta)$.

We can describe very explicitly the elements of $\mathcal{H}^\beta(p)$, in analogy with Proposition 2.2. Let $\widehat{K}$ be the function

$$\widehat{K}(\xi) = \frac{1}{1 + p(-|\,\xi|^2)} \,,$$

in which p is a $\mathcal{G}^\beta$-symbol. Assumption (E_β) implies that $\widehat{K} \in L^2(\mathbb{R}^n)$. It follows that there exists a unique function $K_p \in L^2(\mathbb{R}^n)$ whose Fourier transform $\mathcal{F}(K_p)$ is precisely $\widehat{K}$. We have:

Proposition 2.3. *A measurable function h belongs to the space $\mathcal{H}^\beta(p)$ if and only if $h = K_p * g$ for some $g \in L^2(\mathbb{R}^n)$. Furthermore, if we endow $\mathcal{H}^\beta(p)$ with the inner product*

$$\langle g_1, g_2 \rangle = \int_{\mathbb{R}^n} \left(1 + p(-|\,\xi|^2)\right)^2 \mathcal{F}(g_1)(\xi)\overline{\mathcal{F}(g_2)(\xi)} \, d\xi \,,$$

then $\mathcal{H}^\beta(p)$ is a Hilbert space and the transformation $\mathcal{K} : L^2(\mathbb{R}^n) \to \mathcal{H}_p(\mathbb{R}^n)$ given by

$$\mathcal{K}(g) = K_p * g$$

is an isometric isomorphism.

This result appears in our paper [17]. Proofs of the following observations also appear in this reference:

Lemma 2.3. *Let p be a $\mathcal{G}^\beta$-symbol. We have:*

1. *For each $s \in \mathbb{R}$ with $s \leq \beta$, the embedding $\mathcal{H}^\beta(p) \hookrightarrow H^s(\mathbb{R}^n)$ holds. In other words, $\|p\|_{H^s(\mathbb{R}^n)} \leq C(s,\beta)\|p\|_{\mathcal{H}^\beta(p)}$ for some constant $C(s,\beta) > 0$.*
2. *For each $k \geq 1$ such that $n/2 + k < s \leq \beta$, the embedding $\mathcal{H}^\beta(p) \hookrightarrow C^k(\mathbb{R}^n)$ holds.*
3. *For each $0 < \alpha < 1$ such that $n/2 + \alpha = s \leq \beta$, the embedding $\mathcal{H}^\beta(p) \hookrightarrow C^\alpha(\mathbb{R}^n)$ holds, in which $C^\alpha(\mathbb{R}^n)$ is the space of Hölder continuous functions of order α.*

3. Nonlocal operators

In this section we show how to define the operator L_c given by (6) correctly, as an operator on the space $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$. More generally, we explain how to define the operator (9) on the space $\mathcal{H}^\beta(p)$.

For example, let us define

$$p(s) = s\exp(-c\,s), \text{ for } s \in \mathbb{R}\,. \tag{10}$$

In order to understand the operator L_c given by (6), we need to define the action of the operator $p(\Delta)$. As we remarked in Section 1, our plan is to interpret L_c in such a way that the equation

$$\Delta e^{-c\,\Delta}\phi - U(x,\phi) = 0\,, \quad c > 0\,. \tag{11}$$

retains the intuitive meaning of an equation with infinite derivatives [2, 3, 4, 5]. We begin with a technical lemma.

Lemma 3.1. *Assume that $G \in C^2 \cap L^2(\mathbb{R}^n)$, and that $f \in L^2(\mathbb{R}^n)$. Then, $(\Delta G) * f = \Delta(G * f)$.*

Proof. We set

$$W(x) = \int_{\mathbb{R}^n} G(x-y)f(y)dy\,,$$

and define $\tau_x(g)(y) = g(x-y)$ for any function $g \in L^2(\mathbb{R}^n)$. Using the mean value theorem we see that

$$\left|\frac{W(x+h)-W(x)}{h} - \int_{\mathbb{R}^n}\frac{\partial}{\partial x}G(x-y)f(y)dy\right|$$
$$\leq \left(\int_{\mathbb{R}^n}\left|\tau_{x_h}(\frac{\partial}{\partial x}G)(y) - \tau_x(\frac{\partial}{\partial x}G)(y)\right|^2 dy\right)^{1/2}\|f\|_2\,.$$

The right-hand side of this inequality tends to zero as x_h tends to x. □

This elementary lemma allows us to use the machinery of analytic vectors due to E. Nelson [26] (see also [28] for an exposition of the theory). We recall this important notion:

Definition 3.1. *If A is a closed operator in a Banach space X, a vector $u \in C^\infty(A) = \cap_{n\geq 0} D(A^n)$, where $D(A)$ is the domain of A, is called an analytic vector for A if the series*

$$\sum_{k=0}^{\infty} \frac{t^k}{k!} A^k u$$

converges for some $t > 0$. More generally, a vector $u \in C^\infty(A) = \cap_{n\geq 0} D(A^n)$, where $D(A)$ is the domain of A, is called an entire vector for A if the series

$$\sum_{k=0}^{\infty} \frac{z^k}{k!} A^k u$$

converges for all $z \in \mathbb{C}$.

Entire vectors first appeared in the paper [14] by R. Goodman. The following proposition is crucial for us:

Proposition 3.1. *For $u \in \mathcal{H}^{c,\infty}(\mathbb{R}^n)$, the following facts are verified:*

(i) *The functions $\Delta^k u$, $k \in \mathbb{N}$, and $|\xi|^2 e^{c|\xi|^2} \mathcal{F}(u)$, are in $L^2(\mathbb{R}^n)$.*

(ii) *Let $\mathcal{E}(\Delta)$ be the set of all entire vectors of Δ in $L^2(\mathbb{R}^n)$, let $f \in \mathcal{E}(\Delta)$ and set $u = K * f$. Then*

$$\Delta \sum_{n=0}^{\infty} \frac{(-c)^n}{n!} \Delta^n u \in L^2(\mathbb{R}^n) \, .$$

Proof. Let $u \in \mathcal{H}^{c,\infty}(\mathbb{R}^n)$. We notice that $u \in C^m(\mathbb{R}^n)$ for every $m \geq 0$ due to Lemma 2.3. Moreover, Proposition 2.2 tells us that $u = K * f$ for some $f \in L^2(\mathbb{R}^n)$, and it follows that

$$(\Delta^k u)^\wedge(\xi) = (-|\xi|^2)^k \, \widehat{K}(\xi) \widehat{f}(\xi) \, ,$$

where $\wedge$ stands for the Fourier transform. Now, since K belongs to the Schwartz space, the product $(-|\xi|^2)^k \, \widehat{K}(\xi)$ is a bounded function. On the other hand $\widehat{f} \in L^2(\mathbb{R}^n)$, and therefore the right-hand side of the above identity is in $L^2(\mathbb{R}^n)$. The first part of claim (i) then follows. The second part is trivial since $u \in \mathcal{H}^{c,\infty}(\mathbb{R}^n)$.

We now prove (ii).

Proposition 2.2 implies that $u = K * f$ belongs to $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$, and (i) tells us that $-|\xi|^2 e^{c|\xi|^2} \mathcal{F}(u)$ belongs to $L^2(\mathbb{R}^n)$. We have

$$-|\xi|^2 e^{c|\xi|^2} \mathcal{F}(u) = -|\xi|^2 e^{c|\xi|^2} \widehat{K} \widehat{f} \tag{12}$$

$$= (\Delta K)^\wedge e^{c|\xi|^2} \widehat{f} \, . \tag{13}$$

On the other hand, $\sum_{k=0}^{\infty} \frac{(-c)^k}{k!}(\Delta^k f)$ converges in $L^2(\mathbb{R}^n)$ since $f \in \mathcal{E}(\Delta)$. Therefore $\sum_{k=0}^{\infty} \frac{(-c)^k}{k!}(\Delta^k f)^\wedge$ is also in $L^2(\mathbb{R}^n)$ by continuity of the Fourier transform. But then,

$$\left(e^{c|\,\xi|^2}\right)\widehat{f} = \left(\sum_{k=0}^{\infty} \frac{(-c)^k}{k!}(-|\xi|^2)^k\right)\widehat{f} \tag{14}$$

$$= \sum_{k=0}^{\infty} \frac{(-c)^k}{k!}(\Delta^k f)^\wedge \,. \tag{15}$$

Thus, from (13) we obtain, using again continuity of the Fourier transform

$$(\Delta K)^\wedge e^{c|\,\xi|^2}\widehat{f} = (\Delta K)^\wedge \sum_{k=0}^{\infty} \frac{(-c)^k}{k!}(\Delta^k f)^\wedge \tag{16}$$

$$= \Big(\Delta K * \sum_{k=0}^{\infty} \frac{(-c)^k}{k!}\Delta^k f\Big)^\wedge \,. \tag{17}$$

Using Lemma 3.1 we conclude that

$$\Big(\Delta K * \sum_{k=0}^{\infty} \frac{(-c)^k}{k!}\Delta^k f\Big)^\wedge = \left(\Delta\Big(K * \sum_{k=0}^{\infty} \frac{(-c)^k}{k!}\Delta^k f\Big)\right)^\wedge \,. \tag{18}$$

Thus, Equations (16) and (18) allow us to conclude that

$$(\Delta K)^\wedge e^{c|\,\xi|^2}\widehat{f} = \left(\Delta\Big(K * \sum_{k=0}^{\infty} \frac{(-c)^k}{k!}\Delta^k f\Big)\right)^\wedge \,, \tag{19}$$

$$= \left(\Delta\Big(\sum_{k=0}^{\infty} \frac{(-c)^k}{k!}K * \Delta^k f\Big)\right)^\wedge \tag{20}$$

$$= \Big(\Delta \sum_{k=0}^{\infty} \frac{(-c)^k}{k!}\Delta^k (K * f)\Big)^\wedge \,, \tag{21}$$

in which we have used continuity of convolution and Lemma 3.1. Since the left-hand side of (21) is in $L^2(\mathbb{R}^n)$, assertion (ii) now follows by applying the inverse Fourier transform to Equation (21). □

By Proposition 3.1, the action of the operator $L_c = \Delta e^{-c\Delta} - Id$ on $u = K * f \in \mathcal{H}^{c,\infty}(\mathbb{R}^n)$, where $f \in \mathcal{E}(\Delta)$, can be naturally defined as

$$L_c u = \Delta \sum_{k=0}^{\infty} \frac{(-c)^k}{k!} \underbrace{\Delta \circ \cdots \circ \Delta}_{k\text{-times}} u - u \,, \tag{22}$$

since the series in the right-hand side of (22) converges in $L^2(\mathbb{R}^n)$. For any $u \in \mathcal{H}^{c,\infty}(\mathbb{R}^n)$ we now prove:

Theorem 3.1. *The operator* $L_c = \Delta e^{-c\Delta} - Id$ *can be represented as*

$$L_c u = -\mathcal{F}^{-1}\left(\mathcal{F}(u) + |\,\xi|^2 e^{c|\,\xi|^2}\mathcal{F}(u)\right)\,, \tag{23}$$

for any $u \in \mathcal{H}^{c,\infty}(\mathbb{R}^n)$. *Furthermore,* L_c *is an isometry from* $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$ *into* $L^2(\mathbb{R}^n)$.

Proof. Let $u_f := K * f$ for f in $\mathcal{E}(\Delta)$. Then by the above remark

$$L_c u_f = \Delta e^{-c\Delta} u_f - u_f = \Delta \sum_{k=0}^{\infty} \frac{(-c)^k}{k!}\Delta^k u_f - u_f\,. \tag{24}$$

But then, taking Fourier transform we obtain

$$\mathcal{F}(L_c u_f) = -|\,\xi|^2 \sum_{k=0}^{\infty} \frac{(-c)^k}{k!}(-|\,\xi|^2)^k \mathcal{F}(u_f) - \mathcal{F}(u_f) = -\left(1 + |\,\xi|^2 e^{c|\,\xi|^2}\right)\mathcal{F}(u_f)\,,$$

and we notice that the definition of the norm for $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$ implies that

$$\|u_f\|_{\mathcal{H}^{c,\infty}} = \|L_c u_f\|_2\,. \tag{25}$$

Now we use the fundamental fact that the Laplacian operator Δ in $L^2(\mathbb{R}^n)$ is the generator of an analytic semigroup with angle $\pi/2$, see [1], and that therefore the set $\mathcal{E}(\Delta)$ of entire vectors of Δ is dense [13]. It follows from our remarks after Proposition 2.2 that the set of all the $u_f \in \mathcal{H}^{c,\infty}(\mathbb{R}^n)$ for $f \in \mathcal{E}(\Delta)$ is dense in $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$, and so Equations (23) and (25) are valid for all $u \in \mathcal{H}^{c,\infty}(\mathbb{R}^n)$. □

Certainly, we can generalize these constructions to the class of $\mathcal{G}^\beta$-symbols p. We follow our paper [17]: in view of Theorem 3.1, it is natural to define $p(\Delta)\,u$, $u \in \mathcal{H}^\beta(p)$, as

$$p(\Delta)u = \mathcal{F}^{-1}\left(\,p(-|\xi|^2)\,\mathcal{F}(u)(\xi)\,\right)\,. \tag{26}$$

Indeed, if $u \in \mathcal{H}^\beta(p)$, the function $p(-|\xi|^2)\,\mathcal{F}(u) \in L^2(\mathbb{R}^n)$, and $p(\Delta)u$ makes sense. Thus, $p(\Delta)$ is a well-defined bounded linear operator from $\mathcal{H}^\beta(f)$ to $L^2(\mathbb{R}^n)$.

We remark that Equation (26) reproduces formally the classical definition of a pseudo-differential operator in the sense of Hörmander [21, p. 68] but, as we already observed in the previous section, our "symbols" p fall outside the class of symbols considered in [21].

Definition 3.2. *Let* p *be a* $\mathcal{G}^\beta$*-symbol. The operator* $L = p(\Delta) + Id$ *acts on functions* $u \in \mathcal{H}^\beta(p)$ *as*

$$Lu = \mathcal{F}^{-1}\left(\,\mathcal{F}(u) + p(-|\xi|^2)\,\mathcal{F}(u)\,\right)\,. \tag{27}$$

Since $u \in \mathcal{H}^\beta(p)$, we can immediately check that $Lu \in L^2(\mathbb{R}^n)$ using the Parseval identity.

4. Generalized Euclidean bosonic string equations

4.1. The linear equation for L_c

We are in position to show that the linear problem $L_c u = g$, $g \in L^2(\mathbb{R}^n)$, can be solved completely using our set-up:

Theorem 4.1. *For each $c > 0$ and $g \in L^2(\mathbb{R}^n)$, there exists a unique solution $u_g \in \mathcal{H}^{c,\infty}(\mathbb{R}^n)$ to the linear problem*

$$L_c u = g \, . \tag{28}$$

Moreover, the following equation

$$\|u_g\|_{\mathcal{H}^{c,\infty}(\mathbb{R}^n)} = \|g\|_{L^2(\mathbb{R}^n)} \tag{29}$$

holds.

Proof. It is easy to see that u_g given by

$$u_g = -\mathcal{F}^{-1}\left(\frac{\mathcal{F}(g)}{1+|\xi|^2 e^{c|\xi|^2}}\right) = -K * g \, ,$$

is an element of $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$ which solves Equation (28). Now, applying Fourier transform we get

$$\left(1+|\xi|^2 e^{c|\xi|^2}\right)\mathcal{F}(u_g) = \mathcal{F}(g) \, ,$$

and so the Plancherel theorem implies that $\|u_g\|_{\mathcal{H}^{c,\infty}(\mathbb{R}^n)} = \|g\|_{L^2(\mathbb{R}^n)}$. Equation (29) tells us that the operator L_c has trivial kernel. Uniqueness then follows immediately. □

The solution to the linear problem (28) is not only smooth, but also real-analytic. This fact was shown by a direct computation in our paper [15]. In fact, "super-analyticity" of the solution follows as a corollary of Theorem 4.1 and our structural result Theorem 2.1:

Theorem 4.2. *Let us assume $g \in L^2(\mathbb{R}^n)$. Then, the unique solution u_g to problem (28) belongs to the Gevrey space $G^{1/2}$ and to the Gevrey spaces $G^{\sigma,s}$. In particular, the function u_g real-analytic, i.e., $u_g \in C^\omega(\mathbb{R}^n)$.*

4.2. The nonlinear equation for L_c: radial case

In this section we consider radial functions. Our aim is to prove existence of solutions to the nonlocal equation (2) if the nonlinearity U is spherically symmetric with respect to x, that is, if it satisfies $U(x,y) = U(|x|,y)$.

We denote by $\mathcal{H}^{c,\infty}_r(\mathbb{R}^n)$ the closed subspace of all radial functions in $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$. Our first observation is that if the non-homogeneity f appearing in problem (28) is a radial function, so is its unique solution:

Theorem 4.3. *If $f \in L^2_r(\mathbb{R}^n)$, then the unique solution $u \in \mathcal{H}^{c,\infty}(\mathbb{R}^n)$ to problem (28) is a radial function. Moreover, the identity*

$$\|u\|_{\mathcal{H}^{c,\infty}_r(\mathbb{R}^n)} = \|f\|_{L^2_r(\mathbb{R}^n)}$$

holds.

This result is a straightforward consequence of Proposition 2.2 and the explicit formula for the solution to Equation (28) appearing in Theorem 4.1.

We now state an existence result for nonlinear nonlocal equations. The following theorem was announced in [15] under growth assumptions which turned out to be a little too optimistic:

Theorem 4.4. *Let us assume that V is spherically symmetric with respect to x, and let us assume that there exist a constant $\alpha > 1$, and functions $h \in L^2(\mathbb{R}^n)$, $f \in L^{\frac{2\alpha}{\alpha-1}}(\mathbb{R}^n)$ such that the following two inequalities hold:*

$$|U(x,y) - y| \leq C(|h(x)| + |y|^\alpha), \quad \left|\frac{\partial}{\partial y}\left(U(x,y) - y\right)\right| \leq C\left(|f(x)| + |y|^{\alpha-1}\right) \quad (30)$$

for some constant $C > 0$. Then, there exist $0 < \epsilon < 1$ and $0 < \rho_\epsilon < 1$ such that whenever $\|h\|_2 < \rho_\epsilon$, there is a radial solution $u \in \mathcal{H}_r^{c,\infty}(\mathbb{R}^n)$ to the equation

$$\Delta e^{-c\Delta}\phi = U(x,\phi)\ . \quad (31)$$

with $\|u\|_{L_r^{2\alpha}(\mathbb{R}^n)} \leq \epsilon$.

Proof. Set

$$V_u(x) = U(x, u(x)) - u(x) \quad (32)$$

for $u \in L_r^{2\alpha}(\mathbb{R}^n)$, so that the nonlinear Equation (31) is formally equivalent to $L_c u = V_u$. Since U is radial and $u \in L_r^{2\alpha}(\mathbb{R}^n)$, V_u is a radial function. The function V_u belongs to $L^2(\mathbb{R}^n)$, since assumption (30) implies that

$$\|V_u\|_{L^2} = \|U(\cdot, u(\cdot)) - u(\cdot)\|_{L^2} \leq C\|h\|_{L^2} + C\| \, |u|^\alpha\|_{L^2}\ , \quad (33)$$

and this is finite because $h \in L^2(\mathbb{R}^n)$ and $u \in L_r^{2\alpha}(\mathbb{R}^n)$.

We prove existence of solutions via a fixed point argument. We anticipate one technical difficulty. Since we work on the whole of $\mathbb{R}^n$, standard reasoning based on the Rellich-Kondrakov theorem does not apply. Nevertheless, since we deal with radial spaces, we can use Lions' theorem on Sobolev spaces of functions possessing spherical symmetry (see [24, Theorem II.1], [20]):

For fixed $\epsilon > 0$ we define the set

$$X_\epsilon = \left\{u \in L_r^{2\alpha}(\mathbb{R}^n) : \|u\|_{L^{2\alpha}} \leq \epsilon\right\}.$$

It is easy to see that X_ϵ is a bounded, closed, convex and nonempty subset of the Banach space $L^{2\alpha}(\mathbb{R}^n)$. We define a map $\mathcal{G}$ as follows:

$$\mathcal{G} : X_\epsilon \to L_r^{2\alpha}(\mathbb{R}^n), \quad \mathcal{G}(u) = \tilde{u}\ ,$$

where $\tilde{u}$ is the unique solution to the non-homogeneous linear problem

$$L_c\tilde{u} = V_u\ . \quad (34)$$

There exists $\epsilon > 0$ such that $\mathcal{G} : X_\epsilon \to X_\epsilon$. Indeed, set $s_\alpha = \frac{n}{2}\left(\frac{\alpha}{\alpha+1}\right)$. Since $2 < 2\alpha < 2^* = \frac{2n}{n-2s_\alpha} = 2(\alpha+1)$, the Sobolev embedding theorem gives us the inclusion

$$H^{s_\alpha}(\mathbb{R}^n) \hookrightarrow L^{2\alpha}(\mathbb{R}^n)\ . \quad (35)$$

Let us take $u \in X_\epsilon$. By the Sobolev inequality and Lemma 2.2 we have

$$\|\mathcal{G}(u)\|_{L^{2\alpha}} \leq c\|\mathcal{G}(u)\|_{H^{s_\alpha}} \leq c_\alpha \|\mathcal{G}(u)\|_{\mathcal{H}^{c,\infty}(\mathbb{R}^n)} , \tag{36}$$

in which c_α is a generic constant depending on the embedding (35). Therefore, Theorem 4.1 implies

$$\|\mathcal{G}(u)\|_{L^{2\alpha}} \leq c_\alpha \|\mathcal{G}(u)\|_{\mathcal{H}^{c,\infty}(\mathbb{R}^n)} = c_\alpha \|V_u\|_{L^2} = c_\alpha \, \|U(\cdot, u(\cdot)) - u(\cdot)\|_{L^2} .$$

Thus, using (30) and the Sobolev embedding theorem as in (35) and (36), we find that

$$\begin{aligned} \|\mathcal{G}(u)\|_{L^{2\alpha}} \leq c\|\mathcal{G}(u)\|_{H^{s_\alpha}} &\leq c_\alpha \, C \, (\|h\|_{L^2} + \|u\|^\alpha_{L^{2\alpha}}) \\ &\leq c_\alpha \, C \, (\|h\|_{L^2} + \epsilon^\alpha) . \end{aligned} \tag{37}$$

It follows that if $\|h\|_{L^2}$ is suitably small, we can fix $0 < \epsilon < 1$ so that $c_\alpha \, C \, (\|h\|_{L^2} + \epsilon^\alpha) < \epsilon$. This implies that $\mathcal{G} : X_\epsilon \to X_\epsilon$, as claimed.

Next, we show that the map $\mathcal{G}$ is compact. We take any sequence u_n bounded in the space $L^{2\alpha}_r(\mathbb{R}^n)$. By inequality (37), the sequence $\mathcal{G}(u_n)$ is bounded in $H^{s_\alpha}_r(\mathbb{R}^n)$. Then, by Lemma 2.3 and Lions' theorem ([24, Theorem II.1], [20]) we obtain that the inclusion (35)

$$H^{s_\alpha}_r(\mathbb{R}^n) \hookrightarrow L^{2\alpha}_r(\mathbb{R}^n)$$

is compact and so the map $\mathcal{G}$ is compact. Next, we need to show that $\mathcal{G}$ is continuous, but this fact follows by a standard argument using the Mean Value Theorem and the assumption (30) on the y-derivative of U.

We conclude, therefore, that the map $\mathcal{G} : X_\epsilon \to X_\epsilon$ is compact and continuous. Schauder's fixed point theorem implies that there exists a radial regular solution to the nonlinear problem (40). □

From Theorems 4.4 and 4.2 we obtain a "maximal regularity" property for the solution to problem (40):

Corollary 4.1. *Let us assume that the function U appearing in the right-hand side of* (31) *satisfies the hypothesis of Theorem* 4.4. *Then, there exists a $G^{1/2}$-solution to problem* (31). *In particular, Equation* (31) *admits real-analytic solutions.*

4.3. The linear equation for general symbols L

In this subsection we summarize our results for equations depending on general $\mathcal{G}^\beta$-symbols. The result analogous to our Theorem 4.1 is:

Theorem 4.5. *Let p be a $\mathcal{G}^\beta$-symbol. For each $g \in L^2(\mathbb{R}^n)$, there exists a unique solution $u_g \in \mathcal{H}^\beta(p)$ to the linear problem*

$$Lu = g . \tag{38}$$

Moreover, the equation

$$\|u_g\|_{\mathcal{H}^\beta(p)} = \|g\|_{L^2(\mathbb{R}^n)}$$

holds.

It follows from the embedding results appearing in Lemma 2.3 that the solution to the linear equation (38) is regular. Under some extra assumptions on the symbol p, the solution u is in fact real-analytic:

Theorem 4.6. *Let us assume that $p \in \bigcap_{\beta>0} \mathcal{G}^\beta$ and that there exists $c > 0$ such that*

$$\lim_{m\to\infty} \frac{c^m}{m!} \int_0^\infty \frac{r^{2m+n-1}}{[1+p(-r^2)]^2} dr = 0 \,. \tag{39}$$

If $g \in L^2(\mathbb{R}^n)$, then the solution u to problem (28) is real-analytic, i.e., $u \in C^\omega(\mathbb{R}^n)$.

Proof. We sketch the proof, full details are in [17]. Let us fix $z \in \mathbb{R}^n$. The solution to problem (38) is of the form

$$u(z) = -\int_{\mathbb{R}^n \times \mathbb{R}^n} \frac{e^{2\pi i \xi(z-y)} g(y)}{1+p(-|\xi|^2)} d\xi dy.$$

The Lebesgue theorem, the Schwarz inequality and the Plancherel theorem yield

$$|D^k u(z)| \le (2\pi)^{|k|} \|g\|_{L^2} \left(\int_{\mathbb{R}^n} \left(\frac{|\xi|^{|k|}}{1+p(-|\xi|^2)} \right)^2 d\xi \right)^{\frac{1}{2}} ,$$

and we observe that introducing polar coordinates we can replace the last integral by

$$C \int_0^\infty \frac{r^{2|k|+n-1}}{[1+p(-r^2)]^2} dr \,.$$

The Taylor series for u at z is $\sum_k \frac{D^k u(z)}{k!}(x-z)^k$, where the sum is taken over all multi-indices. The remainder term

$$R_m(x) = \sum_{|k|=m} \frac{D^k u(z+t(x-z))(x-z)^k}{k!} \,, \quad t \in [0,1] \,,$$

is dominated by

$$\sqrt{C} \|f\|_{L^2} \frac{(2\pi n^2 R)^m}{m!} \left(\int_0^\infty \frac{r^{2m+n-1}}{[1+p(-r^2)]^2} dr \right)^{\frac{1}{2}} ,$$

and our assumption (39) yields $|R_m(x)| \to 0$. □

Certainly, this result includes our previous observation that solutions to the linear problem $L_c = g$ are real-analytic. Indeed, [17], if we consider the function $p(s) = -s\exp(-c\,s)$ we have again, this time as a corollary of Theorem 4.6:

Proposition 4.1. *The solutions ϕ to the linear bosonic string equation*

$$(\Delta e^{-c\Delta} + Id)\,\phi = g \,, \qquad g \in L^2(\mathbb{R}^n)$$

are real-analytic.

4.4. The nonlinear equation for general symbols L

In this section we consider the nonlinear equation

$$p(\Delta)\, u - U(\cdot, u) = 0 \tag{40}$$

following our work [17]. We can prove existence of solutions in two settings: first, in the case $U(x,y) = y + \varphi(x)V(x,y)$, where $x \in \mathbb{R}^n$, $y \in \mathbb{R}$, and $\varphi \in C_0^\infty(\mathbb{R}^n)$, and then in the case when the non-linearity $U : \mathbb{R}^n \times \mathbb{R} \to \mathbb{C}$ is spherically symmetric with respect to x. Since the proofs are similar in spirit to the one we summarized in Subsection 4.2, we only write down the statements of the theorems:

Theorem 4.7. *Let us assume that $f \in \mathcal{G}^\beta$, where $\beta > \frac{n}{2}$, and consider the function U_δ, $\delta > 0$, given by*

$$U_\delta(x,y) = -y + \delta\, \varphi(x) V(x,y)\,, \tag{41}$$

where $\varphi \in C_0^\infty(\mathbb{R}^n)$ and V is a differentiable function on $\mathbb{R}^n \times \mathbb{R}$. If there exist a constant $\alpha \geq 1$, a constant $C > 0$ and a function $h \in L^2(\mathbb{R}^n)$ such that the following inequalities hold,

$$|V(x,y)| + \left|\frac{\partial}{\partial x_i} V(x,y)\right| \leq C(h(x) + |y|^\alpha)\,, \qquad i = 1, \ldots, n\,, \tag{42}$$

$$\left|\frac{\partial}{\partial y} V(x,y)\right| \leq C(1 + |y|^\alpha)\,, \tag{43}$$

then, for small δ there exists a solution $u \in \mathcal{H}^\beta(f)$ to problem (40) *with the non-linearity U given by* (41).

In some cases, we can show that the solutions we just obtained are real-analytic:

Corollary 4.2. *Suppose that U is given by* (41)*, that the hypothesis of Theorem* 4.6 *hold, and that the growth assumptions of Theorem* 4.7 *are verified. Then, there exists a C^ω solution to problem* (40).

Now we consider the spherically symmetric case. We denote by $\mathcal{H}_r^\beta(f)$ the closed subspace of all radial functions in $\mathcal{H}^\beta(f)$. As in Subsection 4.2, we can check that if the non-homogeneity g appearing in problem (38) is a radial function, so is its unique solution. We have:

Theorem 4.8. *Let us assume that $p \in \mathcal{G}^\beta$, where $\beta > \frac{n}{2}\left(\frac{\alpha-1}{\alpha}\right)$ and that U is spherically symmetric with respect to x. Assume also that there exist a constant $\alpha > 1$, and functions $h \in L^2(\mathbb{R}^n)$, $g \in L^{\frac{2\alpha}{\alpha-1}}(\mathbb{R}^n)$ such that the following two inequalities hold:*

$$|U(x,y) + y| \leq C(|h(x)| + |y|^\alpha), \quad \left|\frac{\partial}{\partial y}\left(U(x,y) + y\right)\right| \leq C\left(|g(x)| + |y|^{\alpha-1}\right) \tag{44}$$

for some constant $C > 0$. Then, there exist $0 < \epsilon < 1$ and $0 < \rho_\epsilon < 1$ such that whenever $\|h\|_2 < \rho_\epsilon$, there is a radial solution $u \in \mathcal{H}_r^\beta(f)$ to the equation

$$p(\Delta)u - U(\cdot, u) = 0 \tag{45}$$

with $\|u\|_{L_r^{2\alpha}(\mathbb{R}^n)} \leq \epsilon$.

Finally, we comment on the analyticity of solutions:

Corollary 4.3. *Let us assume that U is spherically symmetric with respect to x, that the hypothesis of Theorem* 4.6 *hold, and that the growth assumptions of Theorem* 4.4 *hold. Then, there exists a C^ω solution to problem* (40).

5. Nonlocal equations on compact manifolds

In this section we consider nonlocal equations on a compact, connected, and oriented Riemannian manifold (M, g). We explain in detail how to proceed in the case of the bosonic string equation

$$\Delta_g e^{c\,\Delta_g}\phi - U(x,\phi) = 0\ , \quad c > 0\ , \tag{46}$$

and then we indicate briefly how to generalize our approach to equations of the form

$$p(\Delta_g)\phi = U(x,\phi)$$

for suitable functions p.

We recall [29] that the Laplacian operator Δ_g on a Riemannian manifold (M, g) is defined intrinsically as $\Delta_g f = - * d * d f$, in which d indicates exterior derivative and $*$ is the Hodge star operator. By Hodge's theorem, there exists an orthonormal complete set in $L^2(M)$ consisting of smooth eigenfunctions ω_i of the Laplacian operator Δ_g; all eigenvalues λ_i are non-negative real numbers with finite multiplicity, and they only accumulate at infinity [29].

We use these facts to interpret the left-hand side of Equation (46): If $\phi \in L^2(M)$, we can write $\phi = \sum \phi_i \omega_i$, and then we can compute $\Delta_g\, e^{c\,\Delta_g}\phi$ as

$$\Delta_g\, e^{c\,\Delta_g}\phi = \sum_{i=1}^{\infty} \lambda_i\, e^{c\,\lambda_i}\, \phi_i\, \omega_i\ ,$$

in analogy with the Fourier expansions used in Section 2.

Now we introduce, again in analogy with our previous analysis in the Euclidean space, the space $\widetilde{H}^k(M, g)$. First, we define the Hilbert space

$$l^{2,k}(\mathbb{N}) = \left\{ \alpha = (\alpha_i) : \sum_{i=1}^{\infty} |\alpha_i|^2 (1 + \lambda_i^2)^k < \infty \right\}$$

equipped with the inner product

$$\langle \alpha, \beta \rangle_{l^{2,k}(\mathbb{N})} = \sum_{i=1}^{\infty} \alpha_i \beta_i (1 + \lambda_i^2)^k\ .$$

We set

$$\widetilde{H}^k(M,g)$$
$$= \left\{ f = \sum_{i=1}^{\infty} \alpha_i \omega_i : \sum_{i=1}^{\infty} |\alpha_i|^2 \left(1 + \lambda_i^2\right)^k < \infty \right\} = \left\{ f = \sum_{i=1}^{\infty} \alpha_i \omega_i : (\alpha_i) \in l^{2,k}(\mathbb{N}) \right\}\ .$$

The space $\widetilde{H}^k(M,g)$ endowed with the inner product

$$\langle f,g\rangle_{\widetilde{H}^k(M,g)} = \langle(\alpha_i),(\beta_i)\rangle_{l^{2,k}(\mathbb{N})} = \sum_{i=1}^{\infty}\alpha_i\beta_i\left(1+\lambda_i^2\right)^k \ ,$$

where $f=\sum_{i=1}^{\infty}\alpha_i\,\omega_i$ and $g=\sum_{i=1}^{\infty}\beta_i\,\omega_i$, is a Hilbert space isometrically isomorphic to $l^{2,k}(\mathbb{N})$. The classical Sobolev spaces on Riemannian manifolds (see [18, 29]) coincide with the spaces $\widetilde{H}^k(M,g)$:

Lemma 5.1. *If $k\in\mathbb{N}$ then $\widetilde{H}^k(M,g)=H^k(M,g)$, in which $H^k(M,g)$ is the classical Sobolev space on the Riemannian manifold (M,g). Moreover, there exists a real constant C such that the following inequality holds*

$$\frac{1}{C}\|u\|_{\widetilde{H}^k(M,g)} \leq \|u\|_{H^k(M,g)} \leq C\|u\|_{\widetilde{H}^k(M,g)} \ . \tag{47}$$

Proof. It is enough to show inequality (47) for functions of the form

$$u_N=\sum_{i=1}^{N}\alpha_i\omega_i \ .$$

Hence, let us compute

$$\begin{aligned}\|u_N\|^2_{H^k(M,g)} &= \|u_N\|^2_{L^2(M,g)} + \sum_{l=1}^{k}\int_M \nabla^l u_N\nabla^l u_N dv_g \\ &= \|u_N\|^2_{L^2(M,g)} + \sum_{l=1}^{k}\sum_{i=1}^{N}\sum_{j=1}^{N}\int_M \nabla^l(\alpha_i\omega_i)\nabla^l(\alpha_j\omega_j)dv_g \ ,\end{aligned}$$

where $d\,v_g$ is the standard Riemannian measure on M. Next, integrating by parts k-times we get

$$\|u_N\|^2_{H^k(M,g)} = \sum_{l=0}^{k}\sum_{i=1}^{N}\sum_{j=1}^{N}\int_M \alpha_i\omega_i\alpha_j\omega_j\lambda_j^l dv_g = \sum_{l=0}^{k}\sum_{i=1}^{N}|\alpha_i|^2\lambda_i^l \ .$$

Finally, using the Newton formula we obtain

$$\frac{1}{k!}\|u_N\|^2_{\widetilde{H}^k(M,g)} \leq \|u_N\|^2_{H^k(M,g)} \leq 2^{\frac{k}{2}}\|u_N\|^2_{\widetilde{H}^k(M,g)} \ ,$$

and the lemma follows. □

Now we are ready to introduce a space analog to our $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$. We set

$$\widetilde{H}^{c,\infty}(M,g) = \left\{ f=\sum_{i=1}^{\infty}\alpha_i\omega_i : \sum_{i=1}^{\infty}|\alpha_i|^2\left(1+\lambda_i e^{c\lambda_i}\right)^2<\infty\right\}.$$

Using Lemma 5.1, some basic properties of the exponential map, and the Sobolev theorem on compact Riemannian manifolds [18, 29], we can check the following:

Lemma 5.2. *For each natural number k the embeddings $\widetilde{H}^{c,\infty}(M,g)\hookrightarrow H^k(M,g)$ and $\widetilde{H}^{c,\infty}(M,g)\hookrightarrow C^k(M,g)$ hold.*

Now we are in the position to define the operator $L_c = \Delta_g\, e^{c\,\Delta_g} + Id$ as an operator from $\widetilde{H}^{c,\infty}(M,g)$ to $L^2(M,g)$. We define

$$L_c\phi = \sum \left(\lambda_i\, e^{c\,\lambda_i} + 1\right)\, \phi_i\, \omega_i\ ,$$

where $\phi \in \widetilde{H}^{c,\infty}(M,g)$ and $\phi = \sum \phi_i\, \omega_i$. This construction allows us to solve linear equations, and to prove an existence and regularity result for the nonlinear problem (46) using arguments similar to the ones appearing in the proof of Theorem 4.4. We have:

Lemma 5.3. *For each $f \in L^2(M)$, the linear problem*

$$\Delta_g\, e^{c\,\Delta_g}\phi + \phi = f \tag{48}$$

possesses a unique solution $\phi \in \widetilde{H}^{c,\infty}(M,g)$, and moreover the following equation holds

$$\|\phi\|_{\widetilde{H}^{c,\infty}(M,g)} = \|f\|_{L^2(M,g)}\ .$$

Theorem 5.1. *Let us assume that $U : M \times \mathbb{R} \to \mathbb{R}$, and that there exist constants $\alpha > 1$, $\beta \geq 1$, $C > 0$, and a function $h \in L^2(M)$, such that the following two inequalities hold:*

$$|U(x,y) + y| \leq C(h(x) + |y|^{\alpha}), \quad \left|\frac{\partial}{\partial y}(U(x,y) + y)\right| \leq C\left(1 + |y|^{\beta}\right). \tag{49}$$

If $\|h\|_{L^2}$ is suitably small, there exists a C^{∞} solution ϕ on M to the nonlinear problem

$$\Delta_g e^{c\,\Delta_g}\phi - U(x,\phi) = 0\ . \tag{50}$$

Proof. We see that the nonlinear Equation (50) is equivalent to $L_c u = V(.,u)$, where $V(\cdot,u) = U(\cdot,u) + u$. We fix a real number $s > \frac{n}{2}$. By the Sobolev theorem we get the inclusions

$$H^s(M) \hookrightarrow L^{\infty}(M)\ . \tag{51}$$

Note that if $u \in H^s(M)$, then conditions (49) and the Sobolev embedding (51) imply that the function V belongs to $L^2(M)$.

We define the set

$$Y_{\epsilon} = \{u \in H^s(M) : \|u\|_{H^s} \leq \epsilon\}\ ,$$

so that Y_{ϵ} is a bounded, closed, convex and nonempty subset of the Banach space $H^s(M)$. We define a map $\mathcal{J}$ as follows:

$$\mathcal{J} : Y_{\epsilon} \to H^s(M), \quad \mathcal{J}(u) = \tilde{u}\ ,$$

where $\tilde{u}$ is the unique solution to the non-homogeneous linear problem

$$L_c\tilde{u} = V(.,u)\ .$$

It can be proved using (49) that there exists $\epsilon > 0$ such that $\mathcal{J} : Y_{\epsilon} \to Y_{\epsilon}$. The Rellich-Kondrakov theorem can be now invoked to show that the map $\mathcal{J}$ is compact, while the Mean Value Theorem and our assumptions on the derivative

of V imply that $\mathcal{J}$ is continuous. Application of Schauder's fixed point theorem finishes the proof. □

Finally, we consider briefly the general case $p(\Delta_g)\phi = U(\cdot\,, \phi)$ for suitable functions p. We assume that the "symbol" p satisfies the ellipticity condition

$$M\,(1+\lambda_i^2)^{k/2} \leq p(\lambda_i) \tag{52}$$

in which λ_i, $i = 1, 2, \ldots$, are the eigenvalues of the Laplacian operator Δ_g. We introduce the space

$$\widetilde{H}_p(M,g) = \left\{ h = \sum_{i=1}^{\infty} \alpha_i \omega_i : \sum_{i=1}^{\infty} |\alpha_i|^2 \left(1 + p(\lambda_i)\right)^2 < \infty \right\}.$$

Note that (52) implies that the continuous inclusions

$$\widetilde{H}_p(M,g) \hookrightarrow H^k(M,g)$$

hold for all k. In particular, if $h \in \widetilde{H}_p(M,g)$ then, see for instance [19, p. 34], h is a smooth function on M.

Now we define the operator $L = p(\Delta_g) + Id$ as an operator from $\widetilde{H}_p(M,g)$ to $L^2(M,g)$. We set

$$L\phi = \sum \left(p(\lambda_i) + 1\right)\, \phi_i\, \omega_i\ ,$$

where $\phi \in \widetilde{H}_p(M,g)$ and $\phi = \sum \phi_i\, \omega_i$. Instead of Lemma 5.3 and Theorem 5.1 we have the following two results, see [17]:

Lemma 5.4. *For each $h \in L^2(M)$, the linear problem*

$$p(\Delta_g)\,\phi + \phi = h \tag{53}$$

possesses a unique solution $\phi \in \widetilde{H}_p(M,g)$, and moreover we have,

$$\|\phi\|_{\widetilde{H}_p(M,g)} = \|h\|_{L^2(M,g)}\ .$$

Theorem 5.2. *Let us assume that p satisfies assumption* (52)*, that $U : M \times \mathbb{R} \to \mathbb{R}$, and that there exist constants $\alpha > 1$, $\beta \geq 1$, $C > 0$, and a function $h \in L^2(M)$, such that the following two inequalities hold:*

$$|U(x,y) + y| \leq C(h(x) + |y|^{\alpha}), \quad \left|\frac{\partial}{\partial y}(U(x,y) + y)\right| \leq C\left(1 + |y|^{\beta}\right). \tag{54}$$

If $\|h\|_{L^2}$ is suitably small, there exists a solution ϕ in $\widetilde{H}_p(M,g)$ to the nonlinear problem

$$p(\Delta_g)\,\phi - U(x,\phi) = 0\ . \tag{55}$$

6. Concluding remarks

We stress once again the fact that we arrive at our space $\mathcal{H}^{c,\infty}(\mathbb{R}^n)$ by interpreting $e^{-c\Delta}$ as a power series, so that our equations are really equations in an infinite number of derivatives, as we explained in Section 1. However, as shown in Sections 2 and 3, we can show that this interpretation coincides with the one we would naively impose motivated by the theory of pseudo-differential operators [21]. Once the relationship between equations in an infinite number of derivatives and pseudo-differential operators is understood, it is clear that we can construct suitable spaces for a wide class of symbols p on which $p(\Delta)$ defines a bounded linear operator.

As we have seen in Sections 4 and 5, existence and regularity of solutions to nonlocal equations possed on Euclidean space and compact Riemannian manifolds can be studied in our framework without difficulty. It remains to be investigated whether our methods extend to non-compact manifolds using [18, 19] (and, most probably, the extension of Lions' theorem [24] appearing in [20]) and to consider the physically relevant case of Lorentzian signature.

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Resonances for "Large" Ergodic Systems in One Dimension: A Review

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Abstract. The present note reviews recent results on resonances for one-dimensional quantum ergodic systems constrained to a large box (see [14]). We restrict ourselves to one-dimensional models in the discrete case. We consider two type of ergodic potentials on the half-axis, periodic potentials and random potentials. For both models, we describe the behavior of the resonances near the real axis for a large typical sample of the potential. In both cases, the linear density of their real parts is given by the density of states of the full ergodic system. While in the periodic case, the resonances distribute on a nice analytic curve (once their imaginary parts are suitably renormalized), in the random case, the resonances (again after suitable renormalization of both the real and imaginary parts) form a two-dimensional Poisson cloud.

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0. Introduction

On $\ell^2(\mathbb{N})$, consider V a bounded potential and the operator $H = -\Delta + V$ satisfying the Dirichlet boundary condition at 0.

The potentials V we will consider are of two types:

- V periodic;
- $V = V_\omega$ random, e.g., a collection of i.i.d. random variables.

The spectral theory of such models has been studied extensively (see, e.g., [11]) and it is well known that, when considered on $\ell^2(\mathbb{Z})$, the spectrum of H is purely absolutely continuous when V is periodic ([27]) while it is pure point when $V = V_\omega$ is the Anderson potential ([2, 22]). On $\ell^2(\mathbb{N})$, the picture is the same except for possible discrete eigenvalues outside the essential spectrum which coincides and is of the same nature as the essential spectrum of the operator on $\ell^2(\mathbb{Z})$.

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Let $L > 0$. The object of our study is the following operator on $\ell^2(\mathbb{N})$

$$H_L = -\Delta + V\mathbf{1}_{[\![0,L]\!]} \tag{0.1}$$

when L becomes large. Here, $-\Delta$ is the free Laplace operator defined by $-(\Delta u)(n) = u(n+1) + u(n-1)$ for $n \geq 0$ where $u = (u(n))_{n\geq 0} \in \ell^2(\mathbb{N})$ and $u(-1) = 0$ (Dirichlet boundary condition at 0), and $[\![0, L]\!] = \{0, 1, \ldots, L\} \subset \mathbb{N}$.

Clearly, the essential spectrum of H_L is that of the discrete Laplace operator, that is, $[-2, 2]$, and it is absolutely continuous. Moreover, outside this absolutely continuous spectrum, H_L has only discrete eigenvalues associated to exponentially decaying eigenfunctions.

We are interested in the resonances of the operator H_L. These can be defined as the poles of the meromorphic continuation of the resolvent of H_L through the continuous spectrum of H_L (see, e.g., [28]). One proves that

Theorem 1. *The operator-valued holomorphic function $z \in \mathbb{C}^+ \mapsto (z - H_L)^{-1}$ admits a meromorphic continuation from $\mathbb{C}^+$ to $\mathbb{C} \setminus ((-\infty, -2] \cup [2, +\infty))$ (see Fig. 1) with values in the operators from $\ell^2_{\mathrm{comp}}(\mathbb{N})$ to $\ell^2_{\mathrm{loc}}(\mathbb{N})$.*

FIGURE 1. The spectrum of H_L and the analytic continuation of $(z - H_L)^{-1}$

Moreover, the number of poles of this meromorphic continuation in the lower half-plane is at most equal to L.

As said, we define the resonances as the poles of this meromorphic continuation. The resonance widths, the imaginary part of the resonances, play an important role in the large time behavior of e^{-itH_L}, especially the smallest width that gives the leading order contribution (see [28, 29, 19]).

As $L \to +\infty$, H_L converges to H in the strong resolvent sense. Thus, it is natural to expect that the differences in the spectral nature between the cases V periodic and V random should reflect into differences in the behavior of the resonances. As we shall see, this is the case.

Our goal is to describe the resonances or, rather, their statistical properties and relate them (the distribution of the resonances, the distribution of their widths) to the spectral characteristics of $H = -\Delta + V$. In the periodic case, we expect that the Bloch-Floquet data for the operator $-\Delta + V$ on $\ell(\mathbb{Z})$ will be of importance; in the random case, this role should be taken over by the distribution of the eigenvalues of $-\Delta + V_\omega$.

The scattering theory or the closely related study of resonances for the operator (0.1) or for similar one-dimensional models has already been discussed in various works both in the mathematical and physical literature [6, 5, 16, 25, 3, 17,

1, 15, 26, 18]. The proofs of the result we present below will be released elsewhere ([14]). Though we will restrict ourselves to the discrete model, the continuous model can be dealt with in a very similar way.

Let us now describe our results. We start with the periodic case and turn to the random case in the next section.

1. The periodic case

We assume that, for some $p > 0$, one has

$$V_{n+p} = V_n \quad \text{for all} \quad n \geq 0. \tag{1.1}$$

Let Σ' be the spectrum of H acting on $\ell^2(\mathbb{N})$ and Σ_0 be the spectrum of $-\Delta + V$ acting on $\ell^2(\mathbb{Z})$. One then has the following description for the spectra:

- on $\ell^2(\mathbb{Z})$, $\Sigma_0 = \bigcup_{j=1}^{p} [a_j^-, a_j^+]$ for some $a_j^- < a_j^+$ $(p \geq 1)$ and the spectrum is purely absolutely continuous (see, e.g., [27]); the spectral resolution can be obtained via a Bloch-Floquet decomposition;
- on $\ell^2(\mathbb{N})$, one has (see, e.g., [23])
  - $\Sigma' = \Sigma_0 \cup \{v_j; 1 \leq j \leq n\}$ and Σ_0 is the a.c. spectrum of H;
  - the $(v_j)_{0 \leq j \leq n}$ are isolated simple eigenvalues associated to exponentially decaying eigenfunctions.

When L get large, it is natural to expect that the interesting phenomena are going to happen near energies in Σ'. In $\Sigma' \cap [(-\infty, -2) \cup (2, +\infty)]$, one can check that H_L has only discrete eigenvalues. We will now describe what happens for the resonances near $[-2, 2]$.

1.1. An auxiliary operator

On $\ell^2(\mathbb{Z}_-)$ (where $\mathbb{Z}_- = \{n \leq 0\}$), consider the operator $H_k^- = -\Delta + \tau_k V$ with Dirichlet boundary condition at 0; $\tau_k V$ is the potential V shifted k times to the left i.e. $\tau_k V(\cdot) = V(\cdot + k)$. Let $\Sigma_k^- = \sigma(H_k^-)$.

As is the case for H, the essentially spectrum of H_k^- is purely absolutely continuous and one has $\sigma_{\text{ess}}(H_k^-) = \Sigma_0$ (see e.g. [24, Chapter 7]). H_k^- may also have discrete eigenvalues in $\mathbb{R} \setminus \Sigma_0$. Let dN_k^- be the spectral measure associated to H_k^- and the vector δ_0 i.e.

$$\text{for Im } E \neq 0, \quad \int_{\mathbb{R}} \frac{dN_k^-(\lambda)}{\lambda - E} := \langle \delta_0, (H_k^- - E)^{-1} \Delta_0 \rangle.$$

Then, dN_k^- is a positive measure that is absolutely continuous on Σ_0. Moreover, its density is real analytic on $\overset{\circ}{\Sigma}_0$.

Let I be a compact interval in $(-2,2)\cap\overset{\circ}{\Sigma}_0$. For $E\in\overset{\circ}{\Sigma}_0$, define

$$S_k^-(E)=\text{p.v.}\left(\int_{\mathbb{R}}\frac{dN_k^-(\lambda)}{\lambda-E}\right):=\lim_{\varepsilon\downarrow 0}\left(\int_{-\infty}^{E_0-\varepsilon}\frac{dN_k^-(\lambda)}{\lambda-E}-\int_{E_0+\varepsilon}^{+\infty}\frac{dN_k^-(\lambda)}{\lambda-E}\right)\quad(1.2)$$

The existence and regularity of the Cauchy principal value S_k^- on $\overset{\circ}{\Sigma}_0$ is guaranteed by the regularity of dN_k^- in $\overset{\circ}{\Sigma}_0$ (see e.g. [10]).

In the lower half-plane $\{\text{Im } E<0\}$, define the function

$$\Xi_k(E):=\int_{\mathbb{R}}\frac{dN_k^-(\lambda)}{\lambda-E}+e^{-i\arccos(E/2)}.\quad(1.3)$$

Here, the function $z\mapsto\arccos z$ is the analytic continuation to the lower half-plane of the determination taking values in $[-\pi,0]$ over the interval $[-1,1]$.

The function Ξ_k vanishes at infinity and is analytic in $\{\text{Im } E<0\}$ and in a neighborhood of $(-2,2)\cap\overset{\circ}{\Sigma}_0$. It vanishes identically if and only if V vanishes identically (see [14]). So, if $V\not\equiv 0$, Ξ_k has only isolated zeros of finite multiplicity in $\{\text{Im } E<0\}$ and on $(-2,2)\cap\overset{\circ}{\Sigma}_0$.

1.2. Resonance free regions

We start with a description of the resonance free region.

Theorem 2. *Let I be a compact interval in $(-2,2)$. Then,*

- *if $I\subset\mathbb{R}\setminus\Sigma'$, then, there exists $C>0$ such that, for L sufficiently large, there are no resonances in $\{\text{Re } z\in I,\ \text{Im } z\geq -1/C\}$;*
- *if $I\subset\Sigma_0$, then, there exists $C>0$ such that, for L sufficiently large, there are no resonances in $\{\text{Re } z\in I,\ \text{Im } z\geq -1/(CL)\}$;*
- *if $\{v_j\}=\overset{\circ}{I}\cap\Sigma'=I\cap\Sigma'$ and $I\cap\Sigma_0=\emptyset=I\cap\Sigma_k^-$, then, for L sufficiently large s.t. $L=k \mod(p)$, there exists a unique resonance in $\{\text{Re } z\in I,\ \text{Im } z\geq -1/C\}$; moreover, this resonance, say z_j, satisfies, for some ρ_j independent of L,*

$$\text{Im } z_j\asymp -e^{-\rho_j L}\quad\text{and}\quad|z_j-v_j|\asymp e^{-\rho_j L}.\quad(1.4)$$

So, in the complex strip below the spectrum of the Laplace operator, i.e., the interval $(-2,2)$, except at the discrete spectrum of H, there exists a resonance free region of width at least of order L^{-1}. Each discrete eigenvalue of H generates a resonance that is exponentially close to the real axis.

1.3. Description of the resonances closest to Σ_0

Let I be a compact interval in $(-2,2)\cap\overset{\circ}{\Sigma}_0$ such that I does not contain any zero of Ξ_k (see (1.3)).

Let $(\lambda_j)_j=(\lambda_j^L)_j$ be the Dirichlet eigenvalues of $(-\Delta+V)_{|[\![0,L]\!]}$ in increasing order (see [27]). We then prove the

Theorem 3. *There exists $C_0 > 0$ such that, for $C > C_0$, there exists $L_0 > 0$ such that for $L > L_0$, for $\lambda_j \in I$ such that $\lambda_{j+1} \in I$, there exists a unique resonance in $[\lambda_j, \lambda_{j+1}] + i[-CL^{-1}, 0]$, say z_j. It satisfies*

$$z_j = \lambda_j + \frac{f_k(\lambda_j)}{L} \cot^{-1}\left(\left[e^{-i \arccos(\lambda_j/2)} + S_k^-(\lambda_j)\right] g_k(\lambda_j)\right) + o\left(\frac{1}{L}\right)$$

where $k \equiv L \mod p$ (p is the period of V) and $(f_k)_{0\le k\le p-1}$ and $(g_k)_{0\le k\le p-1}$ are real analytic functions defined by the Floquet theory of H on $\mathbb{Z}$.

The functions $(f_k)_k$ and $(g_k)_k$ can be computed explicitly in terms of the Floquet reduction (see [14]).

One can also analyze what happens near the real zeros of Ξ (see [14]): one obtains that the resonances leave the real axis to go up to distances of size $\dfrac{\log L}{L}$.

From this quite explicit description of the resonances, one shows that, in $I + i[-C/L, 0]$, for L sufficiently large,

- the resonances when rescaled to have imaginary parts of order 1 accumulate on a real analytic curve;
- the local (linear) density of resonances is given by the density of states of H.

More precisely, one proves

Corollary 1. *Fix I and k as above. Then, there exist $V \supset I$, a neighborhood of I and h_k real analytic on V such that, for C sufficiently large and L sufficiently large s.t. $L \equiv k \mod (p)$,*

- *if $z \in I + i[-CL^{-1}, 0]$ is a resonance of H_L, then*
$$L \cdot \operatorname{Im} z = h_k(\operatorname{Re} z) + o(1); \tag{1.5}$$
- *for $J \subset I$, any interval one has*
$$\frac{\#\{z \in J + i[-CL^{-1}, 0], z \text{ resonance of } H_L\}}{L+1} = \int_J dN(E) + o(1). \tag{1.6}$$
where N is the integrated density of states (see e.g. [22]) defined by
$$N(E) = \lim_{L\to+\infty} \frac{\#\{\text{eigenvalues of } (-\Delta + V)_{|[\![0,L]\!]} \text{ in } (-\infty, E]\}}{L+1}. \tag{1.7}$$

Figure 2 pictures the resonances after rescaling their width by L: these are nicely spaced points interpolating a smooth curve.

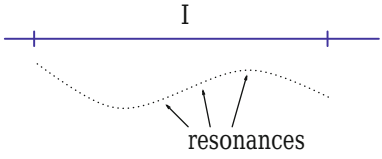

FIGURE 2. The rescaled resonances for a periodic potential

1.4. Description of the low lying resonances

One can also study what happens below the lines $\operatorname{Im} z = -C/L$. As above, let I be a compact interval in $(-2,2) \cap \overset{\circ}{\Sigma}_0$ such that I does not contain any zero of Ξ_k (see (1.3)).

One proves

Theorem 4. *There exists $c > 0$ s.t., for L sufficiently large s.t. $L = k \mod (p)$,*

- *the resonances of H in $I + i[-c, 0]$ are those described in Theorem 3;*
- *the resonances of H in $I + i(-\infty, -c]$ satisfy $|\Xi_k(z)| \leq e^{-cL}$. In particular, there are finitely many of them and they are all exponentially close to some zero of Ξ_k.*

So, by Theorem 3, except for a finite number of resonances that converge to the zeros of Ξ_k, all the resonances of H_L converge to the spectrum of H.

2. The random case

Let now $V = V_\omega$ where $V_\omega(n) = \omega_n$ and $(\omega_n)_{n\geq 0}$ are bounded independent and identically distributed random variables. Assume that the common law of the random variables admits a bounded density, say, g.

Set $H_\omega = -\Delta + V_\omega$ on $\ell^2(\mathbb{N})$. Let $\sigma(H_\omega)$ be the spectrum of H_ω and Σ be the almost sure spectrum of $-\Delta + V_\omega$ acting on $\ell^2(\mathbb{Z})$ (see [11]); one knows that

$$\Sigma = [-2d, 2d] + \operatorname{supp} g$$

One has the following description for the spectra:

- on $\ell^2(\mathbb{Z})$. ω-almost surely, $\sigma(-\Delta + V_\omega) = \Sigma$; the spectrum is purely punctual; it consists of simple eigenvalues associated to exponentially decaying eigenfunctions (Anderson localization, see, e.g., [22, 11]); one can prove that the whole spectrum is dynamically localized;
- on $\ell^2(\mathbb{N})$, one has (see, e.g., [22, 2])
  - ω-almost surely, $\sigma(H_\omega) = \Sigma \cup K_\omega$;
  - Σ is the essential spectrum of H_ω; it consists of simple eigenvalues associated to exponentially decaying eigenfunctions;
  - the set K_ω is the discrete spectrum of H_ω which may be empty and depends on ω.

2.1. The integrated density of states and the Lyapunov exponent

It is defined by (1.7) where $-\Delta + V$ is replaced by $-\Delta + V_\omega$; the limit then exists ω-a.s. and is ω-a.s. independent of ω. N is the distribution function of a probability measure supported on Σ. As the common law of the random variables $(\omega_n)_{n\geq 0}$ admits a bounded density, the integrated density of states $N(E)$ is known to be Lipschitz continuous ([22, 11]). Let $n(E) = \dfrac{dN}{dE}(E)$ be its derivative; it exists for almost every E.

One also defines the Lyapunov exponent, say $\rho(E)$ as follows

$$\rho(E) = \lim_{L\to+\infty} \frac{1}{L+1} \log \left\| \prod_{n=L}^{0} \begin{pmatrix} E - V_\omega(n) & -1 \\ 1 & 0 \end{pmatrix} \right\|. \tag{2.1}$$

For any E, ω-almost surely, this limit is known to exist and to be independent of ω (see, e.g., [22, 2]). Moreover, it is positive and continuous for all E and the Thouless formula states that it is the harmonic conjugate of $n(E)$ (see, e.g., [4]).

2.2. Resonance free regions

Define $H_{\omega,L}$ by (0.1) for $V = V_\omega$. We again start with a description of a resonance free region near the spectrum of $-\Delta$. As in the periodic case, the size of this region will depend on whether an energy belongs to the essential spectrum of H_ω or not. We prove

Theorem 5. *Let I be a compact interval in $(-2, 2)$. Then, one has*

- *there exists $C > 0$ such that, ω-a.s., if $I \subset \mathbb{R} \setminus \sigma(H_\omega)$, then, for L sufficiently large, there are no resonances of $H_{\omega,L}$ in $\{\mathrm{Re}\ z \in I,\ \mathrm{Im}\ z \geq -1/C\}$;*
- *there exists $C > 0$ such that, ω-a.s., if $\{v_j\} = \{v_j(\omega)\} = \overset{\circ}{I} \cap K_\omega = I \cap K_\omega$ and $I \cap \Sigma = \emptyset$, then, for L sufficiently large, there exists a unique resonance in $\{\mathrm{Re}\ z \in I,\ \mathrm{Im}\ z \geq -1/C\}$; moreover, this resonance, say z_j, satisfies (1.4) for some $\rho_j = \rho_j(\omega)$ independent of L.*
- *if $I \subset \overset{\circ}{\Sigma}$, then, there exists $C > 0$ such that, ω-a.s., for L sufficiently large, there are no resonances of $H_{\omega,L}$ in $\{\mathrm{Re}\ z \in I,\ \mathrm{Im}\ z \geq -e^{-2\rho L(1+o(1))})\}$ where ρ is the maximum of the Lyapunov exponent $\rho(E)$ on I.*

When comparing this result with Theorem 2, it is striking that the width of the resonance free region below Σ is much smaller in the random case than in the periodic case. This a consequence of the localized nature of the spectrum, i.e., of the exponential decay of the eigenfunction.

2.3. Description of the resonances close to Σ

We will now see that below the resonance free strip exhibited in Theorem 5 one does find resonances, actually, many of them. We prove

Theorem 6. *Let I be a compact interval in $(-2, 2) \cap \overset{\circ}{\Sigma}$. Then, ω-a.s.,*

- *for any $\kappa \in (0, 1)$, one has*

$$\frac{1}{L} \# \left\{ z \text{ resonance of } H_{\omega,L} \text{ s.t. } \mathrm{Re}\ z \in I,\ \mathrm{Im}\ z \geq -e^{-L^\kappa} \right\} \to \int_I dN(E);$$

- *fix $E \in I$ such that $n(E) > 0$; then, for $\delta > 0$, there exits $\varepsilon > 0$ such that*

$$\liminf_{L\to+\infty} \frac{1}{L} \# \left\{ \text{resonances } z \text{ s.t. } \begin{matrix} \mathrm{Re}\ z \in [E-\varepsilon, E+\varepsilon], \\ \mathrm{Im}\ z \geq -e^{-2(\rho(E)-\delta)L} \end{matrix} \right\} > 0.$$

The striking fact is that the resonances are much closer to the real axis than in the periodic case; the lifetime of these resonances is much larger. The resonant states are quite stable with lifetimes that are exponentially large in the width of the random perturbation.

The structure of the set of resonances is also very different from the one observed in the periodic case (see Fig. 2) as we will see now. Let I be a compact interval in $(-2,2) \cap \overset{\circ}{\Sigma}$ and $\kappa \in (0,1)$. Fix $E_0 \in I$ such that $n(E_0) > 0$.

Let $(z_j^L(\omega))_j$ be the resonances of $H_{\omega,L}$ in $K_L := [E_0-\varepsilon, E_0+\varepsilon]+i\big[-e^{-L^\kappa}, 0\big]$. We first rescale the resonances: define

$$\begin{aligned} x_j = x_j^L(\omega) &= n(E_0)\, L\, (\operatorname{Re} z_j^L(\omega) - E_0) \\ y_j = y_j^L(\omega) &= -\frac{1}{2\rho(E_0)\, L} \log |\operatorname{Im} z_j^L(\omega)|. \end{aligned} \tag{2.2}$$

Let us note that the scaling of the real and of the imaginary of the resonances are very different. According to the conclusions of Theorem 6, this scaling essentially sets the mean spacing between the real parts of the resonances to 1 and the imaginary parts to be of order 1.

Consider now the two-dimensional point process $\xi_L(E_0,\omega)$ defined

$$\xi_L(E_0,\omega) = \sum_{z_j^L \in K_L} \delta_{(x_j,y_j)}. \tag{2.3}$$

We prove

Theorem 7. *The point process ξ_L converges weakly to a Poisson process in $\mathbb{R}\times[0,1]$ with intensity 1. That is, for any $p \geq 0$, if $(I_n)_{1\leq n\leq p}$ resp. $(C_n)_{1\leq n\leq p}$, are disjoint intervals of the real line $\mathbb{R}$ resp. of $[0,1]$, then*

$$\lim_{L\to+\infty} \mathbb{P}\left(\left\{ \omega; \begin{array}{c} \#\left\{ j;\ \begin{array}{l} x_j(\omega,\Lambda) \in I_1 \\ y_j(\omega,\Lambda) \in C_1 \end{array} \right\} = k_1 \\ \vdots \\ \#\left\{ j;\ \begin{array}{l} x_j(\omega,\Lambda) \in I_p \\ y_j(\omega,\Lambda) \in C_p \end{array} \right\} = k_p \end{array} \right\} \right) = \prod_{n=1}^{p} e^{-\mu_n} \frac{(\mu_n)^{k_n}}{k_n!},$$

where $\mu_n := |I_n||C_n|$ for $1 \leq n \leq p$.

Hence, after rescaling the picture of the resonances (see Fig 3) is that of points chosen randomly independently of each other in $\mathbb{R}\times[0,1]$.

This is the analogue of the celebrated result on the Poisson structure of the eigenvalues for a random system (see, e.g., [21, 20, 7])

In [12], we proved decorrelation estimates that can be used in the present setting to prove

Theorem 8. *Fix $E_0 \neq E_0'$ such that $n(E_0) > 0$ and $n(E_0') > 0$. Then, the limits of the processes $\xi_L(E_0,\omega)$ and $\xi_L(E_0',\omega)$ are stochastically independent.*

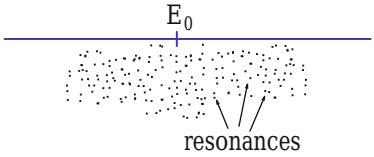

FIGURE 3. The rescaled resonances for a random potential

Due to the rescaling, the above results give a picture of the resonances in a zone of the type

$$E_0 + L^{-1}\left[-\varepsilon^{-1}, \varepsilon^{-1}\right] - i\left[e^{-2(1-\varepsilon)\rho(E_0)L}, e^{-2\varepsilon\rho(E_0)L}\right]$$

For $\varepsilon > 0$ small fixed, when L gets large, this rectangle is of a very small width and located very close to the real axis.

One can get a number of other statistics using the techniques developed for the study of the spectral statistics of the eigenvalues of a random system in the localized phase (see [14, 9, 7, 8, 13]).

2.4. The description of the low lying resonances

It is natural to question what happens deeper in the complex plane. To answer this question, fix two increasing sequences of scales $\ell = (\ell_L)_L$ and $\ell' = (\ell'_L)_L$ such that

$$\ell'_L \leq \ell_L, \quad \frac{\ell'_L}{\log L} \underset{L\to+\infty}{\to} +\infty \quad \text{and} \quad \frac{\ell_L}{L} \underset{L\to+\infty}{\to} 0. \tag{2.4}$$

Fix $\kappa \in (0,1)$. Fix $x_0 \in [0,1]$ and $E_0 \in I$ so that $n(E_0) > 0$. Let $(z_j^L(\omega))_j$ be the resonances of $H_{\omega,L}$ in $\tilde{K}_L := [E_0 - \varepsilon, E_0 + \varepsilon] + i\left[-e^{-\ell'_L}, 0\right)$. Note that $\tilde{K}_L$ is much wider than K_L defined above. We first rescale the resonances using the scale ℓ: define

$$x_j = x_j^{\ell_L}(\omega) = (\operatorname{Re} z_j^L(\omega) - E_0)\ell_L \quad \text{and} \quad y_j = y_j^{\ell_L}(\omega) = \frac{1}{2\ell_L}\log|\operatorname{Im} z_j^L(\omega)|. \tag{2.5}$$

Consider now the two-dimensional point process

$$\xi_{L,\ell,\ell'}(x_0, E_0, \omega) = \sum_{z_j^L \in K_L} \delta_{(x_j, y_j)}. \tag{2.6}$$

We prove

Theorem 9. *For $x_0 \in [0,1)$ and $E_0 \in I$ so that $\nu(E_0) > 0$, the point process $\xi_{L,\ell,\ell'}(x_0, E_0, \omega)$ converges weakly to a Poisson process in $\mathbb{R} \times \mathbb{R}^+$ with density $\frac{n(E_0)}{\rho(E_0)} dxdy$.*

Note that, for any $\alpha > 1$, due to the scaling (2.5), all the resonances that live above the line $\operatorname{Im} z = -e^{-\ell_\Lambda^\alpha}$ are pushed off to infinity and those below the line $\operatorname{Im} z = -e^{-\ell_\Lambda^{1/\alpha}}$ pushed off to the real line. So in Theorem 9, we described the

resonances near the line $\operatorname{Im} z = -e^{-\ell_\Lambda}$. By (2.4), these resonances lie deeper into the lower half-plane than those studied in Theorem 7.

For the processes $(\xi_{L,\ell,\ell'}(x_0, E_0, \omega))_{x_0,E_0}$, one gets an asymptotic independence result analogous to Theorem 8, namely,

Theorem 10. *Fix E_0 and E_0' such that $n(E_0) > 0$ and $n(E_0') > 0$ and x_0 and x_0' such that $(x_0, E_0) \neq (x_0', E_0')$.*

Then, the limits of the processes $\xi_{L,\ell,\ell'}(x_0, E_0, \omega)$ and $\xi_{L,\ell,\ell'}(x_0', E_0', \omega)$ are stochastically independent.

One can also study the resonances that are even further away from the real axis in a way similar to Theorem 4 in the periodic case. Define

$$\tilde{V}_{\omega,L}(n) = \begin{cases} \omega_{L-n} \text{ for } 0 \leq n \leq L, \\ 0 \text{ for } L+1 \leq n. \end{cases}$$

Consider the operator $\tilde{H}_{\omega,L} = -\Delta + \tilde{V}_{\omega,L}$ on $\ell^2(\mathbb{N})$ with Dirichlet boundary condition at 0. As the $(V_\omega(n))_n \geq 0$ are i.i.d. random variables. $\tilde{H}_{\omega,L}$ clearly has the same distribution as $H_{\omega,L}$. Define the measure dN_ω by its Borel transform

$$\text{for } \operatorname{Im} E \neq 0, \quad \int_{\mathbb{R}} \frac{dN_\omega(\lambda)}{\lambda - E} = \langle \delta_0, (H_\omega - E)^{-1} \delta_0 \rangle.$$

We prove

Theorem 11. *Fix $\kappa \in (0,1)$ and $I \subset \overset{\circ}{\Sigma}$. With probability 1, for L sufficiently large, in $I + i\left(-\infty, e^{-L^\kappa}\right]$, a resonance of $\tilde{H}_{\omega,L}$, say E, satisfies*

$$\int_{\mathbb{R}} \frac{dN_\omega(\lambda)}{\lambda - E} + e^{-i \arccos(E/2)} = O\left(e^{-L^\kappa}\right).$$

This should be compared with the results of [16, 17].

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Understanding the Random Displacement Model: From Ground State Properties to Localization

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Abstract. We give a detailed survey of results obtained in the most recent half-decade which led to a deeper understanding of the random displacement model, a model of a random Schrödinger operator which describes the quantum mechanics of an electron in a structurally disordered medium. These results started by identifying configurations which characterize minimal energy, then led to Lifshitz tail bounds on the integrated density of states as well as a Wegner estimate near the spectral minimum, which ultimately resulted in a proof of spectral and dynamical localization at low energy for the multi-dimensional random displacement model.

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47B80 (secondary).

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1. Introduction

By the random displacement model (RDM) we refer to a random Schrödinger operator of the type

$$H_\omega = -\Delta + V_\omega, \quad V_\omega(x) := \sum_{n\in\mathbb{Z}^d} q(x-n-\omega_n) \tag{1}$$

in $L^2(\mathbb{R}^d)$, $d \geq 1$. The potential is generated by randomly displacing translates of the single-site potential q from the lattice sites $n \in \mathbb{Z}^d$. More detailed assumptions on q and the random displacements ω_n will be introduced below as needed.

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The RDM has proven to be much harder to analyze mathematically than the (continuum) Anderson model

$$H^A_{\lambda(\omega)} = -\Delta + \sum_{n\in\mathbb{Z}^d} \lambda_n q(x-n) \tag{2}$$

with random coupling constants $\lambda_n = \lambda_n(\omega)$. A fundamental technical difference between the RDM and the Anderson model lies in their monotonicity properties. If the single-site potential q is sign-definite, then the Anderson model is monotone in the random variables λ_n in quadratic form sense. This is not true for the RDM, independent of sign-assumptions on q.

Many of the rigorous tools which have been developed to study the Anderson model rely on its monotonicity properties. In particular, this is true for most of the proofs of localization for the Anderson model near the bottom of its spectrum. In fact, if one considers the Anderson model with sign-indefinite single-site potential q, and thus looses monotonicity, then localization results are much more recent and far less complete than for the case of sign-definite q, e.g., [40, 32, 24, 34, 35]. The difficulties which arise are in many ways similar to the problems encountered in the RDM. Related phenomena and difficulties also arise in discrete alloy-type models with sign-indefinite single site potential, as recently reviewed in [14].

Among models for continuum random Schrödinger operators, the *structural disorder* described by the RDM can be considered as physically equally natural as the coupling constant disorder in the Anderson model. Another natural model for structural disorder is the Poisson model

$$-\Delta + \sum_i q(x - X_i), \tag{3}$$

with X_i denoting the points of a d-dimensional Poisson process. The RDM as well as the Poisson model were introduced early on in the mathematical literature on continuum random Schrödinger operators, e.g., [26, 36] and references therein. However, progress has been much more limited than for the Anderson model due to the technical difficulties which arise.

An exception is the case $d = 1$, where localization throughout the entire spectrum has been proven for the RDM and the Poisson model in [39, 8, 13]. This was possible based on the powerful dynamical systems methods available to study one-dimensional random operators, in particular those allowing to prove positivity of Lyapunov exponents and to deduce localization from this. However, the non-monotonicity of the RDM and the Poisson model has visible consequences already in the one-dimensional case, for example through the appearance of critical energies in the spectrum at which the Lyapunov exponent vanishes and, in some cases, weaker results (e.g., on dynamical localization, which has not been shown for the one-dimensional Poisson model).

In dimension $d \geq 2$ it is generally expected that "typical" random Schrödinger operators have a localized region at the bottom of the spectrum, at least if the latter corresponds to a *fluctuation boundary* of the spectrum, which describes a

boundary characterized by rare events. The history of localization proofs for the multi-dimensional RDM and Poisson model is told very quickly. For the Poisson model in $d \geq 2$ localization at the bottom of the spectrum was finally proven in [18] for positive single-site potentials and in [19] for negative single-site potentials. In both cases the powerful extension of multi-scale analysis developed by Bourgain and Kenig in [6] was used as a tool.

There were two previous results on localization for the multi-dimensional RDM, [31] and [22]. In [31] a semiclassical version of (1) is considered and localization near the bottom of the spectrum is established for sufficiently small values of a semiclassical coupling parameter at the Laplacian. [22] considers the RDM with an additional periodic term V_{per} and establishes localization for generic (but non-zero) choices of V_{per}. In both works the values of the displacements ω_n have to be sufficiently small and first-order perturbation effects (such as a monotonicity property of Floquet eigenvalues of $-\Delta + V_{\text{per}}$ in [22]) are exploited. What makes the "naked RDM" (1) more difficult to handle is that, as will be pointed out below, one ultimately has to resort to second-order perturbation effects.

The goal of this work is to give a detailed survey of new results for the RDM (1) obtained in the papers [4, 5, 35] and [30], which allowed to understand that the spectral minimum of the RDM is a fluctuation boundary under a natural set of assumptions not requiring additional parameters or smallness of the displacements (other than a non-overlap condition), and ultimately led to a proof of localization in this setting in [30].

The strategy used to prove localization in these works is the one provided by the Fröhlich-Spencer multi-scale analysis [17], as described for continuum models in very accessible form in the book [38], and with state-of-the-art results shown in [20] and surveyed in [29]. In essence, the MSA approach shows that localization, spectral as well as dynamical, can be proven once a smallness result ("Lifshitz tails") for the integrated density of states at the bottom of the spectrum and a Wegner estimate are available as input.

Therefore much of our effort is aimed at proving these two ingredients. However, for the RDM (1) one first needs to address a preliminary problem: Which configurations $\omega = (\omega_n)$ characterize the minimum of the almost sure spectrum of H_ω? To explain that this is a non-trivial issue, let us compare with the Anderson and Poisson models. In the Anderson model (2), due to monotonicity, the spectrum is minimized by choosing all coupling constants λ_n minimal (in the support of their distribution) if q is positive, while all λ_n should be chosen maximal if q is negative. For the Poisson model (3) the spectral minimum is 0 if q is positive, corresponding to regions with widely separated Poisson points. If q is negative, then regions of densely clustered Poisson points lead to spectral minimum $-\infty$. The mechanism for generating the spectral minimum in the RDM is much less apparent (with similar difficulties arising for the Anderson model with non sign-definite single-site potential). In fact, while for the (definite) Anderson and Poisson model the spectrum is minimized by minimizing the potential, for the RDM we

will see that a much more subtle interaction between kinetic and potential energy determines the spectral minimum.

In terms of assumptions to be made, the most important one is that the single-site potential shares the symmetries of the underlying lattice, here $\mathbb{Z}^d$. It is fair to say that in our approach symmetry replaces the lack of any apparent monotonicity properties of the model, ultimately allowing to identify more delicate monotonicity properties which are at the core of our proofs of Lifshitz tail bounds and a Wegner estimate for the RDM.

We find it remarkable how many mathematical ideas and tools had to be invoked and how all this ultimately fit together quite perfectly to lead to a localization proof for the RDM (1). Getting this across to the reader is our main motivation for providing this expository account of our work. Beyond merely stating a series of results, we include frequent discussions of the underlying motivations, often going beyond what we have been able to include in our previously published work. We have also tried to include at least outlines of all proofs, even if we frequently have to refer to the original papers for additional details.

A rough outline of the contents of the remaining sections of this paper is as follows: In Section 2 we reveal how the spectral minimum of the RDM is found. In Section 3 we show how the proof of this is reduced to a spectral minimization property of a related single-site Neumann operator. This operator and its ground state properties are central to almost all our results. In particular, we will revisit this operator in Section 6 and explain why we ultimately needed to know more about it than what is stated in Section 3. To avoid having to interrupt the telling of our localization story, we outline the proofs of these results in Section 10 near the end of the paper.

The rest of the localization story is told in Sections 4, 5, 7, 8 and 9. Section 4 yields information on uniqueness of configurations characterizing the spectral minimum which is necessary for the proof of Lifshitz tail bounds in Sections 5 and 7. The results in the latter two sections work in form of a boot-strap, starting with a Lifshitz tail bound under strong additional assumptions which are then relaxed. Our Wegner estimate for the RDM is presented in Section 8. In Section 9 we state the exact form of our result on localization for the RDM and provide references to the literature on multi-scale analysis, which show how this is proven based on the Lifshitz tail and Wegner bounds. In the very last Section 11 we discuss some open problems related to our work.

2. The spectral minimum of the RDM

We will always assume that the displacement parameters $\omega = (\omega_n)_{n\in\mathbb{Z}^d}$ are independent, identically distributed $\mathbb{R}^d$-valued random variables. Their common distribution is a Borel probability measure on $\mathbb{R}^d$. As usual, we define its support by

$$\operatorname{supp}\mu := \{a \in \mathbb{R}^d : \mu(B_\varepsilon(a)) > 0 \text{ for all } \varepsilon > 0\},$$

which is a closed set. The i.i.d. random variables ω_n can be realized as the canonical projections $\omega \mapsto \omega_n$ in the infinite product probability space

$$(\Omega, \mathbb{P}) = \left(\otimes_{n\in\mathbb{Z}^d}\mathbb{R}^d, \otimes_{n\in\mathbb{Z}^d}\mu\right).$$

Under weak assumptions on μ and the single-site potential q the RDM H_ω is self-adjoint on the second-order Sobolev space in $L^2(\mathbb{R}^d)$ and ergodic with respect to shifts in $\mathbb{Z}^d$ in the sense of, e.g., [10]. Thus its spectrum is almost surely deterministic: There exists $\Sigma \subset \mathbb{R}$ such that

$$\sigma(H_\omega) = \Sigma \quad \text{for } \mathbb{P}\text{-almost every } \omega. \tag{4}$$

In fact, one has

$$\Sigma = \overline{\bigcup_{\omega\in\mathcal{C}_{\mathrm{per}}} \sigma(H_\omega)}, \tag{5}$$

where

$$\mathcal{C}_{\mathrm{per}} := \{\omega \in \mathbb{Z}^d \to \operatorname{supp}\mu \text{ periodic with respect to a sub-lattice of } \mathbb{Z}^d\}. \tag{6}$$

This follows by the same methods which have been used to prove a corresponding result for the Anderson model: That Σ is contained in the right-hand side of (5) follows by approximating any given random configuration with periodic configurations, truncating the random configuration to large cubes and periodically extending from there. On the other hand, one can show that almost every random configuration comes arbitrarily close to any given periodic configuration on arbitrarily large cubes, which is he idea behind the reverse inclusion. For a detailed proof, written for the case of the Anderson model, we refer to [26].

In particular, (5) implies that

$$E_0 := \min\Sigma = \inf\{\min\,\sigma(H_\omega) : \omega \in \mathcal{C}_{\mathrm{per}}\}. \tag{7}$$

It is a non-trivial question to decide if there is a periodic minimizer, i.e., if the infimum in (7) is a minimum. In fact, we do not believe that this is true in general. Our choice of the following assumptions on q and μ is mostly motivated by the fact that they allow to find a periodic minimizer for (7).

(A1) The single-site potential $q : \mathbb{R}^d \to \mathbb{R}$ is bounded, measurable and reflection-symmetric in each variable. Moreover, $\operatorname{supp} q \subset [-r, r]^d$ for some $r < 1/2$.

(A2) Let $d_{\max} := \frac{1}{2} - r$ and $\mathcal{C} := \{(\pm d_{\max}, \ldots, \pm d_{\max})\}$ denote the 2^d corners of the closure $\overline{G}$ of $G := (-d_{\max}, d_{\max})^d$. Then

$$\mathcal{C} \subset \operatorname{supp}\mu \subset \overline{G}.$$

The two support assumptions on q and μ have a simple geometric interpretation for the RDM (1): The support of each single-site term $q(\cdot - n - \omega_n)$ stays in the unit cell centered at n, while it is allowed to "touch" the boundary of the cell. In fact, with positive probability the single-site potentials may move arbitrarily close to each corner of their cell. For a typical configuration of the ω_n see Figure 1 (where the support of q is drawn radially symmetric for aesthetic reasons).

We can now identify a periodic minimizer for (7), stating a result from [4]:

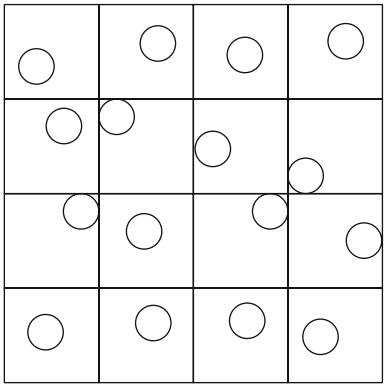

FIGURE 1. The support of V_ω for a typical ω.

Theorem 2.1. *Assume* **(A1)** *and* **(A2)** *and let* $\omega^* = (\omega_n^*)_{n\in\mathbb{Z}^d}$ *be given by*

$$\omega_n^* := ((-1)^{n_1} d_{\max}, \dots, (-1)^{n_d} d_{\max}), \quad n = (n_1, \dots, n_d) \in \mathbb{Z}^d. \tag{8}$$

Then $E_0 = \min \sigma(H_{\omega^*})$.

The potential $V_{\omega^*}(x) = \sum_n q(x - n - \omega_n^*)$ is 2-periodic in each direction and locally consists of densest clusters of 2^d single-site terms placed into adjacent corners of their cells, see Figure 2.

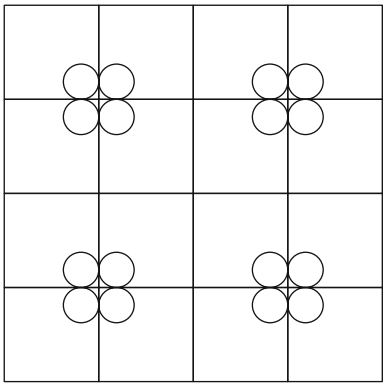

FIGURE 2. Support of V_{ω^*} for $d = 2$.

One may understand this result heuristically by the following strategy to construct test-functions which minimize the quadratic form of H_ω, at least if the single-site potential q is negative: The clusters in V_{ω^*} form wide wells. In these wells one can place localized test functions with relatively small derivative, due to the width of the wells, i.e., small cost in kinetic energy. This gives lower total

energy than the narrower wells given by individual, spatially separated single-site potentials. This is not how Theorem 2.1 is proven. We should also point out that Theorem 2.1 does not impose any sign-restrictions on q, and thus can not be fully explained by the above heuristics. But the heuristics make clear that the spectral minimum of the RDM is determined by a non-trivial interplay between kinetic and potential energy.

Instead we will give a proof of Theorem 2.1 at the end of the next section, based on the answer to a minimization problem for a single-site Neumann operator associated with the RDM.

3. The Neumann problem

Theorem 2.1 provides the answer to an optimization problem involving infinitely many displacement parameters ω_n, $n \in \mathbb{Z}^d$. However, due to the symmetry assumptions on q, it turns out that the proof can be reduced to a related problem involving the optimal placement of just one single-site term.

For this purpose, let $\Lambda_1 := (-\frac{1}{2}, \frac{1}{2})^d$ be the unit cube centered at the origin and $-\Delta^N$ the Neumann-Laplacian on $L^2(\Lambda_1)$, i.e., the unique self-adjoint operator whose quadratic form is $\int_{\Lambda_1} |\nabla f(x)|^2 \, dx$ for $f \in H^1(\Lambda_1)$, the first-order Sobolev space.

For q as in **(A1)** and $a \in \overline{G}$ let

$$H^N_{\Lambda_1}(a) := -\Delta^N + q(x-a)$$

and $E_0(a) := \min \sigma(H^N_{\Lambda_1}(a))$ the non-degenerate lowest eigenvalue of $H^N_{\Lambda_1}(a)$. For a general discussion of properties of operators of this type see Section 2 of [4].

We ask for the optimal placement of $a \in \overline{G}$ to minimize $E_0(a)$ and arrive at the following result.

Theorem 3.1. *Under assumption* **(A1)** *one of the following two alternatives holds:*

(i) $E_0(a)$ *is strictly maximized at* $a = 0$ *and strictly minimized at the corners* $\mathcal{C}$ *of* $\overline{G}$.
(ii) $E_0(a)$ *is identically zero.*

A proof of Theorem 3.1 under the given assumptions can be found in [4]. We will not discuss details of this proof here, as we will later need a strengthened version of Theorem 3.1 for which we will also use somewhat stronger assumptions, see Theorem 6.1 and assumption **(A1)′** in Section 6 below.

The proof of Theorem 3.1 in [4] shows that in each of the two alternatives more can be said:

In case of alternative (i), the function $E_0(a_1, \ldots, a_j, \ldots, a_d)$ is symmetric and strictly unimodal in each variable. Thus, with all other variables fixed, for each j it is a strictly increasing function of a_j in $[-d_{\max}, 0]$ and strictly decreasing in $[0, d_{\max}]$.

On the other hand, if alternative (ii) holds, then the strictly positive ground state eigenfunction $u_0(x,a)$ corresponding to $E_0(a)$ is constant near the boundary of Λ_1 (and thus, by analyticity, constant in the entire connected component of $\Lambda_1 \setminus \operatorname{supp} q(\cdot - a)$ containing the boundary of Λ_1). This reveals a mechanism which can be used to construct non-trivial examples (with non-vanishing q) where alternative (ii) happens:

Let $\phi(x)$ be a positive sufficiently regular function which is constant near the boundary of Λ_1 and then define the potential by setting

$$q(x-a) = \frac{\Delta\phi(x-a)}{\phi(x-a)} \tag{9}$$

as long as $\operatorname{supp} q(\cdot - a) \subset \Lambda_1$. Then $E_0(a)$ vanishes identically for $a \in G$ and $\phi(x-a)$ is the corresponding eigenfunction. As follows from the proof of Theorem 3.1, this is the only mechanism which leads to alternative (ii).

Alternative (i) certainly happens for all non-vanishing sign-definite potentials q, as it follows by perturbation theory that in this case the zero ground state energy 0 of the Neumann Laplacian is pushed either up or down. But alternative (i) is generic also for sign-indefinite potentials, as alternative (ii) will be broken by typical small perturbations of the potential.

Among previously known results, the ones most closely related to Theorem 2.1 can be found in [23] which considers similar questions for the case of the Dirichlet Laplacian $-\Delta^D$ instead of $-\Delta^N$. Also using symmetry assumptions on q, it is found there that the optimal placement of the potential in $-\Delta^D + q(x-a)$ depends strongly on the sign of q. For cubic domains, a special case of the domains considered in [23], it is found that for positive potential the lowest eigenvalue is minimized if the potential is placed in a corner of the cube, while negative potentials should be placed into the center of the cube. This distinction does not happen in the Neumann case, where it is generally true that "bubbles tend to the corners".

While not used in our proof of Theorem 3.1 or in the proofs in [23], one can understand this distinction by perturbative arguments. For this, consider $-\Delta + \lambda q(x-a)$ on $L^2(\Lambda_1)$ for small coupling, with either Dirichlet or Neumann boundary condition. If $E_0^D(a,\lambda)$ denotes the smallest eigenvalue in the Dirichlet case, then by first-order perturbation theory,

$$\partial_\lambda E_0^D(a,0) = \int q(x-a)|\varphi(x)|^2\,dx, \tag{10}$$

where $\varphi(x)$ is the normalized ground state of the Dirichlet Laplacian on Λ_1, i.e., $\varphi(x) = C\prod_{j=1}^d \cos(\pi x_j)$. In the small coupling regime minimizing (10) over a indicates the optimal placement of the potential. If q is positive, then the bubble should be placed into a corner of Λ_1, where $|\varphi|^2$ has the smallest mass. On the other hand, for negative q the bubble should be placed into the center where the mass of $|\varphi|^2$ is largest.

For the Neumann case the heuristics given by first-order perturbation theory is inconclusive. The ground state of the Neumann Laplacian is constant, and thus $\partial_\lambda E_0^N(a,0)$ is independent of a.

However, one gets correct heuristics by going to second-order perturbation theory. We have (for a derivation see Section 2.3 of [4])

$$\partial_\lambda^2 E_0^N(a,0) = -2\sum_{k>0} \frac{(u_0, q(\cdot - a)u_k)^2}{E_k - E_0}. \tag{11}$$

Here $0 = E_0 < E_1 \leq E_2 \leq \cdots$ are the eigenvalues of the Neumann Laplacian and u_k the corresponding eigenfunctions. In $d = 2$ (for simplicity) we have that the first excited state is twice degenerate, $E_1 = E_2 = \pi^2$. Considering only these two terms in (11) (the third term would still give the same result) we get that $\partial_\lambda^2 E_0^N(a,0)$ is approximately given by

$$-\frac{4}{\pi^2}\left[\left(\int q(x-a_1,y-a_2)\sin(\pi x)\,dx\,dy\right)^2 + \left(\int q(x-a_1,y-a_2)\sin(\pi y)\,dx\,dy\right)^2\right],$$

which is non-positive. If q is reflection symmetric, then both integrals are zero for $a = 0$, indicating the position with highest ground state energy in the small coupling regime. If we also assume that q is of fixed sign, then both integrals become maximal in absolute value if a is located near one of the corners of the cube. These are the positions where the ground state energy of $-\Delta^N + \lambda q(x-a)$, $\lambda \approx 0$, is minimal. As opposed to the Dirichlet case, the answer suggested by second-order perturbation theory is the same for positive and negative q.

Let us finally start to get beyond heuristics and show rigorously that Theorem 3.1 implies Theorem 2.1:

Proof of Theorem 2.1, [4]. For any given configuration ω, the restriction of H_ω to the unit cube centered at $n \in \mathbb{Z}^d$ with Neumann boundary conditions is unitarily equivalent (via translation by n) to $H_{\Lambda_1}^N(\omega_n)$, defined as in Theorem 3.1. Thus, by Neumann bracketing and Theorem 3.1,

$$\begin{aligned}\min\sigma(H_\omega) &\geq \min\sigma\left(\bigoplus_{n\in\mathbb{Z}^d} H_{\Lambda_1}^N(\omega_n)\right)\\ &\geq \inf\left\{E_0(a) : a \in [-d_{\max}, d_{\max}]^d\right\}\\ &= E_0(a^*),\end{aligned}$$

where $a^* = (d_{\max}, \ldots, d_{\max})$ is one of the corners $\mathcal{C}$ of $\overline{G}$. This holds for arbitrary configurations ω and thus, by (4), $E_0 = \min\Sigma \geq E_0(a^*)$.

Now consider $\omega^* = (\omega_n^*)_{n\in\mathbb{Z}^d}$ as given by (8). The corresponding potential $V_{\omega^*}(x) = \sum_{n\in\mathbb{Z}^d} q(x - n - \omega_n^*)$ is 2-periodic in x_j for each j. By the Floquet-Bloch theory [37] the bottom of the spectrum of $H_{\omega^*} = -\Delta + V_{\omega^*}$ is given by the smallest eigenvalue E_0^{per} of its restriction to $\Lambda_0^2 := (-\frac{1}{2}, \frac{3}{2})^d$ with periodic boundary conditions, see Figure 3.

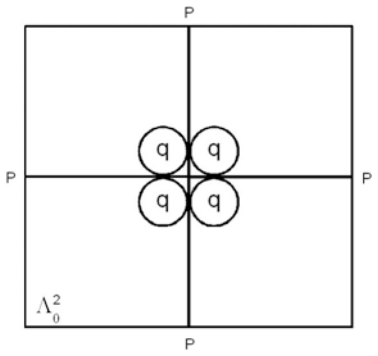

FIGURE 3. The period cell of V_{ω^*} in $d = 2$.

On Λ_0^2 the potential V_{ω^*} is symmetric with respect to all hyperplanes $x_i = 1/2, i = 1, \ldots, d$. Thus E_0^{per} coincides with the smallest eigenvalue of the Neumann problem on Λ_0^2. Again by symmetry of the potential, the latter coincides with the smallest eigenvalue of the Neumann problem on Λ_1. As $\omega_0^* = a^*$, this eigenvalue is $E_0(a^*)$. Together with (7) we have shown that

$$E_0 \leq \min \sigma(H_{\omega^*}) = E_0(a^*).$$

Combined with the previous observation that $E_0(a^*) \leq E_0$ this shows $E_0 = \min \sigma(H_{\omega^*})$. □

4. Uniqueness of the periodic minimizer

After resolving the preliminary problem of characterizing the spectral minimum of the RDM, we could now turn to the other essential ingredients into a localization proof, a Lifshitz tail bound on the IDS and a Wegner estimate. However, a first look at this quickly demonstrates that we also need to address the question of uniqueness in Theorem 2.1. Other than translates of ω^*, are there more periodic configurations which have the same spectral minimum?

To motivate this, let us include a first discussion of Lifshitz tails. For this one considers restrictions $H_{\omega,L}$ of H_ω to $L^2(\Lambda_L)$, where Λ_L is a cube of side-length L centered at the origin. As boundary condition one can generally choose what is most convenient in a given model, for us this will be Neumann conditions. By a Lifshitz tail bound we mean a result which says that the probability of $H_{\omega,L}$ to have an eigenvalue close to E_0, the minimum of the infinite volume spectrum, is exponentially small in L. The meaning of "close" will be made more precise later.

If ω coincides with ω^* on Λ_L or is very close to it, this will give a low lying eigenvalue of $H_{\omega,L}$. Our chances of getting a useful Lifshitz tail bound would worsen if there are many other periodic configurations with the same spectral minimum as ω^*, as this would increase the probability that random configurations

are close to one of the minimizing configurations on Λ_L and thus have low lying eigenvalues.

From this it is immediately clear that for all further considerations we will have to assume that alternative (i) of Theorem 3.1 holds, as under alternative (ii) it follows that $H_{\omega,L}$ has spectral minimum E_0 for *every* configuration ω. The following result is taken from [5].

Theorem 4.1. *Assume* **(A1)**, **(A2)**, *alternative* (i) *of Theorem* 3.1, $d \geq 2$ *and* $r < 1/4$. *Then* ω^* *as given by* (8) *is, up to translations, the unique periodic configuration with* $\min \sigma(H_{\omega^*}) = E_0$.

Two additional assumptions were made here which deserve comment: For the "radius" r of the single-site potential q we require $r < 1/4$ rather then just $r < 1/2$ assumed earlier. This is a technical assumption, which we need to apply an analyticity argument in the proof, see below. Our guess is that this assumption is not necessary for Theorem 4.1 to hold.

However, Theorem 4.1 indeed only holds in the multi-dimensional case $d \geq 2$ In the case $d = 1$ there are many periodic minimizers, as also proven in [5]:

Theorem 4.2. *Assume* **(A1)**, **(A2)**, *alternative* (i) *of Theorem* 3.1 *and* $d = 1$. *Then an* L*-periodic configuration* $\omega = (\omega_n)_{n\in\mathbb{Z}}$, $\omega_{n+L} = \omega_n$ *for all* $n \in \mathbb{Z}$, *satisfies* $\min \sigma(H_\omega) = E_0$ *if and only if*

(i) *all* ω_n *are maximally displaced, i.e.,* $\omega_n = \pm d_{\min}$ *for all* n,
(ii) L *is even, and*
(iii) *in each period* L *equally many* ω_n *are displaced to the left and to the right.*

It is easy to see that a periodic configuration ω with these properties is a minimizer. Let φ_0 be the positive ground state of $-d^2/dx^2 + q(x - d_{\max})$ on $(-1/2, 1/2)$ with Neumann boundary conditions. It can be shown that alternative (i) implies that

$$h := \varphi_0(-1/2) \neq \varphi_0(1/2) =: k.$$

For a configuration satisfying (i), (ii) and (iii) of Theorem 4.2 the Neumann ground state over the period L is found by pasting together scaled copies of φ_0, compare Figure 4 for an example with $L = 4$. The number of steps up is equal to the number of steps down, which allows for periodic extension, showing that $\min \sigma(H_\omega) = E_0$.

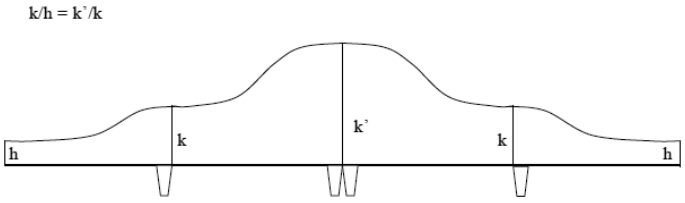

FIGURE 4. A 4-periodic minimizer in $d = 1$.

Lemma 4.4 below, which holds in arbitrary dimension, establishes the necessity of (i). The above construction of the Neumann ground state for the period L now shows that (ii) and (iii) must hold for the Neumann ground state to coincide with the periodic ground state. For a more detailed proof of Theorem 4.2 see [5].

Theorem 4.2 has surprising implications for the integrated density of states $N(E)$ of the one-dimensional RDM. The most extreme situation occurs if μ is the Bernoulli measure with equal weights at the endpoints of $[-d_{\max}, d_{\max}]$, i.e.,

$$\mu = \frac{1}{2}\delta_{d_{\max}} + \frac{1}{2}\delta_{-d_{\max}}. \tag{12}$$

Theorem 4.3. *Let H_ω be the one-dimensional RDM with distribution μ given by* (12)*. Then there exists $C > 0$ such that*

$$N(E) \geq \frac{C}{(\log(E - E_0))^2} \tag{13}$$

for E sufficiently close to E_0.

While similar phenomena have been found for Schrödinger operators with almost-periodic potentials, this is the first known example of a random Schrödinger operator with non-Hölder-continuous IDS. The density $n(E) = N'(E)$ of eigenvalues near the bottom of the spectrum is even higher than for the one-dimensional Laplacian where the IDS has a square-root type singularity $N(E) = CE^{1/2}$ at $E_0 = 0$. Thus the randomness has the effect of pulling more eigenvalues towards the bottom of the spectrum, rather than pushing them away from the bottom as in the more common fluctuation boundary regime described by Lifshitz tails. The reason behind (13) is Theorem 4.2 combined with the law of large numbers. For the symmetric Bernoulli distribution (12) it has very high probability that in a large even period L almost equally many ω_n take values $d_{\max}$ and $-d_{\max}$, leading to a ground state energy very close to E_0. For a detailed proof of Theorem 4.3 see [5].

We now turn back to the original goal of this section, the proof of Theorem 4.1 on the uniqueness of the periodic minimizer in $d \geq 2$. For this we consider a configuration $\omega \in \mathcal{C}_{\text{per}}$ (as defined in (6)) and let Λ be the corresponding rectangular period cell. We let $H^P_{\omega,\Lambda}$ and $H^N_{\omega,\Lambda}$ be the restriction of H_ω to $L^2(\Lambda)$ with periodic and Neumann boundary conditions, respectively, and $E_0(H^P_{\omega,\Lambda})$ and $E_0(H^N_{\omega,\Lambda})$ their lowest eigenvalues. In follows from general facts that

$$\min \sigma(H_\omega) = E_0(H^P_{\omega,\Lambda}) \geq E_0(H^N_{\omega,\Lambda}). \tag{14}$$

We assume that $\min \sigma(H_\omega) = E_0$ and have to show that, up to a translation, ω coincides with ω^*. This is done in two steps.

The first step establishes that all ω_n sit in corners and that the ground state of $H^N_{\omega,\Lambda}$ satisfies Neumann conditions not only on Λ, but on every unit cell contained in Λ:

Lemma 4.4. *Let ω be a periodic configuration with $\min \sigma(H_\omega) = E_0$. Then $\omega_n \in \mathcal{C}$ for all $n \in \mathbb{Z}^d$. Moreover, in this case $E_0(H^P_{\omega,\Lambda}) = E_0(H^N_{\omega,\Lambda})$ and the ground state*

eigenfunction ψ_ω of $H^N_{\omega,\Lambda}$ satisfies Neumann boundary conditions on the boundary of each unit cube Λ_n centered at $n \in \Lambda \cap \mathbb{Z}^d$.

The core of the proof of Lemma 4.4 is the following calculation, based on Neumann bracketing and the characterization of ground state energies as minimizers of the quadratic form:

$$\begin{aligned} E_0(H^N_{\omega,\Lambda}) &= \frac{\int_\Lambda |\nabla\psi_\omega|^2 + \int_\Lambda \sum_{n\in\Lambda\cap\mathbb{Z}^d} q(x-n-\omega_n)|\psi_\omega|^2}{\int_\Lambda |\psi_\omega|^2} \\ &= \sum_{n\in\Lambda\cap\mathbb{Z}^d} \frac{\int_{\Lambda_n} |\nabla\psi_\omega|^2 + \int_{\Lambda_n} q(x-n-\omega_n)|\psi_\omega|^2}{\int_{\Lambda_n} |\psi_\omega|^2} \cdot \frac{\int_{\Lambda_n} |\psi_\omega|^2}{\int_\Lambda |\psi_\omega|^2} \\ &\geq \sum_{n\in\Lambda\cap\mathbb{Z}^d} E_0(\omega_n) \frac{\int_{\Lambda_n} |\psi_\omega|^2}{\int_\Lambda |\psi_\omega|^2} \geq \sum_{n\in\Lambda\cap\mathbb{Z}^d} E_0 \frac{\int_{\Lambda_n} |\psi_\omega|^2}{\int_\Lambda |\psi_\omega|^2} = E_0, \end{aligned} \tag{15}$$

By (14) and the assumption we conclude that $E_0(H^P_{\omega,\Lambda}) = E_0(H^N_{\omega,\Lambda})$ and that all inequalities in (15) are equalities. We also see that $\omega_n \in \mathcal{C}$ for all $n \in \mathbb{Z}^d$, because otherwise, given alternative (i), the last inequality in (15) would be strict. Finally we see from equality in the second to last inequality in (15) that $\psi_\omega|_{\Lambda_n}$ is the ground state for the Neumann problem on Λ_n, and thus satisfies Neumann conditions on Λ_n.

The second step of the proof of Theorem 4.1 is to show symmetric matching of the bubbles, i.e., that in each pair of neighboring unit cells within Λ the single-site potentials are placed symmetrically with respect to the common boundary of the cells. For this we use the following general fact from [5], to where we refer for the proof:

Lemma 4.5. *Consider a connected open region D in $\mathbb{R}^d$, $d \geq 2$ and a hyperplane P that divides this region into two nonempty subregions. Denote by σ the reflection about P and assume that $D \cap \sigma(D)$ is connected. Let $E \in \mathbb{R}$ and, in D, let u be a solution of the equation*

$$-\Delta u = Eu \tag{16}$$

which satisfies the condition $\frac{\partial u}{\partial n} = 0$ on $P \cap D$. Then u can be extended to a symmetric function w on $D \cup \sigma(D)$ which satisfies the equation $-\Delta u = Eu$ in this region.

To finish the proof of Theorem 4.1 let us assume that ω is a periodic minimizing configuration in which, by Lemma 4.4, all bubbles sit in corners, but that there is at least one non-matching neighboring pair of bubbles. Let us focus on $d = 2$ and the situation in Figure 5 (the general argument in [5] uses the same idea). Circumscribe squares around the supports of the two bubbles and remove these two squares from the union R of the two cells. Choose the resulting region as D in Lemma 4.5, and σ as reflection at the center line. Here (and only here) we need the strengthened assumption $r < 1/4$ in Theorem 4.1 to make sure that $D \cap \sigma(D)$ is connected.

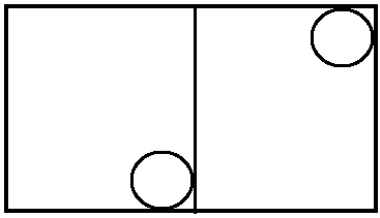

FIGURE 5. A non-matching pair.

Let u be the restriction of the ground state of $H^N_{\omega,\Lambda}$ to D. Then $-\Delta u = E_0 u$ on D and, by Lemma 4.4, u satisfies Neumann conditions on the centerline $P \cap D$. By Lemma 4.5 u can be extended to a symmetric function w on $D \cup \sigma(D)$ satisfying $-\Delta w = E_0 w$. But $D \cup \sigma(D) = R$ and thus w is the ground state of the Neumann Laplacian on R, implying $E_0 = 0$ and that w is constant, a contradiction to alternative (i). This completes the proof of Theorem 4.1.

To end this section let us remark that the fundamental difference in the one-dimensional and multi-dimensional case lies in the possibility to smoothly match Neumann ground states on different unit cells. In $d = 1$ this can always be done by re-scaling as explained by Figure 5. In higher dimension the boundary of cells has much more structure (is not just a point), which ultimately results in matching of ground states only being possible in the trivial reflection-symmetric case.

5. Special Lifshitz tails

After clarifying uniqueness questions in the previous section we finally have enough background information to enter into a discussion of Lifshitz tail properties of the IDS for the random displacement model. In order to use our earlier results we will have to assume from here on that alternative (i) of Theorem 3.1 holds and that $d \geq 2$. We strengthen **(A2)** to require $r < 1/4$ and will in this section also assume that q is continuous to make use of results in [35].

Let $H^N_{\omega,L}$ be the restriction of H_ω to $\Lambda_L = (-L-1/2, L+1/2)^d$ with Neumann boundary conditions. The crucial fact required in localization proofs and also in the proof of Lifshitz tail asymptotics of the IDS is that the probability of $H^N_{\omega,L}$ having an eigenvalue close to E_0 is very small. The first proof of this was given in [35], where it follows as a special case of a more general result. The methods derived in [35] require to assume in **(A2)** that $\operatorname{supp}\mu$ is *finite*. The methods developed later in [30], which are described in Section 7 below, have allowed to remove this additional assumption on μ. However, Theorem 5.1 is crucial as it will serve as the anchor for a bootstrap argument in Section 7. For this it will be sufficient to start with the case $\operatorname{supp}\mu = \mathcal{C}$, i.e., a displacement model where all bubbles sit in corners.

Theorem 5.1. *Let the assumptions listed at the beginning of this section be satisfied and also assume that* $\operatorname{supp}\mu = \mathcal{C}$. *Then there exist* $C > 0$ *and* $\mu > 1$ *such that for all* $L \in \mathbb{N}$,

$$\mathbb{P}\left(\min\sigma(H^N_{\omega,L}) < E_0 + \frac{C}{L^2}\right) < (2L+1)^{d-1}\mu^{-2L}. \tag{17}$$

In the remainder of this section we will discuss the argument from [35] which proves Theorem 5.1, taking some advantage in presentation from only looking at the specific situation which is of interest to us here. However, we will refer to [35] for many of the core analytical parts of the proof.

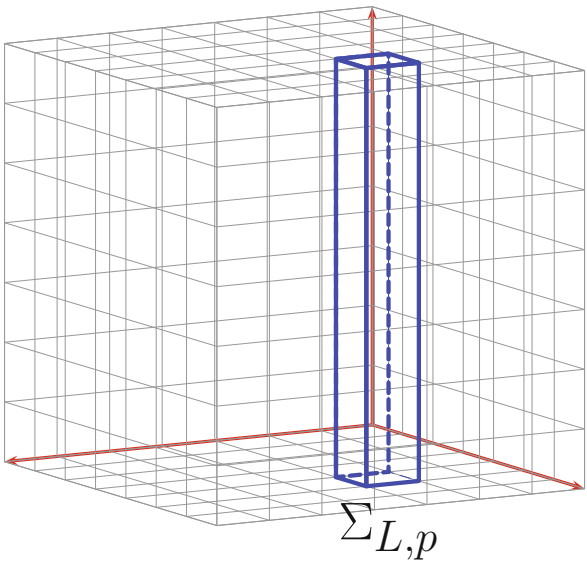

FIGURE 6. A quasi-one-dimensional tube

The argument starts with decomposing the cubes Λ_L into quasi-one-dimensional tubes (see Figure 6) and restricting $H^N_{\omega,L}$ to these tubes under insertion of additional Neumann boundary conditions. Thus let

$$A_L := \{p \in \mathbb{Z}^{d-1} : -L \le p_j \le L \text{ for } j = 1, \dots, d-1\}$$

and, for each $p \in A_L$,

$$\Sigma_{L,p} := \bigcup_{k=-L}^{L} \Lambda_1((p,k)),$$

with $\Lambda_1((p,k))$ denoting unit cubes centered at $(p,k) \in \mathbb{Z}^d$. By $H^N_{\omega,L,p}$ we denote the restriction of H_ω to $L^2(\Sigma_{L,p})$ with Neumann boundary conditions. By

Neumann bracketing we have

$$H^N_{\omega,L} \geq \bigoplus_{p\in A_L} H^N_{\omega,L,p}$$

and therefore

$$\min\sigma(H^N_{\omega,L}) \geq \min_{p\in A_L} \min\sigma(H^N_{\omega,L,p}). \tag{18}$$

For a given ω such that $\omega_n \in \mathcal{C}$ for all n we will say that two neighboring unit cubes are *matching* if the single site potentials in the two cubes are mirror images under reflection at the common boundary of the cubes. For each $p \in A_L$ consider the event

$$X_{L,p} := \{\omega : \Sigma_{L,p} \text{ contains at least one neighboring pair of non-matching cubes}\}$$

and let $X_L := \cap_{p\in A_L} X_{L,p}$.

By independence we have

$$\mathbb{P}(\omega \notin X_{L,p}) \leq \mu^{-2L},$$

where $\mu := 1/\max_{a\in\mathcal{C}} \mu(a)$ (after $\omega_{p,-L}$ is chosen, the other $2L$ values of $\omega_{p,k}$ are determined by matching). This implies that

$$\mathbb{P}(X_L) \geq 1 - (2L+1)^{d-1}\mu^{-2L}. \tag{19}$$

If $\omega \in X_L$, then each tube $\Sigma_{L,p}$ contains at least one non-matching pair of neighboring cubes. Thus by Proposition 5.2 below $\min\sigma(H^N_{\omega,L,p}) \geq E_0 + C/L^2$ for a $C > 0$ independent of p and L. Thus Theorem 5.1 follows from (18) and (19).

In the proposition which was used here we can without loss consider $p = 0$:

Proposition 5.2. *There is a constant $C > 0$, independent of L, such that for every ω with $\omega_n \in \mathcal{C}$ for all n and at least one non-matching pair of cubes in $\Sigma_{L,0}$ it holds that*

$$\min\sigma(H_{\omega,L,0}) \geq E_0 + \frac{C}{L^2}. \tag{20}$$

This, at least essentially, is a result proven in [35]. We will not reproduce the details of the proof, which involve a surprisingly rich combination of analysis tools such as a Poincaré-type inequality, the so-called ground state transform and properties of a Dirichlet-to-Neumann operator, as well as some combinatorics. But we will outline the main idea:

The proof of Proposition 5.2 starts by first arguing that is suffices to assume that

1. the first two cubes $\Lambda_1((0,-L))$ and $\Lambda_1((0,-L+1))$ are non-matched, while
2. all other neighboring pairs are matched.

Seeing this is not entirely trivial and requires a trick as well as some combinatorics. The trick consists in extending the operator $H^N_{\omega,L,0}$ by reflection to a twice longer tube and to consider the resulting operator as an operator on the torus $[-1/2,1/2]^{d-1} \times (\mathbb{R}/2(2L+1)\mathbb{Z})$ with periodic boundary conditions. Due to symmetry this operator has the same spectral minimum as $H^N_{\omega,L,0}$. Now one argues

that the torus can be decomposed into subsegments each of which has a non-matching pair of cubes at one end and otherwise only matching pairs of cubes. Introducing additional Neumann conditions on the subsegments lowers the spectrum and it now suffices to prove the claim for each subsegment (which has length bounded by $2(2L+1)$). Justifying that this decomposition is possible "is an easy combinatorics, though somewhat lengthy to write down using symbols", where we use the words of [35] and omit the details.

Under the additional assumptions (1), (2), Proposition 5.2 is essentially a special case of Theorem 2.1 in [35]. While our situation does not satisfy the exact symmetry assumptions of Theorem 2.1 in [35], the construction of our potential via matching cubes allows to mimic the proof in [35] almost line by line. (We mention, however, that Section 4 of [35] provides a slightly different argument which allows to directly use their Theorem 2.1 to prove Theorem 5.1 above.)

Here the results of Section 4 enter as follows: As the first pair of cubes $\Lambda_1((0,-L))$ and $\Lambda_1((0,-L+1))$ does not match, the lowest eigenvalue of the Neumann problem on the union Λ_2 of these two cubes is strictly larger than E_0. This follows from the arguments in the proof of Theorem 4.1, more specifically the argument at the end of Section 4 which ruled out that in this situation the lowest eigenvalue can be equal to E_0. It is this operator which plays the role of the operator P_0^N in [35]. By the results of Section 4 it is clear that inserting an additional Neumann condition along the surface separating Λ_2 and $\Sigma_{L,0} \setminus \Lambda_2$ strictly lowers the ground state energy of $H^N_{\omega,L,0}$ to E_0. The meaning of Theorem 2.1 of [35] is that it provides the quantitative lower bound CL^{-2} on how much the energy is lowered depending on the length of the attached tube.

The value of the constant $C > 0$ in (20) which is provided by the argument in [35] will depend on the choice of $\omega_{0,-L}$ and $\omega_{0,-L+1}$, after which the remaining values of ω_n are determined by matching. However, as only the finitely many values in the corners $\mathcal{C}$ are allowed, one can ultimately choose the smallest of finitely many values of C.

As indicated earlier, Theorem 5.1 is the result which will be used later, rather than its consequences for the IDS $N(E)$ of H_ω. However, we mention that the following Lifshitz tail bound can be derived from Theorem 5.1 with standard arguments, see [35]:

$$\limsup_{E \downarrow E_0} \frac{\log |\log N(E)|}{\log(E - E_0)} \leq -\frac{1}{2}. \tag{21}$$

The Lifshitz exponent $-1/2$ obtained here is likely not optimal. One would expect that the correct exponent is $-d/2$, as known for the Anderson model or Poisson model. The reason for the discrepancy lies in the essentially one-dimensional argument which enters the proof through the decomposition of cubes into quasi-one-dimensional tubes.

We stress the fundamentally different low energy behavior of the IDS of the RDM in the one-dimensional and multi-dimensional settings. If $\operatorname{supp} \mu = \mathcal{C}$ with

equal probability for all corners, then (21) shows that the IDS has a very thin tail for $d \geq 2$, while by Theorem 4.3 it has a very fat tail (and thus the spectrum does *not* have a fluctuation boundary) for $d = 1$. From this point of view it is a fortunate coincidence that our main goal here is to prove localization in $d \geq 2$ and that, as discussed in the Introduction, localization for the one-dimensional case was already settled by very different methods.

6. The missing link

It is tempting to believe at this point of our work that we are halfway done with verifying the necessary ingredients for a multiscale analysis proof of localization for the RDM. Under suitable assumptions we have shown the Lifshitz-tail bound (17), so it remains to establish a Wegner estimate. Unfortunately, the assumption that $\operatorname{supp}\mu$ be finite in Theorem 5.1 makes us face a dilemma: Most known proofs of Wegner-type estimates, with the exception of some results in $d = 1$ [9, 13], require some smoothness or at least continuity of the distribution of the random parameters, due to the use of averaging techniques involving only finitely many random parameters. For the multi-dimensional continuum Anderson model with Bernoulli distributed random coupling constants a localization proof near the bottom of the spectrum was enabled only recently by the powerful extension of multiscale analysis presented in [6], see also [2] for an extension to the case of arbitrary single site distributions and [21] for a detailed elaboration of the intricate ideas behind [6]. One of the main features of this approach is that the Wegner estimate is not established as an a-priori-ingredient, but its proof is part of the multiscale iteration procedure leading to localization. We mention that due to the use of unique continuation arguments this approach does not work on the lattice, leaving the proof of localization for the multi-dimensional discrete Bernoulli-Anderson model an open problem.

Thus, if we want to complete a localization proof for the RDM based on "traditional" multiscale analysis, the proof of a Wegner estimate will likely require a sufficient amount of regularity of the distribution μ of the displacement parameters ω_n. But this means that we also need to extend the Lifshitz-tail bound to more general distributions μ. The proof discussed in Section 5 above does not extend to this case, as it would require to take an infimum over infinitely many positive constants C with insufficient quantitative information available to guarantee that the resulting constant is strictly positive.

It turned out that the missing link which allowed to overcome both remaining problems, the extension of the Lifshitz-tail bound to a larger class of distributions and the proof of a Wegner estimate for this class, is provided by an inconspicuous but crucial improvement on how bubbles tend to the corners, meaning Theorem 3.1. There it was shown that the function $E_0(a)$, as long as it does not vanish identically, is strictly decreasing in each of its variables away from the origin.

The crucial improvement is that this decrease arises in the form of *non-vanishing derivative*.

This is the first instance where we will have to require some smoothness of q, as differentiability of $E_0(\cdot)$ requires differentiability of q via perturbation theory, see Section 2.1 of [30]. For convenience, we will assume that q is C^∞, even if much less is needed below and in the rest of this paper.

As this is the last time we add assumptions on q, let us restate the full set:

(A1)′ The single-site potential $q : \mathbb{R}^d \to \mathbb{R}$ is infinitely differentiable, reflection-symmetric in each variable and such $\operatorname{supp} q \subset [-r, r]^d$ for some $r < 1/4$. Also assume that $E_0(a) = \min \sigma(H^N_{\Lambda_1}(a))$ does not vanish identically in $a \in \overline{G}$.

We now get

Theorem 6.1. *Assume* **(A1)′**. *Then for all* $a = (a_1, \dots, a_d) \in \overline{G}$ *and all* $i = 1, \dots, d$ *we have*

$$\partial_i E_0(a) \begin{cases} < 0, & \text{if } a_i > 0, \\ = 0, & \text{if } a_i = 0, \\ > 0, & \text{if } a_i < 0. \end{cases}$$

The proof of Theorem 6.1 is far from obvious (at least to us) and is best discussed in the larger context of considering similar questions for more general domains G. In order to not interrupt the presentation of our main story, i.e., the proof of localization for the random displacement model, we postpone this discussion to Section 10 below. But let us point out that the step from Theorem 3.1 to Theorem 6.1 turned out to be far from straightforward. The "smooth methods" behind the proof of Theorem 6.1 are very different from the symmetry-based operator theoretic methods used to prove Theorem 3.1 in [4] and, in particular, explicitly use second-order perturbation theory.

7. General Lifshitz tails

The first of two important applications of Theorem 6.1 is that it allows us to extend the Lifshitz tail bound found in Theorem 5.1 to general distributions μ, not requiring finiteness of the support.

Theorem 7.1. *Assume that* q *and* μ *satisfy* **(A1)′** *and* **(A2)**. *Then there exist* $C_1 > 0$ *and* $\mu > 1$ *such that*

$$\mathbb{P}\left(\min \sigma(H^N_{\omega,L}) < E_0 + \frac{C_1}{L^2} \right) \leq (2L+1)^{d-1} \mu^{-2L} \tag{22}$$

for all $L \in \mathbb{N}$.

We will prove this result by comparing the quadratic form of $H^N_{\omega,L}$ with the quadratic form of a modified displacement model where all bubbles have been moved to the closest corner within their cell. Thus, for $a \in \overline{G}$, let $c(a) \in \mathcal{C}$ be the corner closest to a (if several corners are equally close, any of them can be

chosen). For a displacement configuration $\omega = (\omega_n)_{n\in\mathbb{Z}^d} \in \overline{G}^{\mathbb{Z}^d}$, define $c(\omega) \in \overline{G}^{\mathbb{Z}^d}$ by $(c(\omega))_n = c(\omega_n)$.

From Theorem 3.1 we know that the single-site operator $H^N_{\Lambda_1}(c(a))$ has lower ground state energy than $H^N_{\Lambda_1}(a)$. Theorem 6.1 allows us to quantify this, saying that the distance of the two ground state energies is proportional to $|a - c(a)|$. In particular, there exists $C_2 \in (0,\infty)$ such that

$$E_0(a) - E_0 \geq \frac{1}{C_2} D(a), \tag{23}$$

where $D(a) = \min_{c\in\mathcal{C}} |a-c|$. This is one of the two central ingredients in the proof of the following result. The other one will be Neumann bracketing.

Proposition 7.2. *There exists a constant $C_3 \in (0,\infty)$ such that, in the sense of quadratic forms,*

$$H^N_{\omega,L} - E_0 \geq \frac{1}{C_3}(H^N_{c(\omega),L} - E_0). \tag{24}$$

for all $\omega \in \overline{G}^{\mathbb{Z}^d}$ and all $L \geq 0$.

In particular, (24) implies

$$\min\sigma(H^N_{\omega,L}) - E_0 \geq \frac{1}{C_3}(\min\sigma(H^N_{c(\omega),L} - E_0). \tag{25}$$

The RDM $H_{c(\omega)}$ has i.i.d. distributed displacements supported on $\mathcal{C}$ and thus satisfies the assumptions of Theorem 5.1. Therefore, with C and μ from Theorem 5.1,

$$\begin{aligned}\mathbb{P}\left(\min\sigma(H^N_{\omega,L}) - E_0 < \frac{C}{C_3 L^2}\right) &\leq \mathbb{P}\left(\min\sigma(H^N_{c(\omega),L}) - E_0 < \frac{C}{L^2}\right)\\ &\leq (2L+1)^{d-1}\mu^{-2L},\end{aligned}$$

proving Theorem 7.1.

Thus it remains to prove Proposition 7.2. The strategy for this is to first prove a corresponding result for the single-site operators $H^N_{\Lambda_1}(a)$ and then extend this by Neumann bracketing to the operators $H^N_{\omega,L}$. For the single-site operators one separately considers the cases where a is close to a corner or not close to a corner.

Lemma 7.3. *There exist $C > 0$ and $\delta > 0$ such that, if $D(a) \leq \delta$, then*

$$H^N_{\Lambda_1}(a) - E_0 \geq \frac{1}{C}(H^N_{\Lambda_1}(c) - E_0 + |a-c|). \tag{26}$$

Lemma 7.4. *Fix $\delta \in (0,1)$. There exists $C_\delta \in (0,\infty)$ such that, for $D(a) \geq \delta$ and all $c \in \mathcal{C}$,*

$$H^N_{\Lambda_1}(a) - E_0 \geq \frac{1}{C_\delta}(H^N_{\Lambda_1}(c) - E_0 + |a-c|). \tag{27}$$

Before discussing the proofs of the two Lemmas, let us show how we use them to prove Proposition 7.2. Note that, applying Lemma 7.4 with δ as provided in Lemma 7.3, both Lemmas combined prove the $L = 0$ case. To extend this to general boxes we employ an argument previously used in the proof of Theorem 2.1 in [34]. It is crucial here that we work with Neumann boundary conditions.

For $\psi \in H^1(\Lambda_{2L+1})$, the form domain of $H^N_{\omega,L}$, one has that the restriction of ψ to $\Lambda_1(n)$ is in $H^1(\Lambda_1(n))$ for each $n \in \Lambda'_{2L+1} := \Lambda_{2L+1} \cap \mathbb{Z}^d$. Moreover,

$$\langle (H^N_{\omega,L} - E_0)\psi, \psi\rangle = \sum_{n\in\Lambda'_{2L+1}} \langle (H^N_{\Lambda_1(n)}(\omega_n) - E_0)\psi, \psi\rangle,$$

where we work with the usual slightly abusive notation for quadratic forms.

The same argument may be applied to $H_{c(\omega)}$,

$$\langle (H^N_{c(\omega),L} - E_0)\psi, \psi\rangle = \sum_{n\in\Lambda'_{2L+1}} \langle (H^N_{\Lambda_1(n)}(c(\omega_n)) - E_0)\psi, \psi\rangle.$$

Now Proposition 7.2 follows by applying Lemmas 7.3 and 7.4 for each n, summing, and omitting the positive term $\sum_n \langle |\omega_n - c(\omega_n)|\psi, \psi\rangle_{\Lambda_1(n)}$.

Before we can end this section, we still owe a discussion of the proofs of Lemmas 7.3 and 7.4. To see the latter, note that $D(a) \geq \delta$ implies $H^N_{\Lambda_1}(a) - E_0 \geq \delta/C_2$ by (23). Using the rough bound $|q(x-a) - q(x-c)| \leq 2\|q\|_\infty$ and setting $C := 1 + 2C_2\|q\|_\infty/\delta$ we get

$$(C+1)(H^N_{\Lambda_1}(a) - E_0) - (H^N_{\Lambda_1}(c) - E_0) \geq \frac{C\delta}{C_2} - 2\|q\|_\infty = \frac{\delta}{C_2},$$

and thus

$$H^N_{\Lambda_1}(a) - E_0 \geq \frac{1}{C+1}\left(H^N_{\Lambda_1}(a) - E_0 + \frac{\delta}{C_2}\right).$$

As $\delta = \frac{\delta}{|a-c|}|a-c| \geq \frac{\delta}{2d_{\max}\sqrt{d}}|a-c|$, (27) follows with $1/C_\delta$ chosen as the smaller of $1/(C+1)$ and $\delta/(2(C+1)C_2 d_{\max}\sqrt{d})$.

The previous argument doesn't use the full strength of (23), but only that $E_0(\cdot)$ is continuous and strictly minimized in the corners. The proof of Lemma 7.3 is more subtle and depends on the linear growth of $E_0(\cdot)$ away from the corners. To $a \in \overline{G}$ pick $c \in \mathcal{C}$ such that $D(a) = |a-c|$. By smoothness of q we have the Taylor approximation $q(\cdot - a) - q(\cdot - c) = (c-a)\cdot\nabla q(\cdot - c) + o(|a-c|)$ and thus

$$H^N_{\Lambda_1}(c) - E_0 = H^N_{\Lambda_1}(c) - E_0 + (c-a)\cdot\nabla q(\cdot - c) + o(|a-c|). \tag{28}$$

Bounding the left-hand side by (23) we get, in the sense of quadratic forms,

$$H^N_{\Lambda_1}(c) - E_0 + (c-a)\cdot\nabla q(\cdot - c) \geq \frac{1}{C_2}|a-c| + o(|a-c|).$$

Hence, for $\rho \in (0,1)$ sufficiently small and $\sigma \in \mathcal{S}^{d-1}$ with $a = c + \rho\sigma \in \overline{G}$,

$$H^N_{\Lambda_1}(c) - E_0 - \rho\sigma\cdot\nabla q(\cdot - c) \geq \frac{\rho}{2C_2}.$$

We apply Lemma 7.5 below with $A = H^N_{\Lambda_1}(c) - E_0$ and $B = -\rho\sigma \cdot \nabla q(\cdot - c)$ to conclude that for $C_\rho = \max(2, 2C_2/\rho)$ $t \in [0, 1/2]$ and $\sigma \in \mathcal{S}^{d-1}$ with $c + \rho\sigma \in \overline{G}$,

$$H^N_{\Lambda_1}(c) - E_0 - t\rho\sigma \cdot \nabla q(\cdot - c) \geq \frac{1}{C_\rho}(H^N_{\Lambda_1}(c) - E_0 + t).$$

From this and (28) we find for $|a - c| \leq \rho/2$ and $t = |a - c|/\rho$,

$$H^N_{\Lambda_1}(a) - E_0 \geq \frac{1}{C_\rho}(H^N_{\Lambda_1}(c) - E_0 + |a - c|/\rho) + o(|a - c|).$$

This implies (26) if $\delta > 0$ is chosen sufficiently small, completing the proof of Lemma 7.3.

We have used the following simple fact, which was previously used in a similar context in [34].

Lemma 7.5. *Let A be self-adjoint and B bounded and self-adjoint with $A \geq 0$ and $A + B \geq c_0 > 0$, then*

$$A + tB \geq \min\left(\frac{1}{2}, c_0\right) \cdot (A + t)$$

for all $t \in [0, 1/2]$.

This is elementary:

$$A + tB = (1 - t)A + t(A + B) \geq \frac{1}{2}A + tc_0 \geq \min\left(\frac{1}{2}, c_0\right)(A + t).$$

8. Wegner estimate

To describe the ideas behind the proof of a Wegner estimate, we consider H^r_ω, a suitable random Schrödinger operator on $L^2(\mathbb{R}^d)$. Let $L > 0$ and $H^r_{\omega,L}$ be the restriction of H^r_ω to the cube Λ_L with, say, Dirichlet boundary conditions. The boundary conditions are expected not to play a too important role.

A *Wegner estimate* (see [41]) is an estimate on

$$\mathbb{E}(\mathrm{tr}\ \chi_{[E_0-\varepsilon, E_0+\varepsilon]}(H^r_{\omega,L})) = \mathbb{E}(\#\{\text{eigenvalues of } H^r_{\omega,L} \text{ in } [E_0 - \varepsilon, E_0 + \varepsilon]\}) \quad (29)$$

for L large, ε small and a fixed energy E_0. It can also take the form of an estimate on the probability $\mathbb{P}\{H^r_{\omega,L}$ has an eigenvalue in $[E_0 - \varepsilon, E_0 + \varepsilon]\}$ which, by Chebyshev's inequality, is smaller than the previous quantity.

From their very form, it is clear that both quantities should increase with ε and with L. The existence of an integrated density of states for H^r_ω suggests that the optimal upper bound should be proportional to $|\Lambda_L| \sim L^d$. The optimal upper bound in ε is related to the regularity of the integrated density of states. The best bound one may expect is of the form $C\varepsilon L^d$.

Let us give the heuristic underlying such a bound in the simplest case, the case when H^r_ω is the continuous Anderson type model $H^A_{\lambda(\omega)}$ defined in (2), when

q has a fixed sign, say, positive, is continuous and bounded, its support contains Λ_1 and the coupling constants $(\lambda_n)_{n\in\mathbb{Z}^d}$ are i.i.d. and bounded.

Let $(E_j(\omega, L))_j$ denote the eigenvalues of $H^A_{\lambda(\omega),L}$ ordered increasingly. To estimate the quantity $\mathbb{E}(\text{tr } \chi_{[E_0-\varepsilon,E_0+\varepsilon]}(H^A_{\lambda(\omega),L}))$, we can write

$$\begin{aligned}\mathbb{E}(\text{tr } \chi_{[E_0-\varepsilon,E_0+\varepsilon]}(H^A_{\omega,L})) &= \mathbb{E}\left(\sum_j \chi_{[E_0-\varepsilon,E_0+\varepsilon]}(E_j(\omega,L))\right)\\ &\leq \sum_{j\in N_L} \mathbb{P}\left\{E_j(\omega,L)\in[E_0-\varepsilon,E_0+\varepsilon]\right\}.\end{aligned}$$

where, by standard bounds on Schrödinger operators, $\#N_L \lesssim L^d$.

In the case of the continuous Anderson model under the assumptions made above, for $\alpha > 0$, the operator inequality $H^A_{\lambda(\omega)+\overline{\alpha}} - H^A_{\lambda(\omega)} \gtrsim \alpha$ tells us that

$$\forall j, \quad E_j(\lambda(\omega)+\overline{\alpha}, L) - E_j(\lambda(\omega), L) \gtrsim \alpha, \tag{30}$$

where $\overline{\alpha}$ is the vector whose entries are all α.

Based on this and under the assumption that the distribution of the λ_n has a bounded density one can prove that

$$\forall j, \quad \mathbb{P}\left\{E_j(\omega,L)\in[E_0-\varepsilon,E_0+\varepsilon]\right\} \lesssim \varepsilon \tag{31}$$

and obtains the desired bound in εL^d. The proof of (31), while essentially based on the ideas described above, requires additional technical work.

For the discrete d-dimensional Anderson model, the bound

$$\mathbb{E}(\text{tr } \chi_{[E_0-\varepsilon,E_0+\varepsilon]}(H^r_{\omega,L})) \leq C\varepsilon L^d \tag{32}$$

essentially goes back to Wegner's original paper [41], with some technical details filled in later. A detailed proof, essentially following Wegner's original argument, can be found, for example, in the recent survey [28]. Obtaining the bound (32) for the continuum Anderson model was harder, as one can not use the same rank one perturbation methods as in the discrete case to control the spectral shift due to single site terms. Initially, a bound of the form $C\varepsilon L^{2d}$ was obtained for the continuum Anderson model in [27] (for a proof with slightly different methods see also [38]). For q of fixed sign, but without the assumption that the support of q contains Λ_1 and at arbitrary energy, the linear in volume bound (32) was ultimately obtained in [11].

To describe how a Wegner estimate for the random displacement model considered here was found, let us describe a generalization of the idea outlined above which goes back to [31, 32, 33]. To estimate $\mathbb{P}\{E_j(\omega, L) \in [E_0 - \varepsilon, E_0 + \varepsilon]\}$, we study the mapping $\omega \mapsto E_j(\omega, L)$ that realizes a "projection" from the parameter (probability) space onto the real axis; and we want to measure the size (with respect to the probability measure on the parameter space) of the pre-image of some interval. The idea is then to find a vector field $\mathcal{V}$ in the parameters ω such that the eigenvalue $E_j(\omega, L)$ moves when ω moves along the flow of the vector field. The flow of $\mathcal{V}$ foliates the parameter space nicely and the volume we want to measure

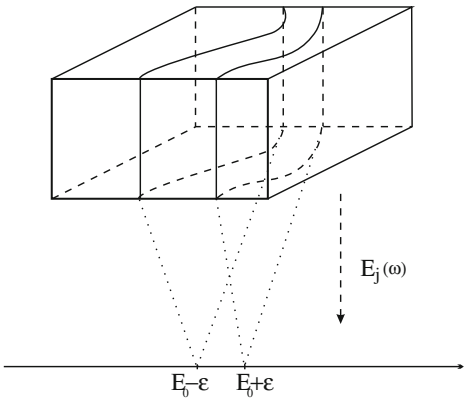

FIGURE 7. Foliation and projection of the probability space

is just the volume contained in a layer between two leaves (see Figure 7). This volume will then be of size the width of this layer at least when the probability measure has a regular density. So if one is able to do this for all the eigenvalues, one gets an estimate of the form εL^d.

To be able to do this for all eigenvalues at a time, one may choose $\mathcal{V}$ so that H_ω^r differentiated along $\mathcal{V}$ has nice properties (e.g., positivity). Let us take the simple example of the continuous Anderson Hamiltonian under the assumptions made above. If we take $\mathcal{V} = \mathrm{div}_{\lambda(\omega)} = \sum_{n\in\Lambda_L} \dfrac{\partial}{\partial\lambda_n(\omega)}$, then $\mathcal{V}H^L_{\lambda(\omega)} \gtrsim \chi_{\Lambda_L}$. This ensures $\mathcal{V}E_j(\omega, L) \gtrsim 1$ which is exactly (30). This is what is needed for a Wegner estimate for the continuous Anderson Hamiltonian when the single site coupling constants admit a bounded density.

The right choice of vector field is model dependent; for the Anderson model, discrete or continuous, in many cases, one may use the divergence vector field as above (for example, see [41, 38]). Another useful vector field with respect to this problem is the generator of the dilations $\sum_n \lambda_n(\omega)\partial_{\lambda_n(\omega)}$. It can be used to get a Wegner estimate for the continuous Anderson model without sign assumptions on V [32, 24] and, in certain cases, for the random displacement models [22]. Other types of randomness may require different types of vector fields, see, e.g., [31, 15].

For the random displacement Hamiltonian H_ω, we will use the same idea and introduce a new vector field. The choice of this vector field is motivated by Theorems 3.1 and 6.1, which indicate that at least low lying eigenvalues should decrease monotonically if the single site potentials are moved towards a corner of their cell.

For a function f on G we set

$$(\partial_c f)(a) := \frac{c(a) - a}{|c(a) - a|} \cdot \nabla f(a),$$

with $c(a)$ denoting the corner closest to a as in Section 7. Thus, ∂_c denotes the directional derivative in the direction of the closest corner, where points a with multiple closest corners will not play a role in the arguments below (starting from (34) below we introduce a cut-off which restricts the values of a relevant for the proof to small neighborhoods of the corners).

By Theorem 6.1 there exist $\delta_0 > 0$ and $r_0 > 0$ such that

$$\partial_c E_0(a) \leq -\delta_0 \quad \text{for all } a \in A_{r_0} := \{a \in G : |c(a) - a| \leq r_0\}, \tag{33}$$

a neighborhood of $\mathcal{C}$.

Let $\eta \in C^\infty(\mathbb{R})$ such that $0 \leq \eta \leq 1$, $\eta(r) = 1$ for $r \leq r_0$ and $\eta(r) = 0$ for $r \geq 2r_0$. Using this function as a cut-off, we localize the vector fields associated with ∂_c onto a neighborhood of the corners, defining

$$(\partial_c' f)(a) := \eta(|c(a) - a|)(\partial_c f)(a). \tag{34}$$

For each $n \in \mathbb{Z}^d$, we write

$$\partial'_{c,\omega_n} H_\omega = \partial'_{c,\omega_n} q(\cdot - n - \omega_n) = -\eta(|c(\omega_n) - \omega_n|) \frac{c(\omega_n) - \omega_n}{|c(\omega_n) - \omega_n|} \cdot (\nabla q)(\cdot - n - \omega_n). \tag{35}$$

If $\psi \in H^1(\Lambda_{2L+1})$, the form domain of $H^N_{\omega,L}$, then $\psi_n := \psi|_{\Lambda_1(n)} \in H^1(\Lambda_1(n))$, the form domain of $H_n(\omega_n)$, and, with the usual abuse of notation for the quadratic form,

$$\langle \psi, H^N_{\omega,L} \psi \rangle = \sum_{n \in \Lambda'_{2L+1}} \langle \psi_n, H_n(\omega_n) \psi_n \rangle, \tag{36}$$

as well as

$$\sum_{n \in \Lambda'_{2L+1}} \langle \psi, \partial'_{c,\omega_n} H^N_{\omega,L} \psi \rangle = \sum_{n \in \Lambda'_{2L+1}} \langle \psi_n, \partial'_{c,\omega_n} H_n(\omega_n) \psi_n \rangle. \tag{37}$$

Proposition 8.1. *There exist $\delta_1 > 0$ and $\delta_2 > 0$ such that*

$$-\sum_{n \in \Lambda'_{2L+1}} \langle \psi, (\partial'_{c,\omega_n} H^N_{\omega,L}) \psi \rangle \geq \delta_1 \|\psi\|^2 \tag{38}$$

for all $L \in \mathbb{N}$, and $\psi \in H^1(\Lambda_{2L+1})$ with $\langle \psi, (H^N_{\omega,L} - E_0)\psi \rangle \leq \delta_2 \|\psi\|^2$.

Thus, near the bottom of the spectrum of $H_{\omega,L}$, the vector field $-\sum_{n \in \Lambda'_{2L+1}} \partial'_{c,\omega_n}$ satisfies exactly the property we are looking for to proceed according to the heuristics explained above. For the details of the proof of Proposition 8.1 as well as for the proof of the implied Wegner estimate in Theorem 8.2 below we refer to [30].

In order to exploit Proposition 8.1 we formulate the following final set of assumptions for the distribution μ of the i.i.d. random displacement parameters $\omega = (\omega_n)$:

(A2)′ With G and $\mathcal{C}$ as above, let $\mathcal{C} \subset \operatorname{supp} \mu \subset \overline{G}$. Also assume that there exists a neighborhood of $\mathcal{C}$ on which μ has a C^1-density.

More formally, this means that there exists $\varepsilon > 0$ and a C^1-function $\rho : \overline{G} \to \mathbb{R}$, such that for every $S \subset \cup_{a \in \mathcal{C}} \{x : |x - a| < \varepsilon\} \cap \overline{G}$ we have

$$\mu(S) = \int_S \rho(x)\, dx.$$

This guarantees that the random variables $|c(\omega_n) - \omega_n|$, which parametrize the layers of the vector field, have absolutely continuous distribution near 0 (i.e., for values of ω_n near the corners). Thus we have exactly the situation required by the above heuristics, which indeed leads to the following Wegner estimate:

Theorem 8.2. *Assume* **(A1)′** *and* **(A2)′**. *Then there exists* $\delta > 0$ *such that, for any* $\alpha \in (0, 1)$, *there exists* $C_\alpha > 0$ *such that, for every interval* $I \subset [E_0, E_0 + \delta]$ *and* $L \in \mathbb{N}$,

$$\mathbb{E}(tr\, \chi_I(H^N_{\omega,L})) \leq C_\alpha |I|^\alpha L^d. \tag{39}$$

We finally need to comment on the reason for the appearance of the exponent $\alpha \in (0, 1)$ in (39). This is a final price we pay for the non-monotonicity (as well as non-analyticity) of our model in the random parameters. The latter necessitate some additional changes in the original strategy of Wegner. The proof of Theorem 8.2 in [30] uses an adaptation of a Wegner estimate proof developed in [24] to handle Anderson models with sign-indefinite single-site potentials. Their argument is based on L^p-bounds for Krein's spectral shift function proven in [12]. These bounds only hold for $p < \infty$ and not for $p = \infty$, which is the reason that we can't choose $\alpha = 1$ in Theorem 8.2.

9. Localization

At this point we have essentially reached the end of the story which was to be told here. As explained in the introduction, with the Lifshitz tail bound of Theorem 7.1 and the Wegner estimate of Theorem 8.2 available, localization for the RDM can be proven via multi-scale analysis. The MSA method is as powerful as the details of carrying it out are intricate. Presenting these details is not a goal of this article. Very good introductions into the mathematics of MSA can be found in the book [38] and the surveys [29] and [28], which also provide extensive bibliographies.

The main task left to us is to state state the exact result on localization for the RDM which was obtained in [30]. Here χ_x denotes the characteristic function of a unite cube centered at x, $\chi_I(H)$ the spectral projection onto I for the operator H, and $\|\cdot\|_2$ the Hilbert-Schmidt norm.

Theorem 9.1. *Assume* **(A1)′** *and* **(A2)′**. *Then there exists* $\delta > 0$ *such that* H_ω *almost surely has pure point spectrum in* $[E_0, E_0 + \delta]$ *with exponentially decaying eigenfunctions.*

Moreover, H_ω is dynamically localized in I, in the sense that for every $\zeta < 1$, there exists $C < \infty$ such that

$$\mathbb{E}\left(\sup_{|g|\leq 1} \|\chi_x g(H_\omega)\chi_I(H_\omega)\chi_y\|_2^2\right) \leq Ce^{-|x-y|^\zeta} \tag{40}$$

for all $x, y \in \mathbb{Z}^d$. The supremum is taken over all Borel functions $g : \mathbb{R} \to \mathbb{C}$ with satisfy $|g| \leq 1$ pointwise.

We note that dynamical localization in the physical sense is covered by (40) in choosing $g(H) = e^{-itH}$ and taking the supremum over $t \in \mathbb{R}$.

The subexponential decay in $|x - y|$ found in (40) is the strongest type of dynamical localization which has been obtained through MSA. This is a result of Germinet and Klein in [20], who used a four times bootstrapped version of the MSA argument, allowing to conclude strong forms of localization from rather weak forms of initial length estimates provided by the Lifshitz tail bound. As described in some more detail in [30], the survey paper [29] provides a very useful resource in explicitly singling out all the properties of a model, which go into the argument in [20]. In addition to the crucial Lifshitz-tail and Wegner bounds proven in Theorems 7.1 and 8.2, the RDM has all other required properties.

In this context we also recommend the book [38] as a very readable account of MSA. Similar to [29] it clearly exhibits the properties of a model which are needed to prove localization via MSA. It uses a version of MSA less sophisticated than what is done in [20], essentially bootstrapping the MSA scheme just twice, to conclude spectral localization and a weaker form of dynamical localization, that is

$$\mathbb{E}\left(\sup_{|g|\leq 1} \||X|^p g(H_\omega)\chi_I(H_\omega)\chi_0\|\right) < \infty \tag{41}$$

for all $p > 0$ in a p-dependent neighborhood I of E_0, giving power-decay rather than subexponential decay in (40). Here $|X|$ is the multiplication operator by the length of the variable $x \in \mathbb{R}^d$.

10. Bubbles tend to the corner

10.1. Bubbles tend to the boundary

The Lifshitz tail estimate as well as the Wegner estimate have as a basic input an estimate on the ground state energy of a Neumann problem as a function of the position of the potential.

It is convenient to take a more general point of view for this problem in which the unit cell Λ_1 is replaced by a bounded domain D with smooth boundary, and to consider the non-degenerate lowest eigenvalue $E_0(a)$ of the operator

$$-\Delta_N + q(x - a) \; . \tag{42}$$

Here Δ_N is the Laplace operator with Neumann boundary conditions on ∂D. We shall assume that the potential q is smooth and has compact support such that the set

$$G = \{a \in \mathbb{R}^d : \text{supp } q(\cdot - a) \subset D\}$$

is not empty. Thus, G is an open and bounded set. We shall, in addition, assume that it is connected.

The following second-order perturbation theory result sets the stage for our investigation. Denote by $\partial_a = w \cdot \nabla_a$ and likewise $\partial_x = w \cdot \nabla_x$ where w is a fixed vector and the subscript denotes the variable in which we differentiate.

Lemma 10.1 (Second-order perturbation theory). *The lowest eigenvalue as a function of a satisfies the equation*

$$\partial_a^2 E_0 - 4\partial_a E_0 \langle u_0, \partial_x u_0 \rangle = 2 \int_D \nabla \cdot (\partial_x u_0 \nabla \partial_x u_0) dx - 2 \sum_{k \neq 0} \frac{B(u_k, \partial_x u_0)^2}{E_k - E_0} \ . \quad (43)$$

Here $B(u, v)$ denotes the bilinear form

$$B(u, v) = (u, \Delta v) - (\Delta u, v) \ ,$$

and $u_k(x; a)$ is the eigenfunction associated with the eigenvalue

$$E_k(a), \quad k = 0, 1, 2, \ldots .$$

The proof of this lemma can be found in [4], with additional modifications in [30]. By Gauss's theorem, the first term on the right side can be written as

$$2 \int_{\partial D} \partial_x u_0 N(x) \cdot \nabla (\partial_x u_0) dS(x) \ ,$$

where $N(x)$ is the outward normal at the point $x \in \partial D$. The following computations should reveal somewhat the geometric structure of this term. For any fixed point x we can extend $N(x)$ to a smooth vector field in a neighborhood of x. We write

$$\begin{aligned} N(x) \cdot \nabla (\partial_x u_0) &= \sum_{i,j} w_j N_i(x) \partial_j \partial_i u_0 \quad (44) \\ &= \sum_{i,j} w_j^{\perp}(x) N_i(x) \partial_j \partial_i u_0 + (w \cdot N(x)) \sum_{i,j} N_j(x) N_i(x) \partial_j \partial_i u_0 \ , \end{aligned}$$

where

$$w^{\perp}(x) = w - (w \cdot N(x)) N(x)$$

is the projection of w onto the plane tangent to ∂D at the point x. For the first term on the right side of (44) we write

$$\sum_{i,j} w_j^{\perp}(x) N_i(x) \partial_j \partial_i u_0 = - \sum_{i,j} w_j^{\perp}(x) (\partial_j N_i(x)) \partial_i u_0 + \sum_{i,j} w_j^{\perp}(x) \partial_j (N_i(x) \partial_i u_0)$$

and note that the last term vanishes. Indeed, this term is a tangential derivative of the function $N(x) \cdot \nabla u_0$ which vanishes identically on ∂D (u_0 is the Neumann ground state). Also,

$$\sum_{i,j} w_j^{\perp}(x)(\partial_j N_i(x))\partial_i u_0 = w^{\perp}(x) \cdot K(x)\nabla u_0,$$

where $K(x) = (K_{j,i}(x)) = (\partial_j N_i(x))$ is the curvature matrix of ∂D at the point x. Thus we have that

$$N(x) \cdot \nabla(\partial_x u_0) = -w^{\perp}(x) \cdot K(x)\nabla u_0 + (w \cdot N(x)) \sum_{i,j} N_j(x) N_i(x) \partial_j \partial_i u_0 \ .$$

Once again, since $N \cdot \nabla u_0 = 0$,

$$\partial_x u_0 = w \cdot \nabla_x u_0 = w^{\perp}(x) \cdot \nabla_x u_0$$

and hence

$$\begin{aligned} 2 \int_{\partial D} & \partial_x u_0 N(x) \cdot \nabla(\partial_x u_0) dS(x) \\ &= -2 \int_{\partial D} w^{\perp}(x) \cdot \nabla_x u_0 w^{\perp}(x) \cdot K(x) \nabla u_0 dS(x) \\ &\quad + 2 \int_{\partial D} w^{\perp}(x) \cdot \nabla_x u_0 (w \cdot N(x)) \sum_{i,j} N_j(x) N_i(x) \partial_j \partial_i u_0 dS(x) \ . \end{aligned}$$

To summarize we have

Lemma 10.2 (Second-order perturbation theory). *The lowest eigenvalue as a function of a satisfies the equation*

$$\begin{aligned} \partial_a^2 E_0 - 4 & \partial_a E_0 \langle u_0, \partial_x u_0 \rangle \\ &= -2 \int_{\partial D} w^{\perp}(x) \cdot \nabla_x u_0 \, w^{\perp}(x) \cdot K(x) \nabla_x u_0 \, dS(x) \\ &\quad + 2 \int_{\partial D} w^{\perp}(x) \cdot \nabla_x u_0 (w \cdot N(x)) \sum_{i,j} N_j(x) N_i(x) \partial_j \partial_i u_0 dS(x) \\ &\quad - 2 \sum_{k \neq 0} \frac{B(u_k, \partial_x u_0)^2}{E_k - E_0} \ . \end{aligned} \tag{45}$$

This formula remains correct if applied to a rectangular parallelepiped and a derivative ∂_a *parallel* to the edges of the domain. While the curvature matrix becomes singular along the corners and edges of the parallelepiped one may argue that these singularities do not contribute to the right-hand side of (45) because the derivatives of u_0 vanish in the directions in which K is singular. A direct argument for this case is provided in [30]. In this case no curvature term appears as the faces of the parallelepiped are flat. Moreover, the second term in (45) vanishes since one of the two terms $w^{\perp}(x)$ or $w \cdot N(x)$ always vanishes. Thus, one gets

Corollary 10.3. *If the domain is rectangular, then for all derivatives ∂_a parallel to the edges of the domain we have*

$$\partial_a^2 E_0 - 4\partial_a E_0 \langle u_0, \partial_x u_0 \rangle = -2 \sum_{k \neq 0} \frac{B(u_k, \partial_x u_0)^2}{E_k - E_0} \ . \tag{46}$$

The point of this formula is that the right side has a definite sign. Corollary 10.3 will be the crucial input for showing that the energy minimizing position is when the potential sits in the corners.

Let us expand the scope a little bit by considering smooth domains D. For such domains, by summing over the canonical basis of unit vectors w one obtains the formula

$$\Delta E_0 - 4(u_0, \nabla u_0) \cdot \nabla E_0 = -2 \int_{\partial D} \nabla u_0 \cdot K(x) \nabla u_0 \, dS - 2 \sum_{k \neq 0} \frac{\sum_i B(u_k, \partial_i u_0)^2}{E_k - E_0} \ . \tag{47}$$

This is best seen by only using the first identity in (44) in the above argument without introducing $w^\perp$, see also [4] for a direct proof. The right side of (47) has a definite sign for the case where the boundary has a positive curvature matrix, i.e., is a convex surface. Assuming that the right side of (47) is given, this equation can be considered as a second-order elliptic equation for the eigenvalue $E_0(a)$ and hence it is amenable to a strong minimum principle (see, e.g., [16] Theorem 3 on p. 349) provided we know that the right side of (47) is strictly negative. It is then a consequence of the strong minimum principle that if $E_0(a)$ attains its minimum over $\overline{G}$ at an interior point of G, then $E_0(a)$ is constant throughout G.

One case where one may try to exploit this reasoning is if the domain D is strictly convex in the sense that the curvature matrix $K(x)$ is positive definite at every point of the boundary ∂D. If the eigenvalue $E_0(a)$ attains its minimum at $a_0 \in G$ then $\nabla E_0(a_0) = 0$ and $\Delta E_0(a_0) \geq 0$. Hence the right side of (47) must vanish. Since $K(x)$ is assumed to be strictly positive at all points of ∂D we have that ∇u_0 vanishes on ∂D, i.e., $u_0(x, a_0)$ is constant there. Using this it is not hard to prove the following theorem.

Theorem 10.4 (Strong minimum principle for E_0). *If $E_0(a_0) = \inf_{a \in G} E_0(a)$ for some $a_0 \in G$, then $E_0(a)$ is identically zero. In this case the wave function is constant in the connected component of the complement of the support of the potential that touches the boundary ∂D.*

In other words, if $E_0(a)$ is not identically zero, then it attains its minimum on the boundary of G.

Theorem 10.4 corresponds to Theorem 1.4 in [4] where a proof is given. Theorem 1.4 as stated there is slightly inaccurate since it is implicitly assumed that the complement of the support of the potential has only one connected component (the exterior component touching ∂D).

For a given domain and potential it is in general not easy to verify if the lowest eigenvalue is independent of the position of the potential. A construction

of examples with this property, starting with the ground state eigenfunction, was described in Section 3, see (9). But it is relatively easy to verify non-constancy of $E_0(a)$ in a number of cases. One has to exhibit one position of the potential where the ground state energy is not zero. This is obvious if the potential has a fixed sign. Likewise, if the potential is not identically zero and if its average is less than or equal to zero, we can use the constant function as a trial function and see that the ground state energy is strictly negative, for if it were zero, the constant function would be the eigenfunction and the potential would be identically zero.

An interesting conclusion can be drawn using Hopf's lemma. Since the domain is smooth, every point satisfies an interior ball condition. Thus, by Hopf's lemma (see, e.g., [16] p. 347) we conclude that the derivative of $E_0(a)$ at the point where the minimum is attained and normal to the boundary is strictly positive.

While all these ideas put us on the right track, we cannot apply them directly to our situation. The underlying domain Λ_1 is not strictly convex and its boundary is obviously not smooth. Moreover, we need the minimal configuration to be in the corners and not just on the boundary, and most importantly we need estimates on how the eigenvalue increases away from the boundary. Note that Hopf's lemma will not do, since at the corners the interior ball condition is not satisfied. Nevertheless, by a refined analysis we can show that these statements remain true for the case where the domain is a rectangular parallelepiped.

10.2. E_0 has a non-vanishing derivatives

Let us consider formula (46) for the case where we take the derivative in the 1-direction. We write $G = I \times G'$ with an open interval I and an open $d-1$-dimensional rectangle G'. As we shall fix the variables $a_2, \dots, a_d$ in G' we shall suppress them from the notation and just write $E_0(a_1)$. Thus, the variable a_1 varies over the open interval I which is symmetric with respect to the origin. (46) takes the form

$$E_0'' - 4E_0' \langle u_0, \partial_1 u_0 \rangle = -2 \sum_{k \neq 0} \frac{B(u_k, \partial_1 u_0)^2}{E_k - E_0} \ . \tag{48}$$

The following dichotomy is of interest for us.

Theorem 10.5. *Assume that the right side of* (48) *vanishes for some* $a_{1,0} \in I$. *Then* $E_0(a_1) = 0$ *identically in* I *and for every* $a_1 \in I$ *the eigenfunction* $u_0(x, a_1)$ *is constant in the connected component of the complement of the support of* q_a *that touches the boundary of* D

Let us give a sketch of the proof, for more details see [30]. If this function vanishes for some value of $a_{1,0}$, then we must have that

$$B(u_k, \partial_1 u_0) = 0, \ k = 0, 1, 2, \dots \ .$$

In other words

$$\langle u_k, \Delta \partial_1 u_0 \rangle = \langle \Delta u_k, \partial_1 u_0 \rangle, \ \ k = 0, 1, 2, \dots \ .$$

This can be used to show that $\partial_1 u_0$ satisfies a Neumann condition on the faces S_1 and T_1 of G perpendicular to the 1-direction, see the proof of Lemma 2.4 in [30]. Thus $u_{x_1,x_1} = 0$ on S_1 and T_1. Since $a_{1,0} \in I$ and $(a_2, \ldots, a_d) \in G'$ the potential is zero in a neighborhood of the boundary ∂D. On the faces S_1 and T_1 the function u_0 satisfies the equation $-\Delta' u_0 = E_0 u_0$, where $\Delta' = \Delta - \frac{\partial^2}{\partial x_1^2}$. Recalling that all the first derivatives of u_0 vanish on the intersections of the faces (e.g., on the intersections of S_1 and T_1 with other faces of G), u_0 must satisfy a Neumann condition on the boundary of the faces S_1, T_1. Since u_0 is non-negative it is the ground state eigenfunction of $-\Delta' u_0 = E_0 u_0$ and hence must be constant. Thus, $E_0 = 0$ and u_0 is harmonic outside the support of the potential. If we pick a point x_0 on S_1 away from the support of the potential (such that the potential is zero near x_0), we may assume by the reflection principle, that the function $u_0(x, a_{1,0})$ is harmonic in a neighborhood U of x_0. Moreover, $u_0(x, a_{1,0})$ is constant on $U \cap S_1$ and $\partial_1 \partial_j u_0(x, a_{1,0}) = 0$ for $j = 1, 2 \ldots, d$. From this one can easily conclude that $u_0(x, a_{1,0})$ must be constant in U (see [30]) and hence in the component of the complement of the support of q_a that touches the boundary. This proves Theorem 10.5, with the ground state being obtained by shifting the potential and u_0 simultaneously.

Armed with this information we can prove Theorem 6.1 easily. It suffices to consider the 1-direction. Returning to (48) we may introduce an integrating factor $F(a_1)$ such that $F'(a_1) = -4\langle u_0, \partial_1 u_0 \rangle$ and rewrite this equation as

$$\left(e^F E_0'\right)'(a_1) = -2e^{F(a_1)} \sum_{k \neq 0} \frac{B(u_k, \partial_1 u_0)^2}{E_k - E_0} \ .$$

By Theorem 10.5 and assumption **(A1)′** the right-hand side is strictly negative. Since we assume that the potential is symmetric with respect to reflections about the 1-direction, we know that the eigenvalue $E_0(a_1)$ is a symmetric function, i.e., $E_0(-a_1) = E_0(a_1)$ and hence $E_0'(0) = 0$. Thus, for $a_1 > 0$, by integrating we obtain

$$E'(a_1) = -2e^{-F(a_1)} \int_0^{a_1} e^{F(\alpha)} \sum_{k \neq 0} \frac{B(u_k, \partial_1 u_0)^2}{E_k - E_0} d\alpha < 0 \ , \tag{49}$$

which implies Theorem 6.1.

11. Open problems

The main reason for presenting this expository account of our results on the random displacement model is that the methods developed have led to a satisfactory understanding of localization for this model, where multiple pieces of a puzzle eventually fell into place to reveal a complete picture. Thus, to some extend, this is the end of a story. Nevertheless, various aspects of our work reveal natural and non-trivial questions for further work. We end our presentation by describing some of them.

11.1. Bubbles tend to the boundary

Our work has led to two types of results about the optimal placement of a potential to minimize the lowest eigenvalue of the Neumann problem (42) on a given domain G. While Theorem 10.4 shows that for general convex domains the minimizing position is at the boundary, Theorems 3.1 and 6.1 characterize corners as the exact minimizing positions for the special case of a rectangular domain. It is natural to believe that corners are good candidates for minimizers for other polyhedral domains, in particular for regular n-gons in $d = 2$, but our methods do not allow to prove this for any $n \neq 4$. The second term in (45) does not vanish unless the domain is a rectangular parallelepiped! Of course, in this case one would assume that the potential shares the symmetries of the domain. Radially symmetric potentials would be the most natural candidates and it might also help to choose them sign-definite. Particularly interesting would be a proof of this for equilateral triangles, $n = 3$, because all the other results presented in this paper would then apply to get a localization proof for the RDM on triangular lattices.

It is natural to conjecture that on smooth convex domains the minimizing position of the potential along the boundary should be at a point of maximal curvature, as long as the potential has sufficiently small support to smoothly fit into the boundary at this point. A case where one could hope to formulate and prove this rigorously is an elliptic domain G in $\mathbb{R}^2$ with a small radially symmetric potential.

11.2. Periodic minimizers

Formula (5), characterizing the almost sure spectrum of the RDM in terms of periodic displacement configurations, holds under very weak assumptions on μ and the single-site potential q. Is it necessary to take the closure on the right-hand side? That we were able to prove the existence of a periodic minimizer in Theorem 2.1 was due to a number of lucky coincidences (or of well-chosen assumptions, for that matter). One might ask if for more general cases the existence of a periodic minimizer in (5) is the rule or more likely to be an exception.

For example, what happens if we keep all the assumptions in **(A1)** and **(A2)** above, with the exception that $\operatorname{supp}\mu$ may not contain *all* the corners $\mathcal{C}$ of G? Our simple method of constructing a minimizer by multiple reflections breaks down. It is not clear at all, and maybe not likely, that a periodic minimizer exists. The same problem arises if we don't require that the single-site potential is reflection symmetric in each coordinate. One might be led to believe that periodic minimizers hardly ever exist, but for the moment we do not know a single counterexample.

One may also look at non-rectangular lattices, while keeping all the desired symmetry assumptions on q and $\operatorname{supp}\mu$. If, as suggested in Section 11.1, bubbles tent to the corners for regular triangles, then a periodic minimizer for the triangular lattice in $\mathbb{R}^2$ could be constructed by repeated reflection, as in the case of rectangles. However, the same does not work for a hexagonal lattice, where contradictory positions of some of the bubbles arise after just a few reflections. Is there nevertheless a periodic minimizer for the hexagonal RDM?

11.3. The fractional moments method

In our proof of localization for the RDM we followed the strategy provided by multi-scale analysis, which yields spectral and dynamical localization based on the Lifshitz tail bound and Wegner estimate provided by Theorems 7.1 and 8.2. Another method which has provided localization proofs for multi-dimensional random operators is the fractional moments method (FMM) originally introduced by Aizenman and Molchanov in [3] to give a simple proof of localization for the multi-dimensional discrete Anderson model. This method has meanwhile been extended to show localization for continuum Anderson models [1, 7]. While likely not being as universally applicable as MSA (and quite certainly not extendable to situations as considered in [6]), an interesting feature of the FMM is that, in situations where it is applicable, it yields a stronger form of dynamical localization than what has been obtained via MSA. Instead of (40) one gets the stronger

$$\mathbb{E}\Big(\sup_{|g|\leq 1} \|\chi_x g(H_\omega)\chi_I(H_\omega)\chi_y\|_2^2\Big) \leq Ce^{-\eta|x-y|} \tag{50}$$

for some $\eta > 0$ and intervals I in the localized regime.

It would be interesting to find out if the FMM applies to the random displacement model under the assumptions of Theorem 9.1. While the FMM uses Lifshitz tail bounds in a similar way as MSA, one would need to replace the Wegner estimate by another technical tool, the fractional moment bound

$$\sup_{E\in I,\varepsilon>0} \mathbb{E}(\big\|\chi_x(H_\omega - E - i\varepsilon)^{-1}\chi_y\big\|^s) \leq Ce^{-\eta|x-y|} \tag{51}$$

for suitable $s \in (0,1)$. In fact, it would already be a major step to establish finiteness of the left-hand side of (51) as an a priori bound. We believe that the properties of the RDM which went into our proof of a Wegner estimate can also lead to a proof of this a priori bound.

11.4. Non-generic single site potentials

We have argued above that alternative (i) of Theorem 3.1 is the generic case and we have proven our localization results under this assumption. Nevertheless, we also observed that via formula (9) one gets a rich reservoir of examples in which the ground state of the single-site Neumann operator $H^N_{\Lambda_1}(a)$ is constant outside the support of the potential and thus $E_0(a)$ identically vanishing. When choosing a single-site potential of this type in defining the random displacement model, one sees that $\min\sigma(H_\omega) = \min\sigma(H^N_{\omega,L}) = 0$ for *all* choices of ω and L. Thus we are *not* in the fluctuation boundary regime which we exploited above to get the Lifshitz tail bound and thus can not prove low energy localization with our methods.

The determination of the spectral type of H_ω near zero for this case remains an open problem. The fact alone that zero is the deterministic ground state energy for finite volume restrictions of H_ω does not exclude the possibility of Lifshitz tails, as a single non-degenerate eigenvalue does not affect the IDS in the infinite volume limit. On the other hand, the ground state eigenfunction in this model is an essentially uniformly spread out extended state (differing from a constant

only by local random fluctuations). While we don't necessarily believe that this could indicate the existence of absolutely continuous spectrum near zero, it might lead to non-trivial transport, similar to the existence of critical energies in certain one-dimensional random operators such as the dimer model, e.g., [25]. Finding the answer to this will require a much better understanding of excited states of the RDM, a task which we have managed to systematically avoid in all the results presented above.

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On Limiting Eigenvalue Distribution Theorems in Semiclassical Analysis

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Abstract. We give a detailed proof of limiting eigenvalue distribution theorems (LEDT) for eigenvalue clusters associated to suitable bounded perturbations of the spherical Laplacian on S^n and the hydrogen atom Hamiltonian. In order to show the structure of the proof of those theorems, we introduce a LEDT for suitable bounded perturbations of the k-dimensional harmonic oscillator.

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1. Introduction

Let Δ_{S^2} be the Laplacian on the 2-sphere S^2 (the set of unit vectors in the Euclidean space $\mathbb{R}^3$). It is a well-known fact that the spectrum of the operator Δ_{S^2} is equal to the set of eigenvalues $\lambda_\ell = \ell(\ell+1)$, $\ell = 0, 1, \ldots$, with multiplicity $d_\ell = 2\ell + 1$. Let us now consider the Schrödinger operator on S^2:

$$H = \Delta_{S^2} + V \,, \tag{1}$$

with $V : S^2 \to \mathbb{R}$ a continuous function. The effect of introducing the potential V is to create the splitting of the unperturbed eigenvalues λ_ℓ. Thus the spectrum of H is discrete and, since V is bounded and the distance $|\lambda_\ell - \lambda_{\ell+1}| = O(\ell)$, then we have well-defined clusters of eigenvalues around λ_ℓ (at least when we are far enough from the origin). The size of those clusters is no longer than the infinite norm of V and we will have as many eigenvalues in the ℓth cluster as the original multiplicity d_ℓ of the unperturbed eigenvalue λ_ℓ. Let us denote by $\eta_{\ell,m}$, $m = 1, \ldots, d_\ell$ the eigenvalues in the ℓth cluster (we are listing each eigenvalue as many times as its multiplicity).

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A very interesting question is to describe the distribution of eigenvalues in those clusters when we take the high energy semiclassical limit ($\ell \to \infty$). An answer to this question goes as follows: Consider a test function $f \in C_0^\infty$. Then, for each ℓ, consider the average of the real numbers obtained by evaluation of f on the shifts $\eta_{\ell,m} - \lambda_\ell$. Then those averages have a limit when $\ell \to \infty$ involving the averages of the perturbation V along the classical orbits of the unperturbed problem (the geodesic flow). Namely, we have the following

Theorem 1. *Let f and V as above. Then*

$$\frac{1}{d_\ell} \sum_{m=1}^{\infty} f(\eta_{\ell,m} - \lambda_\ell) = \int_{S^2} f\left(\hat{V}(\mathbf{w})\right) dS(\mathbf{w}) \,, \tag{2}$$

where dS denotes the normalized surface measure on S^2 and $V : S^2 \to \mathbb{R}$ can be thought as a kind of a Radon transform whose evaluation at a point $\mathbf{w} \in S^2$ is equal to the average of V along the oriented great circle $\mathcal{C}_\mathbf{w}$ on S^2 orthogonal to $\mathbf{w}$:

$$\hat{V}(\mathbf{w}) = \frac{1}{2\pi} \int_0^{2\pi} V(\mathcal{C}_\mathbf{w}(s)) ds \,, \tag{3}$$

where s is the arc-length.

The theorem above is a particular case of a limiting eigenvalue distribution theorem (LEDT) introduced by A. Weinstein [28] where he actually proves that the theorem holds when we have a compact Riemannian manifold M all of whose geodesics are closed. The limit involves an integral on the space of oriented geodesics Γ of the manifold M. Note that for the case of the 2-sphere, Γ can be identified with the 2-sphere. See articles by H. Widom [29], Y. Colin de Verdiere [26] and V. Guillemin [8] and S. Sternberg [7] for related work on this problem.

It seems a very interesting task to look for other systems where a LEDT can be established. Namely, systems where the discrete spectrum involves degenerated eigenvalues and the associated classical problem has periodic orbits on a given energy surface. A. Uribe and C. Villegas-Blas [25] have studied the case of bounded perturbations of the hydrogen atom using the Moser regularization [20].

The purpose of the present paper is to give a detailed introduction to the LEDT on both the n-sphere and the hydrogen atom problems following reference [25]. In order to show the structure of the proof of the LEDT for those two cases, we first introduce a LEDT for perturbations of the k-dimensional harmonic oscillator (KDHO). As far as we know, a LEDT for the KDHO has not appeared in the published literature, although it is a natural problem to study after the work of A. Weinstein. In a recent work, V. Guillemin, A. Uribe and Z. Wang [9] have considered a LEDT for the KDHO in a more advanced research program. However, their proof is different than ours (we use a Bargmann space representation). We remark that the existence of clusters for perturbations of the KDHO can be obtained as a consequence of work by B. Helffer and D. Robert (see Theorem 3.9 in [11]), but we give our own proof for such a fact. We thank A. Uribe for suggesting to us the basic mechanism to establish a LEDT for the KDHO case.

The paper is organized as follows. We first describe in Section 2 the Bargmann space representation and the corresponding Bargmann transform for the Hilbert space $L^2(\mathbb{R}^n)$. We obtain an expression for the projector associated to a given eigenspace of the KDHO in terms of states concentrated on corresponding classical orbits when the Planck parameter $\hbar$ is small. Then we introduce in Section 3 the LEDT for the KDHO with bounded perturbations given by suitable pseudo-differential operators of order zero by (i) estimating the norm of the difference between the perturbed and unperturbed orthogonal projectors associated to the ℓth cluster with ℓ large and (ii) using the averaging method originally introduced by A. Weinstein [28]. We continue in Section 4 by showing a LEDT for perturbations of the spherical Laplacian on the n-sphere where the perturbation is given by a pseudo-differential operator of order zero (thus Theorem 1 will be a particular case of Section 4). The structure of the proof follows the one given in Section 3 so we mainly show the additional ideas for the proof. In particular we establish a Szegö-type theorem that will be used in the next section on the hydrogen atom case. Finally, in Section 5 we introduce a LEDT for suitable perturbations of the hydrogen atom Hamiltonian. We follow the structure of the proof given in previous sections concentrating mainly in the additional and subtle points for the proof of the hydrogen atom case. Sections 4 and 5 follow reference [25] although the first part of the proof for the LEDT follows Section 3 and additional comments are included. We finish with some comments on further developments for LEDT in other physical systems.

2. The Bargmann representation

In this section we give a brief description of both the Bargmann space representation $\mathcal{B}_k^{(\hbar)}$ of analytical functions and a unitary transform $\mathbf{B}_k^{(\hbar)}$ relating $\mathcal{B}_k^{(\hbar)}$ with $L^2(\mathbb{R}^k)$ (the so-called Bargmann transform). We also give an expression for the orthogonal projector from $\mathcal{B}_k^{(\hbar)}$ onto a subspace of homogeneous polynomials of a given degree in terms of certain states whose concentration property will be shown and used in the next sections in order to prove a limiting eigenvalue distribution theorem for perturbations of the k-dimensional harmonic oscillator. Regarding the description of both $\mathcal{B}_k^{(\hbar)}$ and $\mathbf{B}_k^{(\hbar)}$, we will restrict ourselves to only mention some properties that will be useful for us in the present work. We refer the reader to the references [4] and [10] for a detailed description.

2.1. The Bargmann space

For k a positive integer, let $\mathcal{B}_k^{(\hbar)}$ denote the Bargmann space of complex-valued holomorphic functions on $\mathbf{z} \in \mathbb{C}^k$ which are square integrable with respect to the following measure on $\mathbf{z} \in \mathbb{C}^k$:

$$d\nu_k^{\hbar}(\mathbf{z}) := \frac{1}{(\pi\hbar)^k} \exp\left(-\frac{|\mathbf{z}|^2}{\hbar}\right) d\mu(\mathbf{z}), \tag{4}$$

with $\mathbf{z} = (z_1, \ldots, z_k)$, $|\mathbf{z}|^2 = |z_1|^2 + \cdots + |z_k|^2$, $d\mu$ the Lebesgue measure on $\mathbb{C}^k \simeq \mathbb{R}^{2k}$ and $\hbar > 0$ the Planck's parameter.

The vector space $\mathcal{B}_k^{(\hbar)}$ is a Hilbert space under the following inner product

$$\langle F_1, F_2 \rangle_{\mathcal{B}_k^{(\hbar)}} = \int_{\mathbb{C}^k} F_1(\mathbf{z})\overline{F_2(\mathbf{z})} d\nu_k^{\hbar}(\mathbf{z}), \quad F_1, F_2 \in \mathcal{B}_k^{(\hbar)}. \tag{5}$$

The following orthonormal set of monomials gives a basis for $\mathcal{B}_k^{(\hbar)}$

$$\Gamma_\ell(\mathbf{z}) \equiv \frac{z_1^{\ell_1} \cdots z_k^{\ell_k}}{\hbar^{|\ell|/2}\sqrt{\ell_1! \cdots \ell_k!}}\,, \tag{6}$$

with $\ell = (\ell_1, \ldots, \ell_k)$, $|\ell| \equiv \ell_1 + \cdots + \ell_k$ and $\ell_j \in N^*$, $j = 1, \ldots, k$, where N^* denotes the set of non-negative integer numbers.

Thus the Bargmann space $\mathcal{B}_k^{(\hbar)}$ can be written as a direct sum

$$\mathcal{B}_k^{(\hbar)} = \bigoplus_{s=0}^{\infty} W_s^{(\hbar)} \ , \tag{7}$$

where $W_s^{(\hbar)}$ denotes the vector space of homogeneous polynomials of degree s endowed with the inner product given in Eq. (5).

Let us denote by $\mathbf{w} \cdot \mathbf{z} = \sum_{j=1}^k w_j \overline{z_j}$ the usual inner product in $\mathbb{C}^k$. The Bargmann space $\mathcal{B}_k^{(\hbar)}$ has the key property of having a reproducing kernel. Namely, the function

$$K_k^{(\hbar)}(\mathbf{w}, \mathbf{z}) \equiv \exp\left(\frac{\mathbf{w} \cdot \mathbf{z}}{\hbar}\right) \tag{8}$$

has the property that for all $F \in \mathcal{B}_k^{(\hbar)}$:

$$F(\mathbf{w}) = \langle F(\cdot), K_k^{(\hbar)}(\cdot, \mathbf{w}) \rangle_{\mathcal{B}_k^{(\hbar)}} = \int_{\mathbb{C}^k} F(\mathbf{z}) \exp\left(\frac{\mathbf{w} \cdot \mathbf{z}}{\hbar}\right) d\nu_k^{\hbar}(\mathbf{z}). \tag{9}$$

2.2. The orthogonal projections onto subspaces of homogeneous degree

Let us introduce the following normalized states in $W_s^{(\hbar)} \subset \mathcal{B}_k^{(\hbar)}$: For $\mathbf{z} \neq 0$ and s a non-negative integer number, we define

$$\Phi_{\mathbf{z},s}^{(\hbar)}(\mathbf{w}) = \frac{(\mathbf{w} \cdot \mathbf{z})^s}{\hbar^{s/2}|\mathbf{z}|^s\sqrt{s!}}. \tag{10}$$

Using the Taylor expansion for $\exp\left(\frac{\mathbf{w}\cdot\mathbf{z}}{\hbar}\right)$ and the orthonormal basis for $\mathcal{B}_k^{(\hbar)}$ given above (see Eq. (6)) we can show that the function $\frac{(\mathbf{w}\cdot\mathbf{z})^s}{\hbar^s s!}$ gives the reproducing kernel for the space $W_s^{(\hbar)}$. Thus the following expression for the orthogonal projection $\Lambda_s^{(\hbar)} : \mathcal{B}_k^{(\hbar)} \mapsto W_s^{(\hbar)}$ holds

$$\Lambda_s^{(\hbar)} F = \frac{1}{\hbar^s s!} \int_{\mathbb{C}^k} \left\langle F, \Phi_{\mathbf{z},s}^{(\hbar)} \right\rangle_{\mathcal{B}_k^{(\hbar)}} \Phi_{\mathbf{z},s}^{(\hbar)} |\mathbf{z}|^{2s} d\nu_k^{\hbar}(\mathbf{z}), \quad F \in \mathcal{B}_k^{(\hbar)} \ . \tag{11}$$

It will be very useful to obtain an expression for the projector $\Lambda_s^{(\hbar)}$ in terms of and integral involving $|\mathbf{z}| = 1$ only. Let us write $\mathbf{z} = r\tilde{\mathbf{z}}$ with $r \geq 0$ and $\tilde{\mathbf{z}}$ in

the surface $\Sigma_1 = \{\mathbf{z} \in \mathbb{C}^k \mid |\mathbf{z}| = 1\}$. Let us denote by $d\Omega$ the normalized surface measure on Σ_1 regarded as the unit sphere S^{2k-1} in $\mathbb{R}^{2k}$ and by d_s the dimension of the vector space $W_s^{(\hbar)}$.

After some computation we find the result

$$\Lambda_s^{(\hbar)} F = d_s \int_{\Sigma_1} \left\langle F, \Phi_{\mathbf{z},s}^{(\hbar)} \right\rangle_{\mathcal{B}_k^{(\hbar)}} \Phi_{\mathbf{z},s}^{(\hbar)} d\Omega(\mathbf{z}), \quad F \in \mathcal{B}_k^{(\hbar)}, \tag{12}$$

where we have used that the area of the unit sphere S^{2k-1} is given by $|S^{2k-1}| = \frac{2\pi^k}{(k-1)!}$ and $\int_{r=0}^{\infty} r^{2s+2k-1} \exp(-r^2) dr = \frac{(s+k-1)!}{2}$.

2.3. The Bargmann transform for $L^2(\mathbb{R}^k)$

The Bargmann transform $\mathbf{B}_k^{(\hbar)} : L^2(\mathbb{R}^k) \mapsto \mathcal{B}_k^{(\hbar)}$ is defined by the following integral operator:

$$\mathbf{B}_k^{(\hbar)} \Psi(\mathbf{z}) = \frac{1}{(\pi\hbar)^{k/4}} \int_{\mathbf{x}\in\mathbb{R}^k} \exp\left(-\frac{1}{2\hbar} [\mathbf{z}^2 + \mathbf{x}^2 - 2\sqrt{2}\mathbf{z}\cdot\mathbf{x}] \right) \Psi(\mathbf{x}) d\mathbf{x} \ , \tag{13}$$

with $\mathbf{x} = (x_1, \ldots, x_k)$, $\mathbf{z}^2 = z_1^2 + \cdots + z_k^2$, $\mathbf{x}^2 = x_1^2 + \cdots + x_k^2$, $\mathbf{z}\cdot\mathbf{x} = z_1 x_1 + \cdots + z_k x_k$ and $d\mathbf{x}$ the Lebesgue measure on $\mathbb{R}^k$. The Bargmann transform $\mathbf{B}_k^{(\hbar)}$ is a unitary operator with $L^2(\mathbb{R}^k)$ endowed with the usual inner product:

$$\langle \Psi_1, \Psi_2 \rangle_{L^2(\mathbb{R}^k)} = \int_{\mathbf{x}\in\mathbb{R}^k} \Psi_1(\mathbf{x}) \overline{\Psi_2}(\mathbf{x}) d\mathbf{x}. \tag{14}$$

The integral kernel defining the Bargmann transform $\mathbf{B}_k^{(\hbar)}$ belongs to $L^2(\mathbb{R}^k)$ for $\mathbf{z}$ fixed. Moreover, it has the remarkable property that its complex conjugate gives the canonical coherent states for the k-dimensional harmonic oscillator introduced initially by E. Schrödinger:

$$\Psi_{\mathbf{z},\hbar}(\mathbf{x}) = \frac{1}{(\pi\hbar)^{k/4}} \overline{\exp\left(-\frac{1}{2\hbar} [\mathbf{z}^2 + \mathbf{x}^2 - 2\sqrt{2}\mathbf{z}\cdot\mathbf{x}] \right)}. \tag{15}$$

The system of coherent states $\{\Psi_{\mathbf{z},\hbar}\}_{\mathbf{z}\in\mathbb{C}^k}$ has several relevant properties (see [18]). In particular, the Bargmann transform of the states $\Psi_{\mathbf{z},\hbar}$ gives the reproducing kernel of the Bargmann space $\mathcal{B}_k^{(\hbar)}$. Namely,

$$\mathbf{B}_k^{(\hbar)} \Psi_{\mathbf{z},\hbar}(\mathbf{w}) = \exp\left(\frac{\mathbf{w}\cdot\mathbf{z}}{\hbar} \right) \ . \tag{16}$$

The Bargmann transform $\mathbf{B}_k^{(\hbar)}$ intertwines the standard creation and annihilation operators acting on $L^2(\mathbb{R}^k)$ with the multiplication z_j and $\hbar\partial/\partial z_j$ operators respectively $(j = 1, \ldots, k)$. Namely

$$\mathbf{B}_k^{(\hbar)} \left(\frac{\hat{x}_j - \imath \hat{p}_j}{\sqrt{2}} \right) (\mathbf{B}_k^{(\hbar)})^{-1} = \text{multiplication by } \ z_j, \tag{17}$$

$$\mathbf{B}_k^{(\hbar)} \left(\frac{\hat{x}_j + \imath \hat{p}_j}{\sqrt{2}} \right) (\mathbf{B}_k^{(\hbar)})^{-1} = \hbar \frac{\partial}{\partial z_j}, \tag{18}$$

where $\hat{x}_j =$ multiplication by x_j and $\hat{p}_j = -\imath\hbar \frac{\partial}{\partial x_j}$, with $j = 1, \ldots, k$.

3. The harmonic oscillator

In this section we introduce two equivalent limiting eigenvalue distribution theorems for perturbations of the k-dimensional harmonic oscillator. The proof is based on two steps. The first one involves the estimate of the difference of two orthogonal projections, one involved with the k-dimensional harmonic oscillator and the other one with the perturbed problem. The second step consist in proving a Szegö type theorem by using the averaging method (originally introduced by A. Weinstein [28]) and introducing coherent states concentrated on classical orbits which lie inside the energy surface Σ_1 (see below).

Let us consider the following Hamiltonian associated to the k-dimensional harmonic oscillator:

$$A_\hbar = -\frac{\hbar^2}{2}\Delta_{\mathbb{R}^k} + \frac{1}{2}\mathbf{x}^2 - \frac{\hbar k}{2}\,, \tag{19}$$

with $\Delta_{\mathbb{R}^k}$ the usual Laplacian on the Euclidean space $\mathbb{R}^k$. We will use the notation $A \equiv A_1$ for the case $\hbar = 1$. Regarding all of the Schrödinger operators involved in this paper, we will be considering their selfadjoint realization on suitable domains.

The spectrum of the operator $A_\hbar$ is the set of eigenvalues

$$S(A_\hbar) \equiv \{\hbar(\ell_1 + \cdots + \ell_k) \mid \ell_1, \ldots, \ell_k \in \mathbb{N}^*\}\,. \tag{20}$$

Note that each eigenvalue in $S(A_\hbar)$ has multiplicity $d_s = \frac{(s+k-1)!}{s!(k-1)!}$ with $s \equiv \ell_1 + \cdots + \ell_k$.

As a consequence of Eqs. (17), the Bargmann transform $\mathbf{B}_k^{(\hbar)}$ intertwines the harmonic oscillator operator $A_\hbar$ with the following operator:

$$\mathbf{B}_k^{(\hbar)}\ (A_\hbar)\ (\mathbf{B}_k^{(\hbar)})^{-1} = \hbar\sum_{j=1}^{k} z_j\frac{\partial}{\partial z_j}\,. \tag{21}$$

Note that the spectrum of the harmonic oscillator and its eigenspaces are much easier to find in the Bargmann space representation than in $L^2(\mathbb{R}^k)$. In particular, we can see that the eigenspaces of the operator $\hbar\sum_{j=1}^{k} z_j\frac{\partial}{\partial z_j}$ are precisely the spaces $W_s^{(\hbar)}$ with $s \in \mathbb{N}^*$.

3.1. Coherent states and classical orbits

For $s \in \mathbb{N}^*$, let us denote by $V_s^{(\hbar)}$ the eigenspace of $A_\hbar$ associated with the eigenvalue $\hbar s$ and endowed with the inner product indicated in Eq. (14). Let $\Pi_s^{(\hbar)} : L^2(\mathbb{R}^k) \mapsto V_s^{(\hbar)}$ be the corresponding orthogonal projection of $A_\hbar$. The Bargmann transform intertwines the projections $\Pi_s^{(\hbar)}$ and $\Lambda_s^{(\hbar)}$:

$$\mathbf{B}_k^{(\hbar)}\ \left(\Pi_s^{(\hbar)}\right)\ (\mathbf{B}_k^{(\hbar)})^{-1} = \Lambda_s^{(\hbar)}\,. \tag{22}$$

Thus, using Eq. (12) we can obtain the following integral representation for the projector $\Pi_s^{(\hbar)}$ in terms of an integral involving the surface Σ_1:

$$\Pi_s^{(\hbar)}\Psi = d_s\int_{\Sigma_1}\left\langle\Psi, \Psi_{\mathbf{z},s}^{(\hbar)}\right\rangle_{L^2(\mathbb{R}^k)}\Psi_{\mathbf{z},s}^{(\hbar)}d\Omega(\mathbf{z}), \quad \Psi \in L^2(\mathbb{R}^k), \tag{23}$$

where, for $\mathbf{z} \neq 0$, $\Psi^{(\hbar)}_{\mathbf{z},s} \equiv (\mathbf{B}^{(\hbar)}_k)^{-1}\Phi^{(\hbar)}_{\mathbf{z},s}$. Note that in Eq. (23), the region Σ_1 can be regarded as the energy surface $G = 1$ corresponding to the classical harmonic oscillator Hamiltonian $G : T^*\mathbb{R}^k \to \mathbb{R}^k$ given by

$$G(\mathbf{x}, \mathbf{p}) = \frac{\mathbf{p}^2}{2} + \frac{\mathbf{x}^2}{2} = \sum_{j=1}^{k} z_j \overline{z}_j \ , \tag{24}$$

with $z_j = \frac{x_j - \imath p_j}{\sqrt{2}}$, $j = 1, \ldots, k$. The measure $d\Omega$ is the normalized Liouville measure on the energy surface $G = 1$ (i.e., $d\Omega$ is the normalized measure obtained by restriction of the volume form on $\mathbb{R}^{2k}$ associated to the symplectic 2-form $\sum_{j=1}^{k} dp_j \wedge dx_j$). Note that the Hamiltonian flow determined by G in terms of the variable $\mathbf{z}$ is just motion on a circle of radius equal to the magnitude of the initial condition. Namely, if $\boldsymbol{\eta}$ is the initial condition, then the solution to the Hamilton equations related to G at time t is $\mathbf{z}(t) = \exp(\imath t)\boldsymbol{\eta}$.

Remark 2. *Since the states $\Psi^{(\hbar)}_{\mathbf{z},s}$ provide a resolution of the identity for the space $V^{(\hbar)}_s$, then we will refer to the them as coherent states. Proposition* (5) *below indicates that, for given $\mathbf{z} \neq 0$, $\hbar = 1/N$ and N large, the state $\Psi^{(\hbar)}_{\mathbf{z},s}$ concentrates on the classical orbit $\exp(\imath t)\mathbf{z}$ but not at a particular point (which is the case for $\Psi_{\mathbf{z},\hbar}$). Thus maybe the states $\Psi^{(\hbar)}_{\mathbf{z},s}$ should be called orbit states. However we will keep the name "coherent states" because similar states for the n-sphere and hydrogen atom problem have been studied before and called coherent states in the literature.*

It will be useful to note that the projections $\Pi^{(\hbar)}_s$ and $\Pi_s \equiv \Pi^{(1)}_s$ are related by dilation operators:

$$\Pi_s = D_{\hbar^{1/2}}\, \Pi^{(\hbar)}_s\, D_{\hbar^{-1/2}} \ , \tag{25}$$

with the unitary dilation operators defined for $r > 0$ in the following way

$$D_r\Psi(\mathbf{x}) = r^{k/2}\Psi(r\mathbf{x}), \quad \Psi \in L^2(\mathbb{R}^k) \ , \tag{26}$$

with the property $(D_r)^{-1} = D_{r^{-1}}$. Equation (25) can be obtained from the equality $D_{\hbar^{1/2}}\, A_\hbar\, D_{\hbar^{-1/2}} = \hbar A$.

3.2. A limiting eigenvalue distribution theorem for perturbations of the harmonic oscillator

Let $N \in \mathbb{N}$ and let us consider the Planck's parameter $\hbar$ taking only discrete values $\hbar = 1/N$. Then consider the family of Schrödinger operators $\{A_{1/N}\}_{N\in\mathbb{N}}$ (see Eq. (19) for the definition of the operator $A_\hbar$). Since, for each $N \in \mathbb{N}$, the spectrum of the operator $A_{1/N}$ is the set $S(A_{1/N}) = \{\frac{1}{N}s \mid s = 0, 1, \ldots\}$ then we find that, for each $N \in \mathbb{N}$, the real number $E = 1$ is an eigenvalue of $A_{1/N}$ with multiplicity $d_N = \frac{(N+k-1)!}{N!(k-1)!}$ (see Eq. (20)). Moreover, since the distance between $E = 1$ and the rest of the spectrum of $S(A_{1/N})$ is $O(1/N)$ then, by introducing a perturbation of size $O(\hbar^{1+\delta})$ with $\delta > 0$, we can create a cluster of eigenvalues around $E = 1$. Namely, for N sufficiently large, the unperturbed eigenvalue $E = 1$ splits into a cluster of d_N eigenvalues (stability property) in an interval of size equal to the

operator norm of the perturbation (we are listing each one of those new eigenvalues in the cluster as many times as its multiplicity). We want to establish a theorem on the distribution of eigenvalues in those clusters in the semiclassical limit $N \to \infty$.

The stability property mentioned above consisting in the equality between the original multiplicity d_N of the eigenvalue $E = 1$ and the multiplicity associated with the cluster of eigenvalues around $E = 1$ is a consequence of the estimate in Eq. (39). Such an estimate shows that the norm of the difference between two related orthogonal projections is $O(\hbar^\delta)$ which in particular is smaller than one for $\hbar$ sufficiently small. Therefore the dimension of the range of both projectors must be the same (see reference [17]).

Thus we are led to consider the following family of Schrödinger operators ($\hbar = 1/N$):

$$H_\hbar \equiv A_\hbar + \epsilon(\hbar) Q_\hbar \, , \tag{27}$$

with $0 < \epsilon(\hbar) = O(\hbar^{1+\delta})$, $\delta > 0$ and $Q_\hbar$ a selfadjoint and $\hbar$-admissible pseudo-differential operator of order zero acting on the Hilbert space $L^2(\mathbb{R}^k)$ and with operator norm uniformly bounded with respect to $\hbar$. Namely, $Q_\hbar$ satisfies the following conditions (see reference [19] for details):

a: Let us consider a function $a : \mathbb{R}^{2k} \times (0, \hbar_0] \to \mathbb{R}$ for some $\hbar_0 > 0$ fixed. We say that a belongs to the space of symbols $S_{2k}(1)$ iff $a = a(\mathbf{z}; \hbar)$ is a smooth function of the variable $\mathbf{z} \in \mathbb{R}^{2k}$ and for any multi-index $\alpha \in (\mathbb{N}^*)^{2k}$ we have

$$\partial_{\mathbf{z}}^\alpha a(\mathbf{z}; \hbar) = O(1) \tag{28}$$

uniformly with respect to $(\mathbf{z}; \hbar) \in \mathbb{R}^{2k} \times (0, \hbar_0]$.

b: The action of $Q_\hbar$ on a function $\Psi \in L^2(\mathbb{R}^k)$ is (formally) given by

$$Q_\hbar \Psi(\mathbf{x}) = \frac{1}{(2\pi\hbar)^k} \int_{\mathbb{R}^{2k}} \exp\left(\imath \, (\mathbf{x} - \mathbf{y}) \cdot \boldsymbol{\xi}/\hbar\right) a\left(\frac{\mathbf{x} + \mathbf{y}}{2}, \boldsymbol{\xi}; \hbar\right) \Psi(\mathbf{y}) d\mathbf{y} d\boldsymbol{\xi} \, . \tag{29}$$

The oscillatory integral in Eq. (29) can be understood in a rigorous manner by introducing an operator inside the integral and obtained by performing a sufficient number of integration by parts. Under the condition in Eq. (28), the operator $Q_\hbar$ must be a bounded operator with operator norm uniformly bounded with respect to $\hbar$ (see the theorem by Calderón-Villancourt in reference [19]).

c: The symbol a is a classical symbol, i.e., a has the following asymptotic expression:

$$a(\mathbf{x}, \boldsymbol{\xi}) \sim \sum_{j=0} \hbar^j a_j(\mathbf{x}, \boldsymbol{\xi}) \, , \tag{30}$$

with $a_j \in S_{2k}(1)$ independent of $\hbar$ and a_0 not identically zero. The function a_0 will be called the principal symbol of the operator $Q_\hbar$ and denoted by $\sigma(Q_\hbar)$.

Let us denote by $\eta_{N,m}$, with $m = 1, \ldots, d_N$, the eigenvalues of the operator $H_{1/N}$ inside the cluster around the eigenvalue $E = 1$.

Theorem 3. *Let f be a continuous function on the real line and assume that $Q_\hbar$ is a selfadjoint and $\hbar$-admissible pseudo-differential operator of order zero as above. Then*

$$\lim_{N\to\infty} \frac{1}{d_N} \sum_{m=1}^{d_N} f\left(\frac{\eta_{N,m}-1}{\epsilon(\hbar)}\right) = \int_{\Sigma_1} f\left(\frac{1}{2\pi}\int_0^{2\pi} \sigma(Q_\hbar)\left(\mathbf{x}(t;\mathbf{z}),\mathbf{p}(t;\mathbf{z})\right) dt\right) d\Omega(\mathbf{z}) \ , \tag{31}$$

where $(\mathbf{x}(t;\mathbf{z}),\mathbf{p}(t;\mathbf{z}))$ is the solution of the Hamilton equations associated to the classical harmonic oscillator Hamiltonian G defined above (see Eq. (24)) with initial condition $(\mathbf{x}_0(\mathbf{z}),\mathbf{p}_0(\mathbf{z})) \equiv (\sqrt{2}\Re(\mathbf{z}), -\sqrt{2}\Im(\mathbf{z}))$, i.e.,

$$(\mathbf{x}(t;\mathbf{z}),\mathbf{p}(t;\mathbf{z})) = \phi_G^t(\mathbf{x}_0(\mathbf{z}),\mathbf{p}_0(\mathbf{z})), \tag{32}$$

with ϕ_G^t the Hamiltonian flow associated to G at time t.

Note that the average of the principal symbol $\sigma(Q_\hbar)$ along the classical orbit $(\mathbf{x}(t;\mathbf{z}),\mathbf{p}(t;\mathbf{z}))$ does not change if we consider a different initial point in the same orbit (determined by a different element $\mathbf{z}\in\Sigma_1$). Thus we introduce the manifold of oriented orbits $\mathcal{O}\equiv\Sigma_1/S^1$ where S^1 denotes the group of rotations on a plane $SO(2)$ acting on Σ_1 according to the 2π periodic flow ϕ_G^t. The manifold $\mathcal{O}$ has a natural measure dm which is the push-forward measure of $d\Omega$ under the projection map $\mathcal{P}:\Sigma_1\to\mathcal{O}$ ($\mathcal{P}$ assigns to a given $\mathbf{z}\in\Sigma_1$ the orbit $\gamma=\{\exp(it)\mathbf{z} \mid t\in\mathbb{R}\}\simeq\{(\mathbf{x}(t;\mathbf{z}),\mathbf{p}(t;\mathbf{z})) \mid t\in\mathbb{R}\}$). Given a function $\sigma:\Sigma_1\to\mathbb{R}$, we define the averaged function $\langle\sigma\rangle:\mathcal{O}\to\mathbb{R}$ as follows

$$\langle\sigma\rangle(\gamma) = \frac{1}{2\pi}\int_0^{2\pi}\sigma(\gamma(t))dt \ . \tag{33}$$

The function $\langle\sigma\rangle$ can be thought of as a kind of a Radon transform of the function σ.

There is another important measure related to the right-hand side of Eq. (31). Namely, let $dm_{\sigma(Q_\hbar)}$ be the push-forward measure of dm under the map $\langle\sigma(Q_\hbar)\rangle$.

Thus the right-hand side of Eq. (31) can be re-written as:

$$\begin{aligned}\int_{\Sigma_1} f\left(\frac{1}{2\pi}\int_0^{2\pi}\sigma(Q_\hbar)\left(\mathbf{x}(t;\mathbf{z}),\mathbf{p}(t;\mathbf{z})\right)dt\right)d\Omega(\mathbf{z}) &= \int_{\mathcal{O}} f\left(\ \langle\sigma(Q_\hbar)\rangle(\gamma)\ \right)dm(\gamma)\\ &= \int_{\mathbb{R}} f(\lambda)dm_{\sigma(Q_\hbar)}(\lambda) \ . \end{aligned} \tag{34}$$

Theorem 3 can be equivalently stated in terms of perturbations of a fixed operator $A\equiv A_1 = -\frac{1}{2}\Delta_{\mathbb{R}^k}+\frac{1}{2}\mathbf{x}^2-\frac{k}{2}$ associated to the harmonic oscillator (independent of $\hbar$). To do that we make use of the dilation operators introduced in Eq. (26). First notice that

$$H_\hbar = \hbar D_{\hbar^{-1/2}}\left(A+\frac{\epsilon(\hbar)}{\hbar}D_{\hbar^{1/2}}Q_\hbar D_{\hbar^{-1/2}}\right)D_{\hbar^{1/2}} \ . \tag{35}$$

Thus, for each value of $\hbar$, the spectrum of the operator

$$F_\hbar \equiv A + \frac{\epsilon(\hbar)}{\hbar} D_{\hbar^{1/2}} Q_\hbar D_{\hbar^{-1/2}} \tag{36}$$

is equal to the spectrum of $H_\hbar$ scaled by the factor $1/\hbar$.

The spectrum of the operator A is the set of non-negative integer numbers. Since the operator norm $\|\frac{\epsilon(\hbar)}{\hbar} D_{\hbar^{1/2}} Q_\hbar D_{\hbar^{-1/2}}\|$ is $O(\hbar^\delta)$, then for $N \in \mathbb{N}$ given and sufficiently large, with $\hbar = 1/N$, there is a well-defined cluster of eigenvalues around the eigenvalue $\tilde{E}_N = N$ of the operator A. Let us denote by $\gamma_{N,m}$ $m = 1, \ldots, d_N$ the eigenvalues of $F_\hbar$ in such a cluster. Then we have:

Theorem 4. *Let f be a continuous function on the real line and assume that $Q_\hbar$ is a selfadjoint and $\hbar$-admissible pseudo-differential operator of order zero as above. Then*

$$\lim_{N\to\infty} \frac{1}{d_N} \sum_{m=1}^{d_N} f\left(\frac{\gamma_{N,m} - N}{\hbar^\delta}\right) = \int_{\Sigma_1} f\left(\frac{1}{2\pi}\int_0^{2\pi} \sigma(Q_\hbar)\left(\mathbf{x}(t;\mathbf{z}), \mathbf{p}(t;\mathbf{z})\right) dt\right) d\Omega(\mathbf{z}) \tag{37}$$

where $(\mathbf{x}(t;\mathbf{z}), \mathbf{p}(t;\mathbf{z}))$ is defined as in Theorem 3.

Notice that in Theorem (3) we are studying clusters of eigenvalues around a fixed point $E = 1$ whereas in Theorem (4) the clusters are around points $(\tilde{E}_N = N)$ moving towards infinity.

Proof. Since both $\left|\frac{\gamma_{N,m}-N}{\hbar^\delta}\right|$ and the size of the orbit $(\mathbf{x}(t;\mathbf{z}), \mathbf{p}(t;\mathbf{z}))$ are $O(1)$ then we only need to prove Theorem 4 for the restriction of the function f to a compact set From the Stone-Weierstrass approximation theorem, we see in turn that it is enough to prove Eq. (37) for a monomial $f(x) = x^q$ with q a non-negative integer.

The proof is based on two main steps: (1) Approximation of the sum appearing on the left-hand side of Eq. (37) by the trace of $(\Pi_N D_{\hbar^{1/2}} Q_\hbar D_{\hbar^{-1/2}} \Pi_N)^q$ where, as above, Π_N is the projector of the operator A associated to the eigenvalue N. Note that the range of Π_N is d_N dimensional. (2) To prove a Szegö type theorem showing that the limit $N \to \infty$ of the trace mentioned in step (1) is equal to the right-hand side of Eq. (37).

3.3. Step (1). The norm of the difference of orthogonal projections

Let P_N be the orthogonal projector of the operator $F_{1/N}$ associated to the cluster of eigenvalues $\gamma_{N,m}$ $m = 1, \ldots, d_N$ around the unperturbed eigenvalue N.

First, let us estimate the operator norm of the difference $P_N - \Pi_N$ by using the integral representation of those projectors in terms of the corresponding resolvent operators. Let $\mathcal{C}$ be a circle of radius smaller than $1/2$ and center N. Then we have

$$\Pi_N = \frac{1}{2\pi\imath}\int_{\xi\in\mathcal{C}} (\xi - A)^{-1}\, d\xi, \quad P_N = \frac{1}{2\pi\imath}\int_{\xi\in\mathcal{C}} \left(\xi - F_{1/N}\right)^{-1} d\xi. \tag{38}$$

Since $\|\frac{\epsilon(\hbar)}{\hbar} D_{\hbar^{1/2}} Q_\hbar D_{\hbar^{-1/2}}\|$ is $O(\hbar^\delta)$ then we can show by using the second resolvent identity (see [13]) that

$$\|P_N - \Pi_N\| = O(\hbar^\delta)\ , \tag{39}$$

where we have used the fact that the operator norm of the resolvents $(\xi - A)^{-1}$ and $\left(\xi - F_{1/N}\right)^{-1}$ are equal to the inverse of the distances between ξ and the spectrum of A and $F_{1/N}$ respectively (which in both cases is $O(1)$). Note that Eq. (39) implies in particular that, for N sufficiently large, $\|P_N - \Pi_N\| < 1$. Hence the dimensions of the ranges of the orthogonal projections P_N and Π_N must be the same (see [17]).

Next, let us write the sum appearing on the left-hand side of Eq. (37) as a trace:

$$\frac{1}{d_N} \sum_{m=1}^{d_N} \left(\frac{\gamma_{N,m} - N}{\hbar^\delta} \right)^q = \frac{1}{d_N} \operatorname{tr} \left(P_N \left(\frac{F_{1/N} - N}{\hbar^\delta} \right) P_N \right)^q\ . \tag{40}$$

Thus we have using the estimate in Eq. (39)

$$P_N \left(\frac{F_{1/N} - N}{\hbar^\delta} \right) P_N = \Pi_N \left(\frac{F_{1/N} - N}{\hbar^\delta} \right) P_N + O(\hbar^\delta) \tag{41}$$

$$= \Pi_N D_{\hbar^{1/2}} Q_\hbar D_{\hbar^{-1/2}} P_N + O(\hbar^\delta) \tag{42}$$

$$= \Pi_N D_{\hbar^{1/2}} Q_\hbar D_{\hbar^{-1/2}} \Pi_N + O(\hbar^\delta)\ , \tag{43}$$

where we have used $\left(\frac{F_{1/N} - N}{\hbar^\delta}\right) P_N = O(1)$ for the first equality in Eq. (41), and $\Pi_N (A - N) P_N = 0$ for the second one in Eq. (42) (note that for all $\Psi, \Phi \in L^2(\mathbb{R}^k)$ we have $\langle \Pi_N (A - N) P_N \Psi, \Phi \rangle_{L^2(\mathbb{R}^k)} = \langle P_N \Psi, (A - N) \Pi_N \Phi \rangle_{L^2(\mathbb{R}^k)} = 0$).

Using Eq. (43), we obtain:

$$\left(P_N \left(\frac{F_{1/N} - N}{\hbar^\delta} \right) P_N \right)^q = P_N \left(\Pi_N D_{\hbar^{1/2}} Q_\hbar D_{\hbar^{-1/2}} \Pi_N \right)^q + P_N O(\hbar^\delta) \tag{44}$$

$$= \left(\Pi_N D_{\hbar^{1/2}} Q_\hbar D_{\hbar^{-1/2}} \Pi_N \right)^q + P_N O(\hbar^\delta)$$
$$+ (P_N - \Pi_N) \left(\Pi_N D_{\hbar^{1/2}} Q_\hbar D_{\hbar^{-1/2}} \Pi_N \right)^q\ .$$

By considering an orthonormal basis for the range of Π_N and extending it to a basis for the whole Hilbert space $L^2(\mathbb{R}^k)$, we can show using Eq. (39) and the fact $\| \left(\Pi_N D_{\hbar^{1/2}} Q_\hbar D_{\hbar^{-1/2}} \Pi_N \right)^q \| = O(1)$ that

$$\frac{1}{d_N} \operatorname{tr} \left((P_N - \Pi_N) \left(\Pi_N D_{\hbar^{1/2}} Q_\hbar D_{\hbar^{-1/2}} \Pi_N \right)^q \right) = O(\hbar^\delta)\ . \tag{45}$$

In a similar way, considering a basis for the range of P_N we can show:

$$\frac{1}{d_N} \operatorname{tr} \left(P_N O(\hbar^\delta) \right) = O(\hbar^\delta)\ . \tag{46}$$

Hence the left-hand side of Eq. (40) can be estimated by:

$$\frac{1}{d_N}\sum_{m=1}^{d_N}\left(\frac{\gamma_{N,m}-N}{\hbar^{\delta}}\right)^q=\frac{1}{d_N}\operatorname{tr}\left(\Pi_N D_{\hbar^{1/2}}Q_\hbar D_{\hbar^{-1/2}}\Pi_N\right)^q+O(\hbar^{\delta})\,. \tag{47}$$

3.4. Step (2). A Szegö type theorem for the harmonic oscillator

We want to show that the limit $N\to\infty$ of the right-hand side of Eq. (47) is the right-hand side of Eq. (37). To do that, we first note that by using Eq. (25):

$$\begin{aligned}\frac{1}{d_N}\operatorname{tr}\left(\Pi_N D_{\hbar^{1/2}}Q_\hbar D_{\hbar^{-1/2}}\Pi_N\right)&=\frac{1}{d_N}\operatorname{tr}\left(D_{\hbar^{-1/2}}\Pi_N D_{\hbar^{1/2}}Q_\hbar D_{\hbar^{-1/2}}\Pi_N D_{\hbar^{1/2}}\right)\\&=\frac{1}{d_N}\operatorname{tr}\left(\Pi_N^{(\hbar)}Q_\hbar\Pi_N^{(\hbar)}\right)\,.\end{aligned} \tag{48}$$

Then using the expression for the projector $\Pi_N^{(\hbar)}$ given in Eq. (23) we obtain

$$\frac{1}{d_N}\operatorname{tr}\left(\Pi_N D_{\hbar^{1/2}}Q_\hbar D_{\hbar^{-1/2}}\Pi_N\right)=\int_{\Sigma_1}\left\langle\Psi_{\mathbf{z},N}^{(\hbar)},Q_\hbar\Psi_{\mathbf{z},N}^{(\hbar)}\right\rangle_{L^2(\mathbb{R}^k)}d\Omega(\mathbf{z})\,. \tag{49}$$

We now estimate the expected value of the operator $Q_\hbar$ between the states $\Psi_{\mathbf{z},N}^{(\hbar)}$ by using the Bargmann transform $\mathbf{B}_k^{(\hbar)}$ and the stationary phase method.

Proposition 5. *Let $Q_\hbar$ be a selfadjoint and $\hbar$-admissible pseudo-differential operator of order zero as above. Then for $\hbar=1/N$:*

$$\left\langle\Psi_{\mathbf{z},N}^{(\hbar)},Q_\hbar\Psi_{\mathbf{z},N}^{(\hbar)}\right\rangle_{L^2(\mathbb{R}^k)}=\frac{1}{2\pi}\int_0^{2\pi}\sigma(Q_\hbar)\left(\mathbf{x}(t;\mathbf{z}),\mathbf{p}(t;\mathbf{z})\right)dt+O(\hbar)\,, \tag{50}$$

uniformly for $\mathbf{z}\in\Sigma_1$.

Proof. We will make use of oscillatory integrals in order to deal with the pseudo-differential operator $Q_\hbar$. We will do that in a non-rigorous manner (dealing with non absolutely convergent integrals) in order not to give a too long proof. It is possible to provide a rigorous proof by following reference [19] and using suitable powers of an operator obtained by doing integration by parts.

First we go to the Bargmann space:

$$\left\langle\Psi_{\mathbf{z},N}^{(\hbar)},Q_\hbar\Psi_{\mathbf{z},N}^{(\hbar)}\right\rangle_{L^2(\mathbb{R}^k)}=\left\langle\Phi_{\mathbf{z},N}^{(\hbar)},\mathbf{B}_k^{(\hbar)}Q_\hbar(\mathbf{B}_k^{(\hbar)})^{-1}\Phi_{\mathbf{z},N}^{(\hbar)}\right\rangle_{\mathcal{B}_k^{(\hbar)}}\,, \tag{51}$$

where the states $\Phi_{\mathbf{z},N}^{(\hbar)}$ are defined in Eq. (10).

Using the following formal expressions for the operators $Q_\hbar$ in Eq. (29) and $(\mathbf{B}_k^{(\hbar)})^{-1}$ given by:

$$(\mathbf{B}_k^{(\hbar)})^{-1}F(\mathbf{y})=\frac{1}{(\pi\hbar)^{k/4}}\int_{\boldsymbol{\eta}\in\mathbb{C}^k}\exp\left(-\frac{1}{2\hbar}[\overline{\boldsymbol{\eta}^2}+\mathbf{y}^2-2\sqrt{2}\overline{\boldsymbol{\eta}}\cdot\mathbf{y}]\right)F(\boldsymbol{\eta})d\nu_k^{\hbar}(\boldsymbol{\eta})\,,$$

we obtain for $|\mathbf{z}| = 1$:

$$\left\langle \Psi_{\mathbf{z},N}^{(\hbar)}, Q_\hbar \Psi_{\mathbf{z},N}^{(\hbar)} \right\rangle_{L^2(\mathbb{R}^k)} = \frac{1}{2^k(\pi\hbar)^{7k/2}\hbar^N N!} \int \exp(\frac{\imath}{\hbar} f(\mathbf{x},\mathbf{y},\boldsymbol{\xi},\mathbf{w},\boldsymbol{\eta}))\,(\mathbf{w}\cdot\mathbf{z})^N \cdot \overline{(\boldsymbol{\eta}\cdot\mathbf{z})}^N a\left(\frac{\mathbf{x}+\mathbf{y}}{2},\boldsymbol{\xi};\hbar\right) d\mathbf{x}d\mathbf{y}d\boldsymbol{\xi}d\mathbf{w}d\boldsymbol{\eta}\,, \tag{52}$$

where

$$f(\mathbf{x},\mathbf{y},\boldsymbol{\xi},\mathbf{w},\boldsymbol{\eta}) = \imath\left(\frac{1}{2}\left[\overline{\mathbf{w}}^2 + \mathbf{x}^2 - 2\sqrt{2}\overline{\mathbf{w}}\cdot\mathbf{x}\right] + \frac{1}{2}\left[\boldsymbol{\eta}^2 + \mathbf{y}^2 - 2\sqrt{2}\boldsymbol{\eta}\cdot\mathbf{y}\right] + \imath\,(\mathbf{x}-\mathbf{y})\cdot\boldsymbol{\xi} + |\mathbf{w}|^2 + |\boldsymbol{\eta}|^2\right). \tag{53}$$

Given $\mathbf{z} \in \mathbb{C}^k$, with $|\mathbf{z}| = 1$, let us consider an orthonormal basis for $\mathbb{C}^k$ given by $\{\mathbf{z}, \mathbf{e}_2, \ldots, \mathbf{e}_k\}$. We will write an arbitrary element $\mathbf{w} \in \mathbb{C}^k$ as $\mathbf{w} = re^{\imath\theta}\mathbf{z} + \mathbf{w}_\perp$ with $\mathbf{w}_\perp = (A_2 + \imath B_2)\mathbf{e}_2 + \cdots + (A_k + \imath B_k)\mathbf{e}_k$ and consider r, θ, $A_2, \ldots, A_k$, $B_2, \ldots, B_k$ as real coordinates for $\mathbb{C}^k$. Thus, in particular, we have for $r > 0$ that

$$\Phi_{\mathbf{z},N}^{(\hbar)}(\mathbf{w}) = \frac{e^{N(\ln(r)+\imath\theta)}}{\hbar^{N/2}\sqrt{N!}}\,. \tag{54}$$

Considering $\hbar = 1/N$ and similar coordinates for $\boldsymbol{\eta} = \rho e^{\imath\alpha} + \boldsymbol{\eta}_\perp$ with $\boldsymbol{\eta}_\perp = (C_2+\imath D_2)\mathbf{e}_2+\cdots+(C_k+\imath D_k)\mathbf{e}_k$, we can evaluate the integral appearing in Eq. (52) by using the stationary phase method (see [15]) with respect to all of the variables involved in that integral but θ. Note that for $\theta \in [0, 2\pi)$ given, the function

$$g = f(\mathbf{x},\mathbf{y},\boldsymbol{\xi},\mathbf{w},\boldsymbol{\eta}) - \imath\,(\ln(r) + \imath\theta + \ln(\rho) - \imath\alpha) \tag{55}$$

has a non-degenerate critical point (denoted by X_0) with coordinates

$$\mathbf{x} = \mathbf{y} = \frac{e^{\imath\theta}\mathbf{z} + e^{-\imath\theta}\overline{\mathbf{z}}}{\sqrt{2}},\ \boldsymbol{\xi} = \frac{\imath\left(e^{\imath\theta}\mathbf{z} - e^{-\imath\theta}\overline{\mathbf{z}}\right)}{\sqrt{2}},\ \mathbf{w} = e^{\imath\theta}\mathbf{z},\ \boldsymbol{\eta} = e^{\imath\theta}\mathbf{z}\,. \tag{56}$$

Moreover,

$$\begin{aligned}\Im(g) &= -\ln|\mathbf{w}\cdot\mathbf{z}| - \ln|\boldsymbol{\eta}\cdot\mathbf{z}| + \frac{|\mathbf{x}-\sqrt{2}\Re(\mathbf{w})|^2}{2} + \frac{|\mathbf{y}-\sqrt{2}\Re(\boldsymbol{\eta})|^2}{2} + \frac{|\mathbf{w}|^2}{2} + \frac{|\boldsymbol{\eta}|^2}{2} \\ &\geq -\ln|\mathbf{w}| - \ln|\boldsymbol{\eta}| + \frac{|\mathbf{w}|^2}{2} + \frac{|\boldsymbol{\eta}|^2}{2} \geq 0\,.\end{aligned} \tag{57}$$

Since $g(X_0) = \imath$ and the determinant of the $(7k-1)\times(7k-1)$ Hessian matrix of g evaluated at the critical point is equal to $\det(g''(X_0)) = (\imath)^{7k-1}2^{5k}$ then we obtain:

$$\left\langle \Psi_{\mathbf{z},N}^{(\hbar)}, Q_\hbar \Psi_{\mathbf{z},N}^{(\hbar)} \right\rangle_{L^2(\mathbb{R}^k)} = \frac{\exp\left(\frac{\imath}{\hbar}g(X_0)\right)}{2^k(\pi\hbar)^{7k/2}\hbar^N N!}\left(\int_0^{2\pi}\left[\det\left(\frac{g''(X_0)}{2\pi\imath\hbar}\right)\right]^{-1/2} \cdot\sigma(Q_\hbar)\left(\frac{e^{\imath\theta}\mathbf{z} + e^{-\imath\theta}\overline{\mathbf{z}}}{\sqrt{2}}, \frac{\imath\left(e^{\imath\theta}\mathbf{z} - e^{-\imath\theta}\overline{\mathbf{z}}\right)}{\sqrt{2}}\right) d\theta + O\left(\hbar^{\frac{7k+1}{2}}\right)\right)\,. \tag{58}$$

Finally, using Stirling's formula $N! = \sqrt{2\pi N} N^N \exp(-N)(1 + O(1/N))$, we conclude Eq. (50). Note that the error term in Eq. (50) is equal to the difference between two continuous functions on the variable $\mathbf{z}$ with $|\mathbf{z}| = 1$. Therefore that error term can be bounded by $C\hbar$ with C independent of $\mathbf{z}$. □

We are now able to establish the following lemma using Proposition 5 and Eq. (49):

Lemma 6. *Let $Q_\hbar$ be a selfadjoint and $\hbar$-admissible pseudo-differential operator of order zero as above. Then*

$$\frac{1}{d_N} \operatorname{tr} \left(\Pi_N D_{\hbar^{1/2}} Q_\hbar D_{\hbar^{-1/2}} \Pi_N\right) = \int_{\Sigma_1} \frac{1}{2\pi} \int_0^{2\pi} \sigma(Q_\hbar)\left(\mathbf{x}(t;\mathbf{z}), \mathbf{p}(t;\mathbf{z})\right) dt d\Omega(\mathbf{z}) + O(\hbar). \tag{59}$$

3.5. The averaging method

We now introduce the averaging method in order to find an operator $\tilde{Q_\hbar}$ that commutes with $A_\hbar$ and whose projection onto the range of $\Pi_N^{(\hbar)}$ coincides with the ones for $Q_\hbar$. These properties of the operator $\tilde{Q_\hbar}$ will reduce the study of the first term in the right-hand side of Eq. (47) to the use of Lemma 6. Thus on base of the mentioned properties of the operator $\tilde{Q_\hbar}$ we will be able to establish the following

Theorem 7. A Szegö type theorem for the harmonic oscillator. *Let $Q_\hbar$ be a self-adjoint and $\hbar$-admissible pseudo-differential operator of order zero as above. Let f be a continuous function on the real line. Then*

$$\lim_{N\to\infty} \frac{1}{d_N} tr f \left(\Pi_N D_{\hbar^{1/2}} Q_\hbar D_{\hbar^{-1/2}} \Pi_N\right) = \int_{\Sigma_1} f\left(\frac{1}{2\pi} \int_0^{2\pi} \sigma(Q_\hbar)\left(\mathbf{x}(t;\mathbf{z}), \mathbf{p}(t;\mathbf{z})\right) dt\right) d\Omega(\mathbf{z}) \,. \tag{60}$$

Proof. It is enough to show the proof when f is a monomial $f(x) = x^q$.

Following A. Weinstein [28] we introduce the operator given by the averaging of $Q_\hbar$ under the dynamics determined by the harmonic oscillator operator $A_\hbar$:

$$\tilde{Q_\hbar} = \frac{1}{2\pi} \int_0^{2\pi} \exp\left(-\frac{\imath t A_\hbar}{\hbar}\right) Q_\hbar \exp\left(\frac{\imath t A_\hbar}{\hbar}\right) dt \,. \tag{61}$$

Since the spectrum of the operator $\frac{1}{\hbar} A_\hbar$ is the set of non-negative integer numbers, then the operators $\exp\left(\pm\frac{\imath t A_\hbar}{\hbar}\right)$ are 2π-periodic and, in particular, $\exp\left(\pm\frac{\imath 2\pi A_\hbar}{\hbar}\right)$ are equal to the identity operator. Thus it can be easily shown that $\tilde{Q_\hbar}$ commutes with $A_\hbar$:

$$\left[\tilde{Q_\hbar}, A_\hbar\right] \equiv \tilde{Q_\hbar} A_\hbar - A_\hbar \tilde{Q_\hbar} = -\imath\hbar \int_0^{2\pi} \frac{d}{dt}\left[\exp\left(-\frac{\imath t A_\hbar}{\hbar}\right) Q_\hbar \exp\left(\frac{\imath t A_\hbar}{\hbar}\right)\right] dt = 0 \,. \tag{62}$$

Moreover, since $\exp\left(\pm\frac{\imath t A_\hbar}{\hbar}\right)\Pi_N^{(\hbar)} = \exp(\pm\imath t N)\Pi_N^{(\hbar)}$, we also have

$$\Pi_N^{(\hbar)}\tilde{Q}_\hbar\Pi_N^{(\hbar)} = \Pi_N^{(\hbar)}Q_\hbar\Pi_N^{(\hbar)} \ . \tag{63}$$

From Eqs. (25), (62) and (63) we obtain

$$\begin{aligned}\frac{1}{d_N}\operatorname{tr}\left(\Pi_N D_{\hbar^{1/2}}Q_\hbar D_{\hbar^{-1/2}}\Pi_N\right)^q &= \frac{1}{d_N}\operatorname{tr}\left(\Pi_N^{(\hbar)}Q_\hbar\Pi_N^{(\hbar)}\right)^q = \frac{1}{d_N}\operatorname{tr}\left(\Pi_N^{(\hbar)}\tilde{Q}_\hbar\Pi_N^{(\hbar)}\right)^q \\ &= \frac{1}{d_N}\operatorname{tr}\left(\Pi_N^{(\hbar)}{\tilde{Q}_\hbar}^q\Pi_N^{(\hbar)}\right) \ . \end{aligned} \tag{64}$$

Applying Lemma 6 to the pseudo-differential operator ${\tilde{Q}_\hbar}^q$, whose principal symbol is denoted by $\sigma({\tilde{Q}_\hbar}^q)$, we obtain from Eq. (64):

$$\begin{aligned}&\frac{1}{d_N}\operatorname{tr}\left(\Pi_N D_{\hbar^{1/2}}Q_\hbar D_{\hbar^{-1/2}}\Pi_N\right)^q \\ &\quad= \int_{\Sigma_1}\frac{1}{2\pi}\int_0^{2\pi}\left(\frac{1}{2\pi}\int_0^{2\pi}\sigma(Q_\hbar)\circ\phi_G^{s+t}(\mathbf{x}_0(\mathbf{z}),\mathbf{p}_0(\mathbf{z}))ds\right)^q dt d\Omega(\mathbf{z}) + O(\hbar) \\ &\quad= \int_{\Sigma_1}\left(\frac{1}{2\pi}\int_0^{2\pi}\sigma(Q_\hbar)\circ\phi_G^{s}(\mathbf{x}_0(\mathbf{z}),\mathbf{p}_0(\mathbf{z}))ds\right)^q d\Omega(\mathbf{z}) + O(\hbar) \ , \end{aligned} \tag{65}$$

where we have used the 2π-periodicity of the flow ϕ_G^t and that the principal symbol $\sigma({\tilde{Q}_\hbar}^q)$ evaluated at $(\mathbf{x},\mathbf{p}) \in T^*\mathbb{R}^k$ is given by

$$\begin{aligned}\sigma({\tilde{Q}_\hbar}^q)(\mathbf{x},\mathbf{p}) &= \left(\sigma(\tilde{Q}_\hbar)(\mathbf{x},\mathbf{p})\right)^q \\ &= \left(\frac{1}{2\pi}\int_0^{2\pi}\sigma\left(\exp\left(-\frac{\imath s A_\hbar}{\hbar}\right)Q_\hbar\exp\left(\frac{\imath s A_\hbar}{\hbar}\right)\right)(\mathbf{x},\mathbf{p})ds\right)^q \\ &= \left(\frac{1}{2\pi}\int_0^{2\pi}\sigma(Q_\hbar)\circ\phi_G^s(\mathbf{x},\mathbf{p})ds\right)^q \ . \end{aligned} \tag{66}$$

Note that we have used Egorov's theorem in the last equality of Eq. (66) and that $\sigma(A_\hbar)(\mathbf{x},\mathbf{p}) = G(\mathbf{x},\mathbf{p})$. Thus from Eqs. (47) and (65) we conclude the proof of Theorem 7 and Theorem 4 as well. □

4. The Laplacian on the n-sphere

In this section we describe a limiting eigenvalue distribution theorem for perturbations of the Laplacian on the n-sphere. As in the case of the k-dimensional harmonic oscillator, we actually describe two equivalent theorems. For such a purpose, we introduce some notation and describe coherent states labelled by elements of a complex manifold which can be identified with the unit cotangent bundle $T_1^*S^n$.

Let S^n be the n-sphere $\{\mathbf{x}\in\mathbb{R}^{n+1} \mid |\mathbf{x}| = 1\}$. Let Δ_{S^n} be the Laplacian on S^n with spectrum the set of eigenvalues $\{\lambda_\ell = \ell(\ell+n-1) \mid \ell\in\mathbb{N}^*\}$. The

multiplicity of λ_ℓ is (see [21]):

$$d_\ell = \frac{(2\ell+n-1)(\ell+n-2)!}{(\ell)!(n-1)!} = \frac{2}{(n-1)!}\ell^{(n-1)} + O(\ell^{(n-2)}). \tag{67}$$

For $\ell \in \mathbb{N}^*$, let $\mathcal{L}_\ell$ denote the vector space of restrictions to S^n of harmonic homogeneous polynomials of order ℓ in $n+1$ real variables (by harmonic we mean that the operator $\Delta_{\mathbb{R}^{n+1}} \equiv \sum_{j=1}^{n+1} \frac{\partial^2}{\partial^2 x_j}$ applied to the polynomial is equal to zero). The space $\mathcal{L}_\ell$ is known as the space of spherical harmonics and is the eigenspace of Δ_{S^n} associated to the eigenvalue λ_ℓ. Let us denote by $\Pi_\ell^S : L^2(S^n) \to \mathcal{L}_\ell$ the corresponding orthogonal projector, where $L^2(S^n)$ denotes the Hilbert space of square integrable functions with respect to the normalized surface measure dS and endowed with the usual inner product

$$\langle \Psi_1, \Psi_2 \rangle_{L^2(S^n)} = \int_{\mathbf{w}\in S^n} \Psi_1(\mathbf{w})\overline{\Psi_2(\mathbf{w})} dS(\mathbf{w}) \, . \tag{68}$$

Thus we have $L^2(S^n) = \bigoplus_{\ell=0}^{\infty} \mathcal{L}_\ell$.

Let us introduce the null quadric

$$Q^n = \{\boldsymbol{\alpha} \in \mathbb{C}^{n+1} \mid \alpha_1^2 + \cdots + \alpha_{n+1}^2 = 0\} \, . \tag{69}$$

Note that $\boldsymbol{\alpha} \in \mathbb{C}^{n+1}$ belongs to Q^n if and only if $|\Re(\boldsymbol{\alpha})| = |\Im(\boldsymbol{\alpha})|$ and $\Re(\boldsymbol{\alpha}) \cdot \Im(\boldsymbol{\alpha}) = 0$. The null quadric with the origin removed $Q^n - \{0\}$ can be identified with the cotangent bundle of the n-sphere with the zero section removed $T^*S^n - \{0\}$ via the following map

$$\begin{aligned} \sigma_n : Q^n - \{0\} &\longrightarrow T^*S^n - \{0\}, \\ \sigma_n(\boldsymbol{\alpha}) &= \left(\frac{\Re(\boldsymbol{\alpha})}{|\Re(\boldsymbol{\alpha})|}, -\Im(\boldsymbol{\alpha}) \right) \, . \end{aligned} \tag{70}$$

Let us denote by

$$\mathcal{A} = \{\boldsymbol{\alpha} \in Q^n \;\mid\; |\Re(\boldsymbol{\alpha})| = |\Im(\boldsymbol{\alpha})| = 1 \} \, . \tag{71}$$

The set $\mathcal{A}$ can be identified with the unit cotangent bundle $T_1^*S^n$ via the map σ_n.

4.1. Coherent states and orthogonal projections onto spaces of spherical harmonics

For $\boldsymbol{\alpha} \in \mathcal{A}$ and $\ell \in N^*$, let us introduce the following state $\Phi_{\boldsymbol{\alpha},\ell} \in L^2(S^n)$:

$$\Phi_{\boldsymbol{\alpha},\ell}(\mathbf{w}) = a(\ell) \left(\boldsymbol{\alpha} \cdot \mathbf{w}\right)^\ell \, , \tag{72}$$

where $a(\ell)$ is a normalization constant chosen such that $\|\Phi_{\boldsymbol{\alpha},\ell}\|_{L^2(S^n)} = 1$. It can be shown that (see Eq. 2.11 in [24])

$$a(\ell) = \left(\frac{\ell}{\pi}\right)^{(n-1)/2} \left(\frac{1}{2\pi} + O(\ell^{-1/2}) \right). \tag{73}$$

The states $\Phi_{\boldsymbol{\alpha},\ell}$ have the following three properties:

(A). For $\boldsymbol{\alpha} \in \mathcal{A}$, the state $\Phi_{\boldsymbol{\alpha},\ell}(\mathbf{w}) \in \mathcal{L}_\ell$ because $(\boldsymbol{\alpha} \cdot \mathbf{x})^\ell$ is a harmonic homogeneous polynomial of order ℓ as a function of $\mathbf{x} \in \mathbb{R}^{n+1}$. Thus $\Phi_{\boldsymbol{\alpha},\ell}$ are eigenstates of Δ_{S^n} with eigenvalue λ_ℓ.

(B). The set $\{\Phi_{\boldsymbol{\alpha},\ell} \mid \boldsymbol{\alpha} \in \mathcal{A}\}$ provides a resolution of the identity for the space $\mathcal{L}_\ell$. Namely, the projector Π_ℓ^S can be written as follows:

$$\Pi_\ell^S \Psi = d_\ell \int_{\boldsymbol{\alpha} \in \mathcal{A}} \langle \Psi, \Phi_{\boldsymbol{\alpha},\ell} \rangle_{L^2(S^n)} \, \Phi_{\boldsymbol{\alpha},\ell} d\mu(\boldsymbol{\alpha}), \quad \Psi \in L^2(S^n), \tag{74}$$

where $d\mu(\boldsymbol{\alpha})$ is the normalized $SO(n+1)$ invariant measure on $\mathcal{A}$. We are denoting by $SO(n+1)$ the group of $(n+1) \times (n+1)$ orthogonal matrices with unit determinant. The group $SO(n+1)$ acts on Q^n (for $R \in SO(n+1)$, we define $R\boldsymbol{\alpha} = R(\Re(\boldsymbol{\alpha})) + \imath R(\Im(\boldsymbol{\alpha}))$).

As a consequence of Eq. (74), given a linear operator $\mathbf{A} : L^2(S^n) \to L^2(S^n)$, we can evaluate the trace of the projection of A on the space $\mathcal{L}_\ell$ using the states $\Phi_{\boldsymbol{\alpha},\ell}$:

$$\operatorname{tr}\left(\Pi_\ell^S \mathbf{A} \Pi_\ell^S\right) = d_\ell \int_{\boldsymbol{\alpha} \in \mathcal{A}} \langle \mathbf{A} \Phi_{\boldsymbol{\alpha},\ell}, \Phi_{\boldsymbol{\alpha},\ell} \rangle_{L^2(S^n)} \, d\mu(\boldsymbol{\alpha}) \, . \tag{75}$$

Equation (74) is a consequence of (i) the fact that the operator on the right-hand side of Eq. (74) commutes with rotations (given $R \in SO(n+1)$, we define $T_R : L^2(S^n) \to L^2(S^n)$ by $T_R \Psi(\mathbf{w}) = \Psi(R^{-1}\mathbf{w})$), (ii) the action of $SO(n+1)$ restricted to $\mathcal{L}_\ell$ is irreducible, and (iii) Schur's lemma. Thus Eqs. (74) and (75) can be established with the integrals on the right-hand side of both equations multiplied by a constant factor. By taking the operator A as the identity operator in Eq. (75), one can check that such a constant factor must be equal to d_ℓ.

(C). Since for $\boldsymbol{\alpha} \in \mathcal{A}$ and $\mathbf{w} \in S^n$ we have

$$|\boldsymbol{\alpha} \cdot \mathbf{w}| = \left((\Re(\boldsymbol{\alpha}) \cdot \mathbf{w})^2 + (\Im(\boldsymbol{\alpha}) \cdot \mathbf{w})^2\right)^{1/2} \leq |\mathbf{w}| = 1 \, , \tag{76}$$

with equality if and only if $\mathbf{w}$ belongs to the great circle on the plane generated by $\Re(\boldsymbol{\alpha})$ and $\Im(\boldsymbol{\alpha})$, then the state $\Phi_{\boldsymbol{\alpha},\ell}$ concentrates on that great circle for ℓ large.

Due to properties (A), (B) and (C), we will refer to the states $\Phi_{\boldsymbol{\alpha},\ell}$ as coherent states (see remark 2 above). Note additionally that the states $\Phi_{\boldsymbol{\alpha},\ell}$ are labelled by elements in the phase space T^*S^n.

4.2. A limiting eigenvalue distribution theorem for perturbations of the Laplacian on the n-sphere

Let us consider the operator

$$A_\hbar = \hbar^2 \Delta_{S^n} + \hbar^2 \left(\frac{n-1}{2}\right)^2$$

with spectrum

$$\left\{ \left(\hbar \left(\ell + \frac{n-1}{2}\right)\right)^2 \mid \ell \in N^* \right\}.$$

Let N be a natural number. Consider $\hbar = \frac{1}{N+\frac{n-1}{2}}$. Then taking $\ell = N$ we can see that $E = 1$ is an eigenvalue of $A_\hbar$ with multiplicity d_N. Since the distance between $E = 1$ and next neighbor eigenvalues is $O(1/N)$, then by introducing a bounded perturbation with operator norm $O(\hbar^{1+\delta})$, $\delta > 0$, we can create well-defined clusters of eigenvalues around $E = 1$ for N sufficiently large. Namely, let us consider the operator

$$H_\hbar = A_\hbar + \epsilon(\hbar)Q_\hbar \, , \tag{77}$$

with $\epsilon(\hbar) = \hbar^{1+\delta}$, $\delta > 0$, and $Q_\hbar$ a selfadjoint and pseudo-differential operator of order zero on the n-sphere. The definition of a pseudo-differential operator on a manifold requires some details that we will omit in this work (see [16]). Roughly speaking, we are requiring the operator $Q_\hbar$, when restricted to a given chart of S^n, to be a pseudo-differential operator on $\mathbb{R}^n$ satisfying conditions (a), (b) and (c) mentioned above (see Eqs. (28), (29) and (30)). Thus the operator norm of $Q_\hbar$ will be uniformly bounded in $\hbar$ as an operator acting on $L^2(S^n)$.

Let us denote by $\eta_{N,m}$, $m = 1, \ldots, d_N$ the eigenvalues of $H_\hbar$ in the cluster around $E = 1$. Let us denote by ϕ_G^s the Hamiltonian flow associated to $G : T^*S^n \to \mathbb{R}$, $G(\mathbf{w}, \boldsymbol{\xi}) = |\boldsymbol{\xi}|$ (where $(\mathbf{w}, \boldsymbol{\xi})$ are local coordinates for $T^*(S^n)$) by endowing T^*S^n with its canonical symplectic form. Thus ϕ_G^s is the geodesic flow on S^n with respect to arc length s when restricted to the unit cotangent bundle $T_1^*S^n$.

We are now ready to state the following limiting eigenvalue distribution theorem:

Theorem 8. *Let f be a continuous function on the real line and assume that $Q_\hbar$ is a selfadjoint and $\hbar$-admissible pseudo-differential operator on S^n of order zero as above. Then*

$$\lim_{N\to\infty} \frac{1}{d_N} \sum_{m=1}^{d_N} f\left(\frac{\eta_{N,m} - 1}{\epsilon(\hbar)}\right) = \int_{\mathcal{A}} f\left(\frac{1}{2\pi}\int_0^{2\pi} \sigma(Q_\hbar)\left(\, \mathbf{w}(s;\boldsymbol{\alpha}), \boldsymbol{\xi}(s;\boldsymbol{\alpha}) \,\right) ds\right) d\mu(\boldsymbol{\alpha}), \tag{78}$$

where $(\, \mathbf{w}(s;\boldsymbol{\alpha}), \boldsymbol{\xi}(s;\boldsymbol{\alpha}) \,)$ denotes the geodesic generated by $\Re(\boldsymbol{\alpha})$ and $\Im(\boldsymbol{\alpha})$, and parametrized by arc length s.

Theorem (8) can be stated in terms of perturbations of the $\hbar$ independent operator $A \equiv \Delta_{S^n} + \left(\frac{n-1}{2}\right)^2$. In the case of the harmonic oscillator we made use of dilation operators for that purpose (that will be the case for the hydrogen atom case as well). In the case of the n-sphere we just need to collect the $\hbar^2$ factor:

$$A_\hbar + \epsilon(\hbar)Q_\hbar = \hbar^2 F_\hbar, \quad F_\hbar \equiv A + \kappa(\hbar)Q_\hbar \, , \tag{79}$$

with $\kappa(\hbar) = \frac{\epsilon(\hbar)}{\hbar^2}$.

Since the distance between the unperturbed eigenvalue $\hat{E}_N = \left(N + \frac{n-1}{2}\right)^2$ and its next neighbor eigenvalues is $O(N)$, and the operator norm of $\kappa(\hbar)Q_\hbar$ is $O(N^{1-\delta})$, then, for N sufficiently large, we have well-defined clusters of eigenvalues

around the eigenvalues $\hat{E}_N$. Let us denote by $\gamma_{N,m}$ the eigenvalues in the cluster around $\hat{E}_N$ with $m = 1, \ldots, d_N$.

Theorem 9. *Let f be a continuous function on the real line and assume that $Q_\hbar$ is a selfadjoint and $\hbar$-admissible pseudo-differential operator on S^n of order zero as above. Then*

$$\lim_{N\to\infty} \frac{1}{d_N} \sum_{m=1}^{d_N} f\left(\frac{\gamma_{N,m} - \hat{E}_N}{\kappa(\hbar)}\right) = \int_{\mathcal{A}} f\left(\frac{1}{2\pi}\int_0^{2\pi} \sigma(Q_\hbar)\left(\, \mathbf{w}(s;\boldsymbol{\alpha}), \boldsymbol{\xi}(s;\boldsymbol{\alpha})\,\right) ds\right) d\mu(\boldsymbol{\alpha})\,. \tag{80}$$

As in the case of the harmonic oscillator (Theorem 3), the right-hand side of Eq. (78) can be re-written in terms of both an integral involving the normalized and $SO(n+1)$ invariant measure dm on the space of oriented geodesics $\mathcal{O} = \mathcal{A}/S^1$ of S^n and in terms of an integral involving a measure $dm_{\sigma(Q_\hbar)}$ on $\mathbb{R}$ given by the push-forward of dm under the Radon transform $\langle\, \sigma(Q_\hbar)\,\rangle : \mathcal{O} \to \mathbb{R}$ of the principal symbol $\sigma(Q_\hbar)$. Since $\mathcal{O}$ is compact, then $\langle\, \sigma(Q_\hbar)\,\rangle\,(\mathcal{O})$ is compact which in turn implies that the support of $dm_{\sigma(Q_\hbar)}$ is compact as well.

We remark that it is clear that the measure $dm_{\sigma(Q_\hbar)}$ can have a discrete part (given by the elements of $\mathbb{R}$ whose inverse image under the Radon transform $\langle\, \sigma(Q_\hbar)\,\rangle$ has positive measure) and an absolutely continuous part (with respect to the Lebesgue measure). However, the existence of a singular continuous part of $dm_{\sigma(Q_\hbar)}$ is not immediate. L. Thomas and C. Villegas-Blas [23] have shown a family of potentials for the 2-sphere (the perturbation $Q_\hbar$ is actually a multiplication operator V) whose associated measures dm_V are singularly continuous with respect to the Lebesgue measure. As a consequence and intuitively speaking, it is possible to have, for large values of N, that the eigenvalues in the clusters around the unperturbed eigenvalues $\hat{E}_N = \left(N + \frac{1}{2}\right)^2$ are distributed like elements of a Cantor set.

Proof. The proof follows both the same structure of the one given above for Theorem 4 and very closely Section 4 of reference [25].

We only need to prove the theorem when f is actually a monomial $f(x) = x^q$. Step (1) follows the same ideas as in the KDHO case, so we just restrict ourselves to make the statement: Let P_N^S be the projector of the operator $F_\hbar$ associated to the cluster around $\hat{E}_N$. Then

$$\begin{aligned}\frac{1}{d_N}\sum_{m=1}^{d_N}\left(\frac{\gamma_{N,m} - \hat{E}_N}{\kappa(\hbar)}\right)^q &= \frac{1}{d_N}\,\mathrm{tr}\left(P_N^S\left(\frac{F_\hbar - \hat{E}_N}{\kappa(\hbar)}\right)P_N^S\right)^q \\ &= \frac{1}{d_N}\,\mathrm{tr}\left(\Pi_N^S Q_\hbar \Pi_N^S\right)^q + O(N^{-\delta})\,. \end{aligned}\tag{81}$$

Thus it is left to show that the limit $N \to \infty$ of the right-hand side of Eq. (81) gives the desired result. This is the content of next subsection.

4.3. A Szegö type theorem for the n-sphere

From the expression for the projector Π_N^S in Eq. (74) in terms of coherent states $\Phi_{\boldsymbol{\alpha},N}$, we see that in order to show that the limit $N \to \infty$ of the right-hand side of Eq. (81) is equal to the right-hand side of Eq. (80), we need to establish a proposition estimating the expected value $\langle \Phi_{\boldsymbol{\alpha},N}, Q_\hbar \Phi_{\boldsymbol{\alpha},N} \rangle$ and then to use the averaging method.

The estimate of $\langle \Phi_{\boldsymbol{\alpha},N}, Q_\hbar \Phi_{\boldsymbol{\alpha},N} \rangle$ is a consequence of the stationary phase method and the $SO(n+1)$ invariance of the measure $d\mu$. Thus we only need to get the estimate for the particular case $\boldsymbol{\alpha} = \mathbf{e}_1 + \imath \mathbf{e}_2$ where $\mathbf{e}_1, \ldots, \mathbf{e}_{n+1}$ is the canonical basis of $\mathbb{R}^{n+1}$. Then by using suitable coordinates for the n-sphere according with our choice for $\boldsymbol{\alpha}$ we can show (see reference [25] for details):

Proposition 10. *Let $Q_\hbar$ be a selfadjoint and $\hbar$-admissible pseudo-differential operator on S^n of order zero as above. Then for $\hbar = \frac{1}{N+\frac{n-1}{2}}$:*

$$\langle \Phi_{\boldsymbol{\alpha},N}, Q_\hbar \Phi_{\boldsymbol{\alpha},N} \rangle = \frac{1}{2\pi} \int_0^{2\pi} \sigma(Q_\hbar)\, (\, \mathbf{w}(s;\boldsymbol{\alpha}), \boldsymbol{\xi}(s;\boldsymbol{\alpha})\,)\, ds + O(\hbar)\ , \tag{82}$$

uniformly for $\boldsymbol{\alpha} \in \mathcal{A}$.

The averaging method for the n-sphere needs to be done more carefully in comparison with the k-dimensional harmonic oscillator. The reason is that, in order to get an operator whose spectrum is $\hbar$ times a subset of the integer numbers (and then a 2π-periodic operator under exponentiation), we need to consider the square root of the operator $A_\hbar$. However, the lowest eigenvalue of $A_\hbar$ goes to zero when $\hbar \to 0$ and the square root function is not smooth at the origin.

Thus let us consider the operator

$$B_\hbar \equiv \phi(A_\hbar) - \hbar \frac{n-1}{2}\ , \tag{83}$$

with ϕ a smooth function, which for $0 < \tau << 1$ small and fixed, is defined by

$$\phi(\lambda) = \begin{cases} 0 & \text{if } \lambda \leq \tau/2 \\ \sqrt{\lambda} & \text{if } \lambda \geq \tau \end{cases}\ . \tag{84}$$

Note that $B_\hbar$ is an $\hbar$-admissible pseudo-differential operator with principal symbol $\sigma(B_\hbar) = \phi(|\boldsymbol{\xi}|^2)$ and spectrum

$$S(B_\hbar) = \left\{ \zeta_\ell = \phi\left(\hbar^2 \left(\ell + \frac{n-1}{2} \right)^2 \right) - \hbar \frac{n-1}{2} \quad \middle| \quad \ell \in N^* \right\}\ . \tag{85}$$

In particular,

$$\sigma(B_\hbar) = |\boldsymbol{\xi}| \quad \text{if } \ |\boldsymbol{\xi}| \geq \sqrt{\tau} \quad \text{and} \tag{86}$$

$$\zeta_\ell = \hbar \ell \quad \text{if} \quad \ell > \frac{\sqrt{\tau}}{\hbar}\ . \tag{87}$$

Let us define the average of $Q_\hbar$ along the flow determined by the operator $B_\hbar$ including a factor taking into account that ζ_ℓ is not $\hbar\ell$ for all $\ell \in N^*$. Thus let

us consider a compactly supported smooth function $\chi(\lambda)$ identically equal to one in a small neighborhood of $\lambda = 1$. Then we define

$$\tilde{Q}_\hbar = \chi(\hbar^2 \Delta_{S^n}) \frac{1}{2\pi} \int_0^{2\pi} \exp\left(-\frac{\imath t B_\hbar}{\hbar}\right) Q_\hbar \exp\left(\frac{\imath t B_\hbar}{\hbar}\right) dt \,. \tag{88}$$

We now claim that $\tilde{Q}_\hbar$ commutes with the projector Π_N^S for N sufficiently large. Let

$$\ell_N \equiv \min\left\{ \ell \;\Big|\; \ell > \sqrt{\tau}\left(N + \frac{n-1}{2}\right)\right\} \,. \tag{89}$$

Note that for $\ell \geq \ell_N$ the eigenvalue of $B_\hbar$ is $\hbar\ell$. Moreover, since τ is taken small, then $N > \ell_N$ for N sufficiently large.

First take $\phi \in \mathcal{L}_N$. Let us consider the following decomposition of $Q_\hbar(\phi)$:

$$Q_\hbar(\phi) = \sum_{\ell=0}^{\infty} \phi_\ell \qquad \text{with} \quad \phi_\ell \in \mathcal{L}_\ell \,. \tag{90}$$

Then, since $N > \ell_N$, after a calculation we find

$$\tilde{Q}_\hbar(\phi) = \phi_N + \frac{1}{2\pi} \sum_{0 \leq \ell < \ell_N} \left(\int_0^{2\pi} \exp\left(-\imath t \left[\frac{\zeta_\ell}{\hbar} - N\right]\right) dt \right) \chi(\hbar^2 \Delta_{S^n})(\phi_\ell) \,. \tag{91}$$

Since $\ell < \ell_N$ implies $\hbar^2 \ell(\ell + n - 1) < \sqrt{\tau}\left(\sqrt{\tau} + \frac{n-1}{N + \frac{n-1}{2}}\right)$. Taking $\chi = 0$ in a small neighborhood around the origin we obtain, for N sufficiently large, $\chi(\hbar^2 \Delta_{S^n})\phi_\ell = 0$ for $0 \leq \ell < \ell_N$. Thus we conclude:

$$\tilde{Q}_\hbar \Pi_N^S(\phi) = \phi_N = \Pi_N^S \tilde{Q}_\hbar(\phi) \,, \qquad \phi \in \mathcal{L}_N \,. \tag{92}$$

By doing a similar computation, we can show that for $\phi \in \mathcal{L}_M$ and $M \neq N$

$$\tilde{Q}_\hbar(\phi) = \begin{cases} \chi(\hbar^2 M(M+n-1))\phi_M & \text{if } M \geq \ell_N \\ 0 & \text{if } M < \ell_N \end{cases} \,. \tag{93}$$

Thus we have

$$\tilde{Q}_\hbar \Pi_N^S(\phi) = 0 = \Pi_N^S \tilde{Q}_\hbar(\phi) \,, \quad \phi \in \mathcal{L}_M, \quad M \neq N. \tag{94}$$

Moreover, since

$$\exp\left(-\frac{\imath t B_\hbar}{\hbar}\right) \Pi_N^S = \exp(-\imath t N) \Pi_N^S$$

and

$$\chi(\hbar^2 \Delta_{S^n}) \Pi_N^S = \chi(\hbar^2 N(N+n-1)) \Pi_N^S = \Pi_N^S$$

for N sufficiently large, then we have:

$$\Pi_N^S \tilde{Q}_\hbar \Pi_N^S = \Pi_N^S Q_\hbar \Pi_N^S \,. \tag{95}$$

We now proceed like in the case of the harmonic oscillator noting that, in a neighborhood of the unit cotangent bundle $T_1^* S^n$, we have both properties: (i) the principal symbol of $\chi(\hbar^2 \Delta_{S^n})$ is equal to one and (ii) that the Hamiltonian flow

associated to $\sigma(B_\hbar)$ is the geodesic flow on the n-sphere parametrized by arc length.

As in the case of the harmonic oscillator, let us state our conclusion in the following:

Theorem 11 (A Szegö type theorem for the n-sphere). *Let $Q_\hbar$ be a selfadjoint and $\hbar$-admissible pseudo-differential operator on S^n of order zero as above. Let f be a continuous function on the real line. Then*

$$\lim_{N\to\infty} \frac{1}{d_N} trf\left(\Pi_N^S Q_\hbar \Pi_N^S\right) = \int_{\mathcal{A}} f\left(\frac{1}{2\pi}\int_0^{2\pi} \sigma(Q_\hbar)\left(\, \mathbf{w}(s;\boldsymbol{\alpha}), \boldsymbol{\xi}(s;\boldsymbol{\alpha})\, \right) ds\right) d\mu(\boldsymbol{\alpha})\,. \tag{96}$$

This concludes the proof of Theorem 9. □

5. The Kepler and hydrogen atom problems

In this section we describe some properties of both the Kepler and hydrogen atom problems that will be used to state and prove a limiting eigenvalue distribution theorem for suitable perturbations of the hydrogen atom. In particular, we introduce coherent states for the hydrogen atom and describe the Moser regularization of the Kepler problem including a subsection providing physical intuition behind such a regularization.

The Kepler problem in n dimensions is defined as the Hamiltonian flow associated to the function $K : T^*\left(\mathbb{R}^n - \{0\}\right) \to \mathbb{R}$

$$K(\mathbf{x},\mathbf{p}) = \frac{\mathbf{p}^2}{2} - \frac{1}{|\mathbf{x}|}\,, \tag{97}$$

which corresponds to motion of a particle under the influence of the center of attraction fixed at the origin $\mathbf{x} = 0$. Let us denote by ϕ_K^t the Hamiltonian flow associated to K at time t. We are endowing $T^*\left(\mathbb{R}^n - \{0\}\right)$ with the canonical symplectic form $\sum_{j=1}^n dp_j \wedge dx_j$. We will assume that $n \geq 2$ (the one-dimensional case will be included in the description of the collision orbits, see below).

The energy K is an integral of motion and we will restrict ourselves to study the case of negative energy. Moreover, we will assume that $K = -1/2$. The case of arbitrary negative energy can be obtained by scaling the particular case $K = -1/2$ that we describe below.

5.1. Physical intuition of the Moser regularization

In order to show the basic idea of the Moser regularization, let us actually assume in this subsection that $n = 2, 3$. The angular momentum vector $\mathbf{L}$ and the Runge-Lenz vector $\mathbf{A}$ are integrals of motion

$$\mathbf{L} \equiv \mathbf{x} \times \mathbf{p} \qquad \mathbf{A} \equiv \mathbf{p} \times \mathbf{L} - \frac{\mathbf{x}}{|\mathbf{x}|} \tag{98}$$

Note that $\mathbf{L} \cdot \mathbf{A} = 0$ and $\mathbf{A}^2 - 2K\mathbf{L}^2 = \mathbf{A}^2 + \mathbf{L}^2 = 1$.

We have two possibilities: either (i) $|\mathbf{L}| \neq 0$ or (ii) $|\mathbf{L}| = 0$.

In case (i), the motion must be on the plane orthogonal to $\mathbf{L}$. Moreover, the vector $\mathbf{A}$ must lie on such a plane. Denoting the angle between $\mathbf{x}$ and $\mathbf{A}$ by θ, we find by considering $\mathbf{x} \cdot \mathbf{A}$ and $\mathbf{L} \times \mathbf{A}$ that

$$|\mathbf{x}| = \frac{|\mathbf{L}|^2}{|\mathbf{A}|\cos(\theta) + 1} , \tag{99}$$

$$\mathbf{p} - \frac{\mathbf{L} \times \mathbf{A}}{|\mathbf{L}|^2} = \frac{\mathbf{L} \times \mathbf{x}}{|\mathbf{L}|^2 |\mathbf{x}|} . \tag{100}$$

Thus we find from Eq. (99) that the trajectory in configuration space must be a conic curve. Since $|\mathbf{A}| < 1$ we conclude that such a trajectory is actually an ellipse. Since $\mathbf{L}$ and $\mathbf{A}$ are integrals of motion, Eq. (100) implies that the trajectory in momentum space must be the circle of radius $\frac{1}{|\mathbf{L}|}$ and center $\frac{\mathbf{L}\times\mathbf{A}}{|\mathbf{L}|^2}$. A nice geometric fact is that such a circle is mapped to a great circle on the sphere S^n not passing through the north pole by the stereographic projection $\mathbf{S} : \mathbb{R}^n \to S^n_o$ (here S^n_o denotes the punctured sphere S^n with the north pole removed) given by $\mathbf{w} = \mathbf{S}(\mathbf{p})$ through the following equations:

$$\begin{aligned} \omega_i &= \frac{2p_i}{|\mathbf{p}|^2 + 1}, \quad i = 1, \ldots, n \\ \omega_{n+1} &= \frac{|\mathbf{p}|^2 - 1}{|\mathbf{p}|^2 + 1}. \end{aligned} \tag{101}$$

Thus, when the momentum $\mathbf{p}$ winds on the circle mentioned above with a paste depending on time t, the corresponding point $\mathbf{w} = \mathbf{S}(\mathbf{p})$ on the sphere winds on the corresponding great circle.

All of the orbits with $K = -1/2$ and $|\mathbf{L}| \neq 0$ are 2π-periodic.

Case (ii). This is the case of one-dimensional motion on a straight line. First note that the trajectory in configuration space is bounded $|\mathbf{x}| \leq 2$ because $K = -1/2$. From conservation of energy we have that the particle will have a collision with the center of attraction in a finite time and with the magnitude of the momentum $\mathbf{p}$ going to infinity when the particle approaches the collision. Thus the trajectory in momentum space corresponds to motion on a unbounded straight line. Such a trajectory corresponds to motion on a great circle approaching the north pole when $|\mathbf{p}| \to \infty$ under the stereographic projection $\mathbf{S}$.

Here is the first step in the regularization of the Kepler problem: Consider a new time parameter s determined by the equation:

$$\frac{d}{ds} = |\mathbf{x}| \frac{d}{dt} \quad . \tag{102}$$

From conservation of energy, we find that the magnitude of the new velocity $\frac{d\mathbf{x}}{ds}$ goes to zero when the particle approaches the collision ($|\mathbf{x}| \to 0$). Moreover, considering this new time parameter s, we can show that the motion on the corresponding great circle on S^n_o takes place with uniform unit speed ($|\frac{d\mathbf{w}}{ds}| = 1$) including when

approaching the north pole. It can be checked that this last property holds for the case (i) as well.

Thus in both cases (i) and (ii), the Hamiltonian flow of the Kepler problem can be mapped into the geodesic flow on S^n. Noting that the geodesic flow on S^n is well defined for all values of time s, including the motion on geodesics passing through the north pole, it makes sense to consider the convention that, in a collision orbit, the particle is reflected back to its initial trajectory after having a collision with the center of attraction. Thus we get that all of the orbits on the energy surface $K = -1/2$ can be regarded as 2π-periodic orbits (including the collision orbits). Such is the main physical intuition behind the Moser regularization.

In the next subsection we give a precise mathematical description of Moser regularization [20] starting with the geodesic flow on S^n with respect to the arc-length parameter s and show that we end up with the Hamiltonian flow of the Kepler problem after the time re-parametrization given in Eq. (102) and considering an extension of the stereographic projection indicated in Eq. (101).

5.2. The Moser Regularization and geodesic flow on S^n

Let us now go back to the arbitrary n-dimensional case and consider the stereographic projection $\mathbf{S} : \mathbb{R}^n \mapsto S^n_o$ from the momentum space $\mathbb{R}^n$ onto the punctured sphere S^n_o, given by equations (101). Let us denote by $\boldsymbol{\xi}$ a vector in $T^*_{\mathbf{w}}S^n$ with $\mathbf{w} \in S^n$. The Moser map $\mathcal{M} : T^*(\mathbb{R}^n) \mapsto T^*(S^n_o)$ is the extension of the stereographic projection determined by requiring that $\mathbf{S}^*(\boldsymbol{\xi}\cdot d\mathbf{w}) = \mathbf{y}\cdot d\mathbf{p}$, with $\mathbf{y} \in T^*_{\mathbf{p}}\mathbb{R}^n$. The Moser map sends the point $(\mathbf{p}, \mathbf{y})$ to the point $(\mathbf{w}, \boldsymbol{\xi})$ under Eq. (101), and the following equations:

$$\begin{aligned} \xi_i &= \frac{|\mathbf{p}|^2 + 1}{2} y_i - (\mathbf{y}\cdot\mathbf{p})p_i, \quad i = 1, \ldots, n. \\ \xi_{n+1} &= \mathbf{y}\cdot\mathbf{p}. \end{aligned} \tag{103}$$

The inverse map $\mathcal{M}^{-1}$ is determined by the equations

$$\begin{aligned} p_i &= \frac{\omega_i}{1-\omega_{n+1}}, \quad i = 1, \ldots, n. \\ y_i &= (1-\omega_{n+1})\xi_i + \xi_{n+1}\omega_i. \quad i = 1, \ldots, n. \end{aligned} \tag{104}$$

The Moser map is a canonical transformation (i.e., $\mathcal{M}$ is a diffeomorphism with the property $\mathcal{M}^*(d\boldsymbol{\xi} \wedge d\mathbf{w}) = d\mathbf{y} \wedge d\mathbf{p}$).

The physical relevance of the Moser map in the Kepler problem appears when we take the position vector $\mathbf{x} = -\mathbf{y}$ and restrict ourselves to the surface of constant energy $K = \frac{\mathbf{p}^2}{2} - \frac{1}{|\mathbf{x}|} = -1/2$. Note that such a surface is mapped onto the unit tangent bundle $T^*_1(S^n_o)$ which is contained in $T^*_1(S^n)$ where the geodesic flow on the n-sphere takes place.

Let us actually consider a geodesic on S^n. The equation of such an orbit can be written as:

$$\begin{aligned}\mathbf{w}(s,\boldsymbol{\alpha}) &= \cos(s)\Re(\boldsymbol{\alpha}) + \sin(s)\Im(\boldsymbol{\alpha}) \ , \\ \boldsymbol{\xi}(s,\boldsymbol{\alpha}) &= -\sin(s)\Re(\boldsymbol{\alpha}) + \cos(s)\Im(\boldsymbol{\alpha}) \ . \end{aligned} \tag{105}$$

for some $\boldsymbol{\alpha} \in \mathcal{A}$ and the parameter s equals to the arc-length. If the geodesic contains the north pole, then we will omit the value of s such that $\cos(s)\Re\alpha_{n+1} + \sin(s)\Im\alpha_{n+1} = 1$. Then, from the expression for the inverse Moser map (104) we obtain:

$$\begin{aligned}\mathbf{x}(s,\boldsymbol{\alpha}) &= (\sin(s) - \Im(\alpha_{n+1}))\Re(\vec{\boldsymbol{\alpha}}) + (-\cos(s) + \Re(\alpha_{n+1}))\Im(\vec{\boldsymbol{\alpha}}) \ , \\ \mathbf{p}(s,\boldsymbol{\alpha}) &= \frac{\cos(s)\Re(\vec{\boldsymbol{\alpha}}) + \sin(s)\Im(\vec{\boldsymbol{\alpha}})}{1 - \cos(s)\Re(\alpha_{n+1}) - \sin(s)\Im(\alpha_{n+1})} \ , \end{aligned} \tag{106}$$

where $\vec{\boldsymbol{\alpha}} = (\alpha_1, \ldots, \alpha_n)$.

From (106) we have $|\mathbf{x}| = |1 - \cos(s)\Re(\alpha_{n+1}) - \sin(s)\Im(\alpha_{n+1})|$ which implies $|\mathbf{x}| = 0$ iff $|\mathbf{p}| = \infty$ and in such a case $\frac{d\mathbf{x}}{ds} = 0$. Additionally, one can check that the curves described by (106) have energy $K = \mathbf{p}^2/2 - 1/|\mathbf{x}| = -1/2$.

Let us now consider the time re-parametrization indicated in Eq. (102). One can check by a straight computation that the orbit ($\mathbf{x}$(s(t),$\boldsymbol{\alpha}$),$\mathbf{p}$(s(t),$\boldsymbol{\alpha}$)) obtained from Eq. (106) is actually a Kepler orbit, i.e., it satisfies Hamilton equations:

$$\begin{aligned}\frac{d\mathbf{x}}{dt} &= \frac{\partial H}{\partial \mathbf{p}}(\mathbf{x}(t),\mathbf{p}(t)) \ , \\ \frac{d\mathbf{p}}{dt} &= -\frac{\partial H}{\partial \mathbf{x}}(\mathbf{x}(t),\mathbf{p}(t)) \ . \end{aligned} \tag{107}$$

5.3. The hydrogen atom, the Fock transformation and coherent states

Let us consider the n-dimensional hydrogen atom Hamiltonian, with $n \geq 2$, given by $A_\hbar : D(A_\hbar) \subset L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, and

$$A_\hbar = \frac{-\hbar^2}{2}\Delta_{\mathbb{R}^n} - \frac{1}{|\mathbf{x}|} \ . \tag{108}$$

The spectrum of $A_\hbar$ is

$$S(A_\hbar) = \left\{ -\frac{1}{2\hbar^2\left(\ell + \frac{n-1}{2}\right)^2} \quad | \quad \ell \in \mathbb{N}^* \right\} \bigcup [0,\infty) \ . \tag{109}$$

Let us denote by $\mathcal{E}_\ell$ the eigenspace of the operator $A \equiv A_1$ associated to the eigenvalue $E_\ell = -\frac{1}{2\left(\ell+\frac{n-1}{2}\right)^2}$, with $\ell \in N^*$. The multiplicity of E_ℓ is d_ℓ, see Eq. (67) (the same multiplicity as the eigenvalue λ_ℓ of the Laplacian on S^n). Let $\Pi_\ell^H : L^2(\mathbb{R}^n) \to E_\ell$ be the orthogonal projector corresponding to the eigenvalue $\mathcal{E}_\ell$. Let us denote by $\mathcal{H}_b$ the Hilbert space generated by the spaces $\mathcal{E}_\ell$.

Let $\mathcal{F}$ be the Fourier transform defined as the unitary extension to $L^2(\mathbb{R}^n)$ of the expression

$$\mathcal{F}(f)(\mathbf{p}) = \frac{1}{(2\pi)^{n/2}} \int \exp(-\imath \mathbf{p}\cdot\mathbf{x}) f(\mathbf{x}) d\mathbf{x} \, . \tag{110}$$

We will use the notation $\hat{f} = \mathcal{F}(f)$ and $\hat{\mathcal{E}}_\ell \equiv \mathcal{F}\mathcal{E}_\ell$.

V. Fock [6] introduced a transformation showing that the inverse of the restriction of $-2A$ to the space $\mathcal{H}_b$ is unitarily equivalent to $\Delta_{S^n} + \left(\frac{n-1}{2}\right)^2$ on S^n. This transformation plays the role of the Moser transformation in quantum mechanics. However, the Fock transformation was introduced much earlier (1928) than the Moser one (1970).

The Fock transformation $\mathbf{F} : \mathcal{H}_b \to L^2(S^n)$ is defined as the linear extension of the following assignment: Let $\Psi \in \mathcal{E}_\ell$, then we define

$$\mathbf{F}\Psi \equiv K^{-1} J^{-1/2} D_{r_\ell}^{-1} \hat{\Psi} \, , \tag{111}$$

where $r_\ell \equiv \ell + (n-1)/2$, $K : L^2(S^n) \to L^2(\mathbb{R}^n)$ and $J : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ are defined by

$$K\Phi(\mathbf{p}) = \left(\frac{2}{|\mathbf{p}|^2+1}\right)^{n/2} \Phi(\mathbf{S}(\mathbf{p})), \qquad \Phi \in L^2(S^n), \tag{112}$$

and

$$J(\hat{\Psi})(\mathbf{p}) = \frac{2}{|\mathbf{p}|^2+1} \hat{\Psi}(\mathbf{p}) \quad \hat{\Psi} \in L^2(\mathbb{R}^n). \tag{113}$$

More explicitly, if we denote by $\Phi = \mathbf{F}\Psi$, then

$$\Phi(\mathbf{w}) = \left(\frac{|\mathbf{p}(\mathbf{w})|^2+1}{2}\right)^{n/2} \left(\frac{|\mathbf{p}(\mathbf{w})|^2+1}{2}\right)^{1/2} r_\ell^{-n/2} \hat{\Psi}(r_\ell^{-1}\mathbf{p}(\mathbf{w})) \, , \tag{114}$$

where $\mathbf{p}(\mathbf{w})$ is given by the inverse map $\mathcal{M}^{-1}$ (see Eq. (104)).

Thus the basic idea of the Fock transformation has the following procedure: (i) Consider an eigenfunction $\Psi \in \mathcal{E}_\ell$ of the operator A solving the corresponding eigenvalue equation. (ii) Go to the momentum space by taking the Fourier transform. Note that $\hat{\Psi}$ is a solution of an integral equation. (iii) Then multiply the dilated function $D_{r_\ell}^{-1}\hat{\Psi}$ by the pre-factor $J^{-1/2} = \left(\frac{|\mathbf{p}|^2+1}{2}\right)^{1/2}$. The dilation operator takes into account the fact that we need to scale the momentum since we are working on the energy level E_ℓ. (iv) Finally, multiply by the factor $\left(\frac{|\mathbf{p}|^2+1}{2}\right)^{n/2}$ and go to the sphere via the stereographic projection. Note that the Jacobian of the stereographic projection is $\left(\frac{2}{|\mathbf{p}|^2+1}\right)^n$. The function $\mathbf{F}(\Psi)$ is a solution of an integral equation on the n-sphere whose solutions in $L^2(S^n)$ are in turn the spherical harmonics (see [3]) for details).

There is a subtle point in the procedure defining the Fock transformation. The introduction of the pre-factor $J^{-1/2}$ (necessary in order to end up with the eigenfunctions of the Laplacian on S^n) preserves the $L^2(\mathbb{R}^n)$ norm of Ψ due to the

virial theorem (see [5]). Moreover, remember that in the Kepler problem we had $|\mathbf{x}| = \frac{2}{|\mathbf{p}|^2+1}$ on the surface energy $K = -1/2$ and the factor $|\mathbf{x}|$ is exactly what enters into Eq. (102) defining the time re-parametrization.

Note that the Fock transformation maps the space $\mathcal{E}_\ell$ onto $\mathcal{L}_\ell$. We can use the Fock transformation to get coherent states $\Psi_{\boldsymbol{\alpha},\ell} \equiv \mathbf{F}^{-1}\Phi_{\boldsymbol{\alpha},\ell}$ for the space $\mathcal{E}_\ell$ giving the following expression for the corresponding orthogonal projector:

$$\Pi_\ell^H \Psi = d_\ell \int_{\mathcal{A}} \langle \Psi, \Psi_{\boldsymbol{\alpha},\ell} \rangle_{L^2(\mathbb{R}^n)} \Psi_{\boldsymbol{\alpha},\ell} d\mu(\boldsymbol{\alpha}), \quad \Psi \in L^2(\mathbb{R}^n) \,. \tag{115}$$

Taking Fourier transform in both sides of Eq. (115) we obtain a similar expression for the projector $\hat{\Pi}_N^H \equiv \mathcal{F}\Pi_N^H\mathcal{F}^{-1}$ in terms of the coherent states $\hat{\Psi}_{\boldsymbol{\alpha},\ell} = \mathcal{F}\Psi_{\boldsymbol{\alpha},\ell}$:

$$\hat{\Pi}_\ell^H \Psi = d_\ell \int_{\mathcal{A}} \left\langle \Psi, \hat{\Psi}_{\boldsymbol{\alpha},\ell} \right\rangle_{L^2(\mathbb{R}^n)} \hat{\Psi}_{\boldsymbol{\alpha},\ell} d\mu(\boldsymbol{\alpha}), \quad \Psi \in L^2(\mathbb{R}^n) \,. \tag{116}$$

5.4. A limiting eigenvalue distribution theorem for perturbations of the hydrogen atom

In this section we introduce limiting eigenvalue distribution theorems for both perturbations of the hydrogen atom Hamiltonian $A_\hbar$ and, equivalently, for the $\hbar$-independent operator A. The structure of both the presentation and proof of these theorems follows Sections 3 and 4. However, the proof for the hydrogen atom case is more involved due to the Coulomb singularity. So we will concentrate more on this last point and will only give a sketch of the ideas for the remaining part of both the proof and presentation of the theorems. We follow reference [25] regarding the statements of the limiting eigenvalue distribution theorems and the proof of a corresponding Szegö type theorem.

Let $H_\hbar : D(H_\hbar) \subset L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ given by

$$H_\hbar = A_\hbar + \epsilon(\hbar) Q_\hbar \,, \tag{117}$$

with $Q_\hbar$ a selfadjoint and $\hbar$-admissible pseudo-differential operator of order zero on $L^2(\mathbb{R}^n)$ as above. Let us assume that $0 < \epsilon(\hbar) = O(\hbar^{1+\delta})$ with $\delta > 0$.

Let N be any natural number and consider $\hbar = \frac{1}{N+\frac{n-1}{2}}$. Then $E = -1/2$ is an eigenvalue of $A_\hbar$ with multiplicity d_N. Moreover, there is a well-defined cluster of eigenvalues of $H_\hbar$ around $E = -1/2$. Let us denote by $\eta_{N,m}$, $m = 1, \ldots, d_N$, the eigenvalues in such a cluster.

Theorem 12. *Let f be a continuous function on the real line and assume that $Q_\hbar$ is a selfadjoint and $\hbar$-admissible pseudo-differential operator of order zero on $L^2(\mathbb{R}^n)$ as above. Then*

$$\begin{aligned} &\lim_{N\to\infty} \frac{1}{d_N} \sum_{m=1}^{d_N} f\left(\frac{\eta_{N,m} - (-1/2)}{\epsilon(\hbar)}\right) \\ &\quad = \int_{\mathcal{A}} f\left(\frac{1}{2\pi}\int_0^{2\pi} \sigma(Q_\hbar)\left(\, \mathbf{x}(t,\boldsymbol{\alpha}), \mathbf{p}(t,\boldsymbol{\alpha}) \,\right) dt\right) d\mu(\boldsymbol{\alpha}) \,, \end{aligned} \tag{118}$$

where $(\mathbf{x}(t,\boldsymbol{\alpha}), \mathbf{p}(t,\boldsymbol{\alpha}))$ *denotes the classical orbit solving the Hamilton equations* (107) *for the Kepler problem and initial condition determined by* $\boldsymbol{\alpha}$ *through the map* σ_n *in Eq.* (70) *and the inverse Moser map in Eq.* (104).

Equivalently, we can state Theorem (12) for perturbations of the operator A by considering dilation operators using the following equation:

$$A_\hbar = \frac{1}{\hbar^2} D_{\hbar^{-2}} \left(A + \hbar^2 \epsilon(\hbar) D_{\hbar^2} Q_\hbar D_{\hbar^{-2}} \right) D_{\hbar^2} \ . \tag{119}$$

Thus taking $\hbar = \frac{1}{N+\frac{n-1}{2}}$, we have well-defined clusters of eigenvalues of $A + \hbar^2\epsilon(\hbar) D_{\hbar^2} Q_\hbar D_{\hbar^{-2}}$ around the unperturbed eigenvalue $E_N = -\frac{1}{2\left(N+\frac{n-1}{2}\right)^2}$. Let us denote those eigenvalues by $\gamma_{N,m}$, $m = 1, \ldots, d_N$.

Theorem 13. *Let* f *be a continuous function on the real line and assume that* $Q_\hbar$ *is a selfadjoint and* $\hbar$*-admissible pseudo-differential operator of order zero on* $L^2(\mathbb{R}^n)$ *as above. Then*

$$\begin{aligned} &\lim_{N\to\infty} \frac{1}{d_N} \sum_{m=1}^{d_N} f\left(\frac{\gamma_{N,m} - E_N}{\hbar^2 \epsilon(\hbar)} \right) \\ &\quad = \int_{\mathcal{A}} f\left(\frac{1}{2\pi} \int_0^{2\pi} \sigma(Q_\hbar)\left(\mathbf{x}(t,\boldsymbol{\alpha}), \mathbf{p}(t,\boldsymbol{\alpha}) \right) dt \right) d\mu(\boldsymbol{\alpha}) \ . \end{aligned} \tag{120}$$

Proof. By studying the norm of the difference of the perturbed and unperturbed orthogonal projectors as above (see step 1 in the proof of Theorem (4)), it is possible to show that

$$\frac{1}{d_N} \sum_{m=1}^{d_N} \left(\frac{\gamma_{N,m} - E_N}{\hbar^2 \epsilon(\hbar)} \right)^q = \frac{1}{d_N} \operatorname{tr} \left(\Pi_N^H D_{\hbar^2} Q_\hbar D_{\hbar^{-2}} \Pi_N^H \right)^q + O(N^{-\delta}) \ . \tag{121}$$

Thus we need to prove a Szegö type theorem in order to evaluate the limit $N \to \infty$ of the right-hand side of Eq. (121). This is the goal of next subsection.

5.5. A Szegö type theorem for the hydrogen atom

Theorem 14. Szegö type theorem for the hydrogen atom in configuration space. *Let* f *be a continuous function on the real line and assume that* $Q_\hbar$ *is a selfadjoint and an* $\hbar$*-admissible pseudo-differential operator of order zero on* $L^2(\mathbb{R}^n)$. *Then*

$$\begin{aligned} &\lim_{N\to\infty} \frac{1}{d_N} \operatorname{tr} f\left(\Pi_N^H D_{\hbar^2} Q_\hbar D_{\hbar^{-2}} \Pi_N^H \right) \\ &\quad = \int_{\mathcal{A}} f\left(\frac{1}{2\pi} \int_0^{2\pi} \sigma(Q_\hbar)\left(\mathbf{x}(t,\boldsymbol{\alpha}), \mathbf{p}(t,\boldsymbol{\alpha}) \right) dt \right) d\mu(\boldsymbol{\alpha}) \ . \end{aligned} \tag{122}$$

Proof. First we go to momentum space via the Fourier transform. Let us define $\hat{Q}_\hbar \equiv \mathcal{F}_\hbar Q_\hbar \mathcal{F}_\hbar^{-1}$. where the $\hbar$-Fourier transform $\mathcal{F}_\hbar$ is defined by

$$\mathcal{F}_\hbar(f)(\mathbf{p}) = \frac{1}{(2\pi\hbar)^{n/2}} \int \exp(-\frac{\imath}{\hbar} \mathbf{p}\cdot\mathbf{x}) f(\mathbf{x}) d\mathbf{x} \ . \tag{123}$$

Note that $\mathcal{F}_\hbar = \mathcal{F}D_\hbar$ and for $r > 0$, $\mathcal{F}D_r = D_{r^{-1}}\mathcal{F}$. It can be checked that the operator $R_N \equiv \Pi_N^H D_{\hbar^2} Q_\hbar D_{\hbar^{-2}} \Pi_N^H$ is isospectral to the operator

$$\hat{R}_N \equiv \hat{\Pi}_N^H D_{\hbar^{-1}} \hat{Q}_\hbar D_\hbar \hat{\Pi}_N^H \tag{124}$$

by considering $\mathcal{F}R_N\mathcal{F}^{-1}$. Note that $\hat{Q}_\hbar$ is an $\hbar$-admissible pseudo-differential operator because $\mathcal{F}_\hbar$ is a Fourier integral operator in the semiclassical sense.

Then we go to the n-sphere S^n using the Fock transform. The operator $\hat{R}_N$ is in turn isospectral to the operator

$$T_N \equiv \Pi_N^S K^{-1} J^{1/2} \hat{Q}_\hbar J^{1/2} K \Pi_N^S \tag{125}$$

which acts on $L^2(S^n)$. This fact can be shown by using two Bargmann-type transforms $U_N : \hat{\mathcal{E}}_\ell \to L^2(\mathcal{A})$ and $V_N : \mathcal{L}_N \to L^2(\mathcal{A})$ to prove that both operators are similar to the same operator acting on $\mathcal{X}_N = \mathcal{Y}_N$ where $\mathcal{X}_N$ and $\mathcal{Y}_N$ denote the range of U_N and V_N in $L^2(\mathcal{A})$ respectively. The transforms U_N and V_N are defined by

$$U_N \hat{\Psi}(\boldsymbol{\alpha}) = \left\langle \hat{\Psi}, \hat{\Psi}_{\boldsymbol{\alpha},N} \right\rangle_{L^2(\mathbb{R}^n)} , \quad V_N \Phi(\boldsymbol{\alpha}) = \langle \Phi, \Phi_{\boldsymbol{\alpha},N} \rangle_{L^2(S^n)} . \tag{126}$$

Let $\hat{R}_N^\sharp : \mathcal{X}_N \to \mathcal{X}_N$ be defined by

$$\hat{R}_N^\sharp F(\boldsymbol{\alpha}) = \int_{\mathcal{A}} \left\langle \hat{R}_N \hat{\Psi}_{\boldsymbol{\alpha},N}, \hat{\Psi}_{\boldsymbol{\beta},N} \right\rangle_{L^2(\mathbb{R}^n)} F(\boldsymbol{\beta}) d\mu(\boldsymbol{\beta}) , \tag{127}$$

with a similar definition for an a function $T_N^\sharp : \mathcal{Y}_N \to \mathcal{Y}_N$. Then by using the resolution of the identity for $\hat{\Pi}_N^H$ we can show that U_N is injective and

$$\hat{R}_N^\sharp U_N F(\boldsymbol{\alpha}) = \left\langle \hat{R}_N F, \hat{\Psi}_{\boldsymbol{\alpha},N} \right\rangle_{L^2(\mathbb{R}^n)} = U_N \hat{R}_N F(\boldsymbol{\alpha}) \tag{128}$$

which in turn implies $\hat{R}_N = U_N^{-1} \hat{R}_N^\sharp U_N$. In a similar way we also have $T_N = V_N^{-1} T_N^\sharp V_N$. The following calculation shows that the Schwartz kernel of $\hat{R}_N^\sharp$ and $T_N^\sharp$ are the same:

$$\begin{aligned} &\left\langle \hat{R}_N \hat{\Psi}_{\boldsymbol{\alpha},N}, \hat{\Psi}_{\boldsymbol{\beta},N} \right\rangle_{L^2(\mathbb{R}^n)} \\ &\quad = \left\langle D_{\hbar^{-1}} \hat{Q}_\hbar D_\hbar D_{r_N} J^{1/2} K \Phi_{\boldsymbol{\alpha},N}, D_{r_N} J^{1/2} K \Phi_{\boldsymbol{\beta},N} \right\rangle_{L^2(\mathbb{R}^n)} , \end{aligned} \tag{129}$$

where we have used that $\hat{\Psi}_{\boldsymbol{\alpha},N} = D_{r_N} J^{1/2} K \Phi_{\boldsymbol{\alpha},N}$ and the definition of $\hat{R}_N$. If we now make the substitution $\hbar = \frac{1}{N + \frac{n-1}{2}}$, then by using that J is selfadjoint and K unitary we obtain

$$\left\langle \hat{R}_N \hat{\Psi}_{\boldsymbol{\alpha},N}, \hat{\Psi}_{\boldsymbol{\beta},N} \right\rangle_{L^2(\mathbb{R}^n)} = \left\langle T_N \Phi_{\boldsymbol{\alpha},N}, \Phi_{\boldsymbol{\beta},N} \right\rangle_{L^2(S^n)} . \tag{130}$$

Once we are on S^n, we need to study the operator $Z_\hbar = K^{-1} J^{1/2} \hat{Q}_\hbar J^{1/2} K$ which is an $\hbar$-admissible pseudo-differential operator on the punctured sphere S_o^n. The symbol of such an operator is not initially defined on the north pole. By

following the transformations involved in the definition of the operator $Z_\hbar$, we can show that the principal symbol of $Z_\hbar$ is given by

$$\sigma_0(\mathbf{w}, \boldsymbol{\xi}) = (1 - w_{n+1})\sigma(Q_\hbar)(-\mathbf{y}(\mathbf{w}, \boldsymbol{\xi}), \mathbf{p}(\mathbf{w}, \boldsymbol{\xi})) \,, \tag{131}$$

where $\mathbf{y}(\mathbf{w}, \boldsymbol{\xi})$ and $\mathbf{p}(\mathbf{w}, \boldsymbol{\xi})$ are given by the inverse Moser map Eq. (104).

Here is the key point: due to the factor $J^{-1/2}$ included in the definition of the Fock transformation, we obtained the factor $(1 - w_{n+1})$ in Eq. (131) which is zero at the north pole. This factor allows us to consider the continuous extension of the symbol σ_0 to the whole cotangent manifold T^*S^n by defining such an extension as zero at the cotangent space of S^n at the north pole. Let us denote such a continuous extension by σ_0 again.

The next step is to approximate σ_0 by smooth symbols on a neighborhood of the unit cotangent bundle and then to apply Section 4 to the operators with those smooth symbols. Namely, given $\epsilon > 0$, we find a smooth symbol f_ϵ on T^*S^n such that $|\sigma_0 - f_\epsilon| < \epsilon$ on a neighborhood of $T_1^*S^n$. Then we use Section 4 to evaluate $\mathrm{tr}(\Pi_N^S Op_\hbar(f_\epsilon)\Pi_N^S)^q$. We finally take the limit $N \to 0$ followed by the limit $\epsilon \to 0$ (see [25]) for details). This concludes the proof of Theorem 14 and Theorem 13 as well. □

We finally remark that Szegö type theorems for the hydrogen atom have been previously established by L. Thomas and C. Villegas-Blas [24] for both momentum and configuration space for the case of multiplication operators which, in the case of configuration space, are assumed to be only polynomially bounded continuous functions (not necessarily bounded).

6. Further developments

As mentioned in the introduction, the initial situation to consider the existence of a limiting eigenvalue distribution theorem is to have a system whose eigenvalues are degenerated with a corresponding periodic classical flow and then to introduce a suitable perturbation. This is the case of the hydrogen atom under the influence of a constant electric field (Stark effect) and a magnetic field (Zeeman effect). There are nice stability theorems in both cases due to J. Avron, I. Herbst and B. Simon (see [1], [2] and [12]). See the work of E. Vock and W. Hunziker [27] as well. The case of the Stark effect has been studied by P. Hislop and Villegas-Blas [14] and the case of the Zeeman effect is work in progress by P. Hislop, D. Ojeda-Valencia and C. Villegas-Blas. We remark that the study of the Stark effect case involves a non bounded perturbation of the hydrogen atom Hamiltonian, the study of non-selfadjoint operators and a statement of a limiting resonance distribution theorem.

Another case of great interest is a particle on a plane under the influence of a perpendicular constant magnetic field. In this case the spectrum is a countable set of eigenvalues equally spaced but each one with infinite multiplicity (the Landau problem). Thus the study of clusters of an infinite number of eigenvalues

around unperturbed eigenvalues after introducing a suitable perturbation is a very interesting problem to consider. This problem has been studied by A. Pushnitski G. Raikov and C. Villegas-Blas [22], it is finished and submitted.

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On Norm Resolvent and Quadratic Form Convergences in Asymptotic Thin Spatial Waveguides

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Abstract. A quantum particle is restricted to Dirichlet three-dimensional tubes built over a smooth curve $r(x) \subset \mathbb{R}^3$ through a bounded cross section that rotates along $r(x)$. Then the confining limit as the diameter of the tube cross section tends to zero is studied, and special attention is paid to the interplay between uniform quadratic form convergence and norm resolvent convergence of the respective Hamiltonians. In particular, it is shown a norm resolvent convergence to an effective Hamiltonian in case of null curvature and unbounded tubes, and, by means of an example, it is concluded that just norm resolvent convergence does not imply the quadratic form convergence.

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1. Introduction

The question of dimensional reduction in quantum systems restricted to planar strips and spatial tubes (i.e., Dirichlet Laplacian) is as interesting as difficult to be mathematically analyzed. However, it has been of great interest in recent years, and many results are related to the confinement of motion from such strips and tubes to curves; see, for instance, [1, 3, 4, 6, 8, 11, 12, 13, 15, 16, 20, 19]. The main questions to be addressed are the action of effective operators and how to approach them, the behavior of the essential spectrum and eigenvalue expansions in terms of the small diameter (with respect to some directions) of the regions.

It should be noted that such theoretical studies are not isolated from other areas of research and applications; without mentioning that it is an alternative approach to quantize constrained systems. For instance, electronic motion in nanos-

tructures and some periodic solids present confining characteristics due to large potential barriers in some directions, particularly in quantum wires and carbon nanotubes (see, for instance, [21]). Dimensional reductions also appear in the quantum network model used to study the motion of valence electrons in aromatic molecules [2], as well as in studies of quantum graphs (see [14] and references therein), in which the limiting dynamics to a graph must define an effective Hamiltonian operator. Under some conditions it is also related to adiabatic dynamics and the Born-Oppenheimer approximation, since the presence of strong barriers induces different scales in the system [22, 20].

In [11, 1] the authors considered the dynamics of a planar particle as the region approaches a broken line, a particular case of a quantum graph, as the limit $\varepsilon \to 0$ of the dynamics in $\mathbb{R}^2$ under a positive potential $W(x,y)/2\varepsilon^2$ that vanishes exactly on the graph. In [13] the hydrogen atom was restricted between two parallel planes in $\mathbb{R}^3$ and the planar limit was studied, whereas in [10] the confinement of the hydrogen atom in a space tube to the real line was investigated, and the main question was about which boundary condition at the origin should be selected.

A possible technique to prove the norm resolvent convergence of a sequence of self-adjoint operators is to consider the uniform convergence of the corresponding sesquilinear forms. We then present a detailed description of this in Subsection 4.1, although it has appeared in some arguments in [17]; we will show that the converse of such result does not necessarily holds true, for we discuss an example of norm resolvent convergence with no form convergence. For this example we consider a quantum particle initially restricted to Dirichlet tubes in $\mathbb{R}^3$ and take the squeezing limit of the particle motion from tubes to lines in space; the known results are in the sense of norm resolvent convergence to effective operators in case of bounded tubes [4, 8], whereas for unbounded tubes the results are restricted to strong resolvent sense [8]. In any event, herein we present a proof of norm resolvent convergence to unbounded tubes in case the curvature of the curve vanishes, that is, if the curve is a straight line (the tube cross section may has a nontrivial rotation; see ahead); the norm resolvent convergence for the general case of nonvanishing curvature remains an open question.

We think that at this point it is worth illustrating the general problem with a well-known simple example. Consider a quantum particle restricted to the box $B_\varepsilon = \{(x,y_1,y_2) \in \mathbb{R}^3 : 0 \le x \le L,\ 0 \le y_1, y_2 \le \varepsilon\}$, and we are interested in the limit $\varepsilon \to 0$. We use units so that the particle mass is $1/2$ and Planck constant $\hbar = 1$; hence the energy of such particle is described by the Laplacian $-\Delta_\varepsilon = -(\partial^2/\partial x^2 + \partial^2/\partial y_1^2 + \partial^2/\partial y_2^2)$ acting in $\mathrm{L}^2(B_\varepsilon)$ with Dirichlet (i.e., vanishing of the wavefunctions) boundary condition at the border ∂B_ε, thus with domain $\mathcal{H}_0^1(B_\varepsilon) \cap \mathcal{H}^2(B_\varepsilon)$. Its eigenvalues are

$$\lambda_{n,l_1,l_2} = \frac{1}{4}\left(n^2/L^2 + (l_1^2 + l_2^2)/\varepsilon^2\right),$$

where $n, l_1, l_2 \in \mathbb{N} = \{1, 2, 3, \dots\}$ are the quantum numbers related to directions x, y_1, y_2, respectively. Since $\varepsilon \ll L$, the bottom of its spectrum is regulated by the

ground states in the transversal directions y_1, y_2, that is, $l_1 = l_2 = 1$. As $\varepsilon \to 0$, the excited states in the transversal directions will play no role in the description of the spectrum of the system. If one looks at the corresponding normalized eigenfunctions

$$\psi_{n,l_1,l_2}(x, y_1, y_2) = \left(\frac{2}{L}\right)^{\frac{1}{2}} \sin\left(\frac{\pi n x}{L}\right) \times \left[\frac{2}{\varepsilon} \sin\left(\frac{\pi l_1 y_1}{\varepsilon}\right) \sin\left(\frac{\pi l_2 y_2}{\varepsilon}\right)\right],$$

one notices a clear decoupling of variables due to the particular symmetry of the box, and in the limit as the box is squeezed to the interval $[0, L]$, that is, $\varepsilon \to 0$, the particle motion is essentially one dimensional and thus one simply disregards the transversal motion and works with the space $\mathrm{L}^2[0, L]$ generated by $\psi_n(x) = (2/L)^{1/2} \sin(\pi n x/L)$, $n \in \mathbb{N}$, and effective energy operator $H_{\text{eff}} = -d^2/dx^2$ (just the restriction of the Laplacian to one coordinate) with Dirichlet boundary condition and eigenvalues $n^2/(4L^2)$.

In case the interval $[0, L]$ is replaced by a more general curve $r(x)$ in $\mathbb{R}^3$ and the square cross section by a bounded open planar set S with diameter ε, thus getting a tube Ω_ε, the asymptotic situation is not so clear. But the example above indicates that, in the limit $\varepsilon \to 0$, one should remove from the initial Laplacian the ground state energy (which depends on ε^{-2}) of the Dirichlet Laplacian in S in order to get finite expectation values. It is known that now the effective operator H_{eff} will depend on geometric properties of the reference curve $r(x)$ (see [4, 12] and references therein), and the techniques to study the problem have to be carefully selected, as well as suitable identifications of operators acting in different spaces. In what follows we are going to be more specific in the description of our setting.

Let $r(x)$ be a curve in $\mathbb{R}^3$, $x \in I$, with I denoting either $\mathbb{R}$ or $[0, L]$, is its arc-length parameter, and denote by $k(x)$ and $\tau(x)$ its curvature and torsion at the point $r(x)$, respectively. Let S be an open, bounded, simply connected and nonempty subset of $\mathbb{R}^2$. We build a tube Ω in $\mathbb{R}^3$ by moving the region S along $r(x)$. At each point the region may present a rotation angle which is denoted by $\alpha(x)$ (assume that $\alpha(0) = 0$). We suppose that the functions $k, (\tau + \alpha') \in \mathrm{L}^\infty(I)$, the Dirichlet condition at the boundary $\partial\Omega$, and we study its behavior as the tube is squeezed to $r(x)$.

The self-adjoint operators associated with this problem are

$$\psi \mapsto -\Delta_\varepsilon \psi, \qquad \psi \in \mathcal{H}_0^1(\Omega_\varepsilon) \cap \mathcal{H}^2(\Omega_\varepsilon),$$

where Ω_ε is the tube generated by the cross-section εS, and Δ_ε denotes the Laplacian in Ω_ε. Observe that, as $\varepsilon \to 0$, the sequence of tubes Ω_ε approaches the curve r. It is expected that there is an effective operator, which should be identified with a one-dimensional operator in $\mathrm{L}^2(I)$, describing such singular limit $\varepsilon \to 0$. However, as $\varepsilon \to 0$, the region Ω_ε becomes narrower and the transverse oscillations of the particle become faster. Let λ_0 be the first (i.e., the lowest) eigenvalue of the Dirichlet Laplacian restricted to S and u_0 the (positive) associated normalized

eigenfunction, that is,

$$-\Delta u_0 = \lambda_0 u_0, \quad u_0 \in \mathcal{H}_0^1(S), \quad u_0 \geq 0, \quad \int_S |u_0|^2 dy = 1.$$

Write [4]

$$C(S) := \int_S |\,(\nabla_y u_0, Ry)\,|^2 dy \quad \text{and} \quad R = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

where ∇_y denotes the gradient in the cartesian variables $y = (y_1, y_2)$ in S. Motivated by the particular box example above, one considers the sequence of operators

$$H_\varepsilon \psi = -\Delta_\varepsilon \psi - \frac{\lambda_0}{\varepsilon^2}\psi, \qquad \operatorname{dom} H_\varepsilon = \mathcal{H}_0^1(\Omega_\varepsilon) \cap \mathcal{H}^2(\Omega_\varepsilon). \tag{1}$$

The term λ_0/ε^2 is intended to renormalize the divergence of the transverse oscillations.

After an appropriate change of variables and regularizations, in case the curve is finite (i.e., $I = [0, L]$), so that the tubes are bounded, in [4] the asymptotic behavior of the eigenvalues λ_j^ε of (1) (with $j \in \mathbb{N}$) were found to be ruled by the eigenvalues of the effective one-dimensional self-adjoint operator

$$Tw := -w'' + C(S)(\tau + \alpha')(x)w - \frac{k(x)^2}{4}w, \tag{2}$$

with $\operatorname{dom} T = \mathcal{H}_0^1(0, L) \cap \mathcal{H}^2(0, L)$. More precisely, if μ_j are the eigenvalues of T, it was shown that, for each $j \in \mathbb{N}$,

$$\lambda_j^\varepsilon \to \mu_j, \quad \varepsilon \to 0. \tag{3}$$

Observe that the operator (2) depends on geometric features of the tube, despite the initial three-dimensional problem had no explicitly potential.

The case of unbounded tubes (more precisely, $I = \mathbb{R}$) was studied in [8] through the variational technique of strong and weak Γ-convergences, and it was found a strong resolvent operator convergence to

$$Tw := -w'' + C(S)(\tau + \alpha')(x)w - \frac{k(x)^2}{4}w, \quad \operatorname{dom} T = \mathcal{H}^2(\mathbb{R}). \tag{4}$$

As a byproduct of [8], the eigenvalue convergence (3) (in case of bounded tubes) was justified as a result of an operator norm resolvent convergence to the effective operator T in (2). It will be convenient to use the same notation for the operators (2) and (4), and it is expected to cause no confusion.

The proof of a kind of norm resolvent convergence also in the case of unbounded tubes $I = \mathbb{R}$, with T in (4) playing the role of an effective operator, thus improving some results of [4, 8], was implicitly conjectured in Remark 4.8 in [4] and proposed as an open problem at the end of [19]. We then tried to get such result by way of uniform quadratic form convergence as employed in [17, 16, 9] (see Subsection 4.1 in this work); however, such technique only works in case $k(x) \equiv 0$, that is, $r(x)$ is a straight line (see Theorem 3). For general nonvanishing curvatures, the analysis of the quadratic form convergence has revealed a counterexample to the

natural question if the norm resolvent convergence implies the uniform form convergence, as discussed in Subsection 4.3.2. We underline that our counterexample just indicates some weakness of the quadratic form approach for certain problems.

Shortly, this is the content of this work. In Section 2 we describe in detail the tube we work with. In Section 3 we introduce the relevant quadratic forms. In Section 4 we state our main results, whereas part of their proofs appear in Section 5.

2. Construction of the tubes

By following [4, 19], let $r : I \to \mathbb{R}^3$ be a simple C^3 curve in $\mathbb{R}^3$ parametrized by its arc-length parameter x. The curvature of r is defined by $k := |r''|$. We choose the orthonormal triad of vector fields $\{T, N, B\}$, called the tangent, normal and binormal vectors, respectively, moving along the curve and defined by

$$T = r', \qquad N = k^{-1}T', \qquad B = T \times N. \tag{5}$$

To justify the construction (5), it is assumed that $k > 0$, but if r is a piece of a straight line (i.e., $k = 0$ identically in this piece), one can choose a constant Frenet frame instead. It is possible to combine constant Frenet frames with the Frenet frame (5) to include other types of curves, for instance, curves with $k > 0$ only on a compact interval of values of x (and so obtaining a global differentiable Frenet frame; see [18], Theorem 1.3.6).

In each situation above we assume that the Frenet frame exists and that the Frenet equations are satisfied, that is,

$$\begin{pmatrix} T' \\ N' \\ B' \end{pmatrix} = \begin{pmatrix} 0 & k & 0 \\ -k & 0 & \tau \\ 0 & -\tau & 0 \end{pmatrix} \begin{pmatrix} T \\ N \\ B \end{pmatrix}, \tag{6}$$

where τ is the torsion of r, actually defined by (6).

Let S be an open, bounded, simply connected and nonempty subset of $\mathbb{R}^2$. The set

$$\Omega = \left\{\mathbf{x} \in \mathbb{R}^3 : \mathbf{x} = r(x) + y_1 N(x) + y_2 B(x),\, x \in I, y = (y_1, y_2) \in S\right\}$$

is obtained by translating the region S along the curve r. At each point $r(x)$ we allow a rotation of the region S by an angle $\alpha(x)$ with respect to $\alpha(0) = 0$, so that the new region is given by

$$\Omega^\alpha = \left\{\mathbf{x} \in \mathbb{R}^3 : \mathbf{x} = r(x) + y_1 N_\alpha(x) + y_2 B_\alpha(x),\, x \in I, (y_1, y_2) \in S\right\},$$

with

$$\begin{aligned} N_\alpha(x) &:= \cos\alpha(x) N(x) + \sin\alpha(x) B(x), \\ B_\alpha(x) &:= -\sin\alpha(x) N(x) + \cos\alpha(x) B(x). \end{aligned}$$

Next, for each $0 < \varepsilon < 1$, we "squeeze" the cross sections of the above region, that is, consider

$$\Omega_\varepsilon^\alpha = \left\{ \mathbf{x} \in \mathbb{R}^3 : \mathbf{x} = r(x) + \varepsilon y_1 N_\alpha(x) + \varepsilon y_2 B_\alpha(x),\, x \in I, (y_1, y_2) \in S \right\}.$$

From now on we will omit the symbol α in most notations and write $d\mathbf{x} = dx dy_1 dy_2$ and $dy = dy_1 dy_2$. The symbol $\nabla = (\partial_x, \nabla_y)$ denotes the gradient in the coordinates (x, y_1, y_2) in $\mathbb{R}^3$.

In this work we study the behavior of a quantum particle that moves in Ω_ε, under Dirichlet condition at the boundary $\partial\Omega_\varepsilon$, in the singular limit $\varepsilon \to 0$, that is, when Ω_ε approaches the curve $r(x)$ as $\varepsilon \to 0$. Thus, we initially consider the family of quadratic forms

$$g_\varepsilon(\psi) := \int_{\Omega_\varepsilon} |\nabla\psi|^2 d\mathbf{x}, \qquad \operatorname{dom} g_\varepsilon = \mathcal{H}_0^1(\Omega_\varepsilon), \tag{7}$$

which is associated with the Dirichlet Laplacian operator $-\Delta_\varepsilon$ in Ω_ε.

Remark 1. *For each closed lower bounded quadratic form, say b with domain* $\operatorname{dom} b$ *in a Hilbert space $\mathcal{H}$, it will tacitly be supposed that $b(\xi) = +\infty$ if $\xi \in \mathcal{H} \setminus \operatorname{dom} b$. It is a convenient way to work in the larger space $\mathcal{H}$ instead of only in the closure of* $\operatorname{dom} b$*; moreover, with such praxis, b becomes explicitly lower semicontinuous. See, for instance, Section* 9.3 *and Chapter* 10 *in* [7].

3. Quadratic forms

As usual, we perform a change of variables so that the integration region in (7) becomes independent of $\varepsilon > 0$. For the singular limit $\varepsilon \to 0$, customary "regularizations" will be employed.

Consider the mapping

$$\begin{array}{rccl} f_\varepsilon : & I \times S & \to & \Lambda_\varepsilon \\ & (x, y_1, y_2) & \mapsto & r(x) + \varepsilon\, (y_1 N_\alpha(x) + y_2 B_\alpha(x)), \end{array}$$

and suppose the boundedness $\|k\|_\infty, \|\tau\|_\infty, \|\alpha'\|_\infty < \infty$. These conditions are to guarantee that f_ε will be a diffeomorphism. With this change of variables we work with a fixed region for all $\varepsilon > 0$; more precisely, the domain of the quadratic form (7) turns out to be $\mathcal{H}_0^1(I \times S)$. On the other hand, the price to be paid is a nontrivial Riemannian metric $G = G_\varepsilon$ which is induced by f_ε, i.e.,

$$G = (G_{ij}), \qquad G_{ij} = \langle e_i, e_j \rangle = G_{ji}, \qquad 1 \le i, j \le 3,$$

where

$$e_1 = \frac{\partial f_\varepsilon}{\partial x}, \qquad e_2 = \frac{\partial f_\varepsilon}{\partial y_1}, \qquad e_3 = \frac{\partial f_\varepsilon}{\partial y_2}.$$

Some calculations show that in the Frenet frame

$$J = \begin{pmatrix} e_1 \\ e_2 \\ e_3 \end{pmatrix} = \begin{pmatrix} \beta_\varepsilon & -\varepsilon(\tau+\alpha')\langle z_\alpha^\perp, y\rangle & \varepsilon(\tau+\alpha')\langle z_\alpha, y\rangle \\ 0 & \varepsilon\cos\alpha & \varepsilon\sin\alpha \\ 0 & -\varepsilon\sin\alpha & \varepsilon\cos\alpha \end{pmatrix},$$

where

$$\beta_\varepsilon(x,y) = 1 - \varepsilon k(x)\langle z_\alpha, y\rangle, \quad z_\alpha := (\cos\alpha, -\sin\alpha), \quad z_\alpha^\perp := (\sin\alpha, \cos\alpha).$$

The inverse matrix of J is given by

$$J^{-1} = \begin{pmatrix} \dfrac{1}{\beta_\varepsilon} & \dfrac{(\tau+\alpha')y_2}{\beta_\varepsilon} & -\dfrac{(\tau+\alpha')y_1}{\beta_\varepsilon} \\ 0 & \dfrac{\cos\alpha}{\varepsilon} & \dfrac{-\sin\alpha}{\varepsilon} \\ 0 & \dfrac{\sin\alpha}{\varepsilon} & \dfrac{\cos\alpha}{\varepsilon} \end{pmatrix}.$$

Note that $JJ^t = G$ and $\det J = |\det G|^{1/2} = \varepsilon^2\beta_\varepsilon(x,y)$. Since k is a bounded function, for ε small enough β_ε does not vanish in $I \times S$. Thus, $\beta_\varepsilon > 0$ and f_ε is a local diffeomorphism. By requiring that f_ε is injective (that is, the tube is not self-intersecting), a global diffeomorphism is obtained.

Introducing the notation

$$||\psi||_G^2 := \int_{I\times S} |\psi(x,y)|^2 \varepsilon^2 \beta_\varepsilon(x,y)\, dxdy,$$

we obtain a sequence of quadratic forms

$$\tilde{t}_\varepsilon(\psi) := \left|\left|J^{-1}\nabla\psi\right|\right|_G, \qquad \operatorname{dom}\tilde{t}_\varepsilon = \mathcal{H}_0^1(I\times S, G).$$

More precisely, the above change of coordinates was obtained by a unitary transformation

$$\begin{aligned} U_\varepsilon : \mathrm{L}^2(\Omega_\varepsilon) &\to \mathrm{L}^2(I\times S, G) &(8)\\ \phi &\mapsto \phi\circ f_\varepsilon &(9)\end{aligned}$$

However, we still denote $U_\varepsilon\psi$ by ψ.

Recall that λ_0 is the lowest eigenvalue of the negative Laplacian with Dirichlet boundary conditions in the cross-section region S, and $u_0 \geq 0$ the corresponding eigenfunction of this restricted problem, and we remove the diverging energy λ_0/ε^2 from their quadratic forms. Therefore, we turn to the study of the sequence of quadratic forms

$$\hat{t}_\varepsilon(\psi) := \varepsilon^{-2}\left(\left|\left|J^{-1}\nabla\psi\right|\right|_G^2 - \frac{\lambda_0}{\varepsilon^2}\|\psi\|_G^2 + c\|\psi\|_G^2\right),$$

where c is a positive constant to be chosen later, and its role is to turn $\hat{t}_\varepsilon$, and t_ε below as well, into strictly positive quadratic forms for all $\varepsilon > 0$. In order to

properly deal with the dimensional reduction, we have introduced a convenient global multiplicative factor ε^{-2}. After the norms are written out, we obtain

$$\hat{t}_\varepsilon(\psi) = \int_{I\times S} \Big[\frac{1}{\beta_\varepsilon(x,y)}\,|\psi' + \nabla_y\psi\cdot Ry(\tau+\alpha')(x)|^2 + \frac{\beta_\varepsilon(x,y)}{\varepsilon^2}\left(|\nabla_y\psi|^2 - \lambda_0|\psi|^2\right) + \beta_\varepsilon(x,y)c|\psi|^2\Big]\,dxdy\ .$$

Note that $\operatorname{dom}\hat{t}_\varepsilon = \mathcal{H}_0^1(I\times S)$ is a subspace of $\mathrm{L}^2(I\times S,\beta_\varepsilon(x,y))$. Since $\beta_\varepsilon(x,y)\to 1$ uniformly, as $\varepsilon\to 0$, the spaces $\mathrm{L}^2(I\times S,\beta_\varepsilon(x,y))$ and $\mathrm{L}^2(I\times S)$ are algebraically equivalent (see Remark 5 in [8]). Due to this fact, we assume that $\operatorname{dom}\hat{t}_\varepsilon$ is a subspace of $\mathrm{L}^2(I\times S)$.

We denote by $\hat{T}_\varepsilon$ the self-adjoint operator associated with the quadratic form $\hat{t}_\varepsilon$, so that

$$\hat{T}_\varepsilon = U_\varepsilon^{-1}H_\varepsilon U_\varepsilon + \beta_\varepsilon(x,y)c,$$

where H_ε and U_ε were introduced in Equations (1) and (8), respectively.

Finally, introduce the quadratic form $\operatorname{dom} t_\varepsilon = \mathcal{H}_0^1(I\times S)$ with action

$$t_\varepsilon(\psi) := \int_{I\times S} dydx\left[|\psi' + \nabla_y\psi\cdot Ry(\tau+\alpha')|^2 + \frac{\beta_\varepsilon}{\varepsilon^2}(|\nabla_y\psi|^2 - \lambda_0|\psi|^2) + c|\psi|^2\right].$$

The form t_ε is obtained from $\hat{t}_\varepsilon$ after replacing both, the multiplication by $1/\beta_\varepsilon$ in the first term inside the integral and the multiplication by β_ε in the last term inside the integral, simply by the constant value 1.

Let T_ε be the self-adjoint operator associated with t_ε. By taking into account the discussion just after Lemma 1, it follows that $\hat{T}_\varepsilon$ and T_ε are strictly positive operators, thus for each $\mu > 0$, we have that $-\mu$ is a common element of the resolvent sets of $\hat{T}_\varepsilon$ and T_ε. See Proposition 1.

4. Main results

The goal here is an analysis of the convergence, or not, of the sequence of quadratic forms $\hat{t}_\varepsilon$ as $\varepsilon\to 0$. It will be shown that one may consider t_ε instead of $\hat{t}_\varepsilon$, and the principal conclusions appear in Subsection 4.3. The proofs of the propositions in this section are postponed to Section 5.

4.1. Uniform quadratic form convergence

In this subsection we describe how the uniform convergence of forms (understood in the sense of (10) below and, in a more general context, in terms of the set of relations (11)–(15)) implies the norm resolvent convergence of the associated operators. We state two theorems and they are based on references [17, 16]; however, we only present the proof of one of them, since their proofs are in fact similar.

Theorem 1. *Let $(a_\varepsilon)_\varepsilon, (q_\varepsilon)_\varepsilon$ be two sequences of positive closed sesquilinear quadratic forms in a separable Hilbert space $\mathcal{H}$ with $\operatorname{dom} a_\varepsilon = \operatorname{dom} q_\varepsilon = \mathcal{D}$, for*

all $\varepsilon > 0$, and $A_\varepsilon, Q_\varepsilon$ the self-adjoint operators associated with $(a_\varepsilon)_\varepsilon$ and $(q_\varepsilon)_\varepsilon$, respectively. Suppose that there is $\lambda > 0$ so that $a_\varepsilon, q_\varepsilon \geq \lambda$, for all $\varepsilon > 0$, and

$$|a_\varepsilon(\psi) - q_\varepsilon(\psi)| \leq q(\varepsilon)\, q_\varepsilon(\psi), \qquad \forall \psi \in \mathcal{D}, \tag{10}$$

with $q(\varepsilon) \to 0$ as $\varepsilon \to 0$. Then, there exists $\tilde{C} > 0$ so that, for $\varepsilon > 0$ small enough,

$$\|A_\varepsilon^{-1} - Q_\varepsilon^{-1}\| \leq \tilde{C}\, q(\varepsilon).$$

Now we discuss a generalization of such theorem, that it is related to the following setting. For each $\varepsilon > 0$, let a_ε be a sequence of positive closed sesquilinear forms in a separable Hilbert space $\mathcal{H}$, and A_ε the corresponding associated positive self-adjoint operators. Let $\mathcal{H}_\varepsilon$ be a closed subspace of $\mathcal{H}$ and $\mathcal{H}^\varepsilon$ the orthogonal complement of $\mathcal{H}_\varepsilon$ in $\mathcal{H}$. Then, through the decomposition $\mathcal{H} = \mathcal{H}_\varepsilon \oplus \mathcal{H}^\varepsilon$, each $\psi \in \mathcal{H}$ can be uniquely written as

$$\psi = \psi_\varepsilon + \psi^\varepsilon, \qquad \psi_\varepsilon \in \mathcal{H}_\varepsilon,\, \psi^\varepsilon \in \mathcal{H}^\varepsilon.$$

Suppose that $\psi \in \operatorname{dom} a_\varepsilon$ implies $\psi_\varepsilon \in \operatorname{dom} a_\varepsilon$; consequently, $\psi^\varepsilon \in \operatorname{dom} a_\varepsilon$ as well. Thus,

$$d_\varepsilon := \{\psi_\varepsilon : \psi \in \operatorname{dom} a_\varepsilon\} \quad \text{and} \quad d^\varepsilon := \{\psi^\varepsilon : \psi \in \operatorname{dom} a_\varepsilon\},$$

are dense subsets in $\mathcal{H}_\varepsilon$ and $\mathcal{H}^\varepsilon$ respectively.

Consider the family of restrictions

$$q_\varepsilon := a_\varepsilon|_{d_\varepsilon}, \qquad b_\varepsilon := a_\varepsilon|_{d^\varepsilon},$$

of quadratic forms in $\mathcal{H}_\varepsilon$ and $\mathcal{H}^\varepsilon$, respectively. Both q_ε and b_ε are positive closed quadratic forms. We denote by Q_ε and B_ε the corresponding associated self-adjoint operators. Thus, the quadratic form a_ε can be written as

$$a_\varepsilon(\psi) = q_\varepsilon(\psi_\varepsilon) + b_\varepsilon(\psi^\varepsilon) + 2\, m_\varepsilon(\psi_\varepsilon, \psi^\varepsilon), \tag{11}$$

and for parameters $p(\varepsilon) > 0, q(\varepsilon) > 0$, suppose that the following conditions hold true:

$$q_\varepsilon(\psi_\varepsilon) \geq c(\varepsilon)||\psi_\varepsilon||^2, \quad \forall \psi_\varepsilon \in d_\varepsilon, \quad c(\varepsilon) \geq c_0 > 0; \tag{12}$$

$$b_\varepsilon(\psi^\varepsilon) \geq p(\varepsilon)||\psi^\varepsilon||^2, \quad \forall \psi^\varepsilon \in d^\varepsilon; \tag{13}$$

$$|m_\varepsilon(\psi_\varepsilon, \psi^\varepsilon)|^2 \leq q(\varepsilon)^2\, q_\varepsilon(\psi_\varepsilon)\, b_\varepsilon(\psi^\varepsilon), \quad \forall \psi \in \operatorname{dom} a_\varepsilon; \tag{14}$$

$$q(\varepsilon) \to 0,\ p(\varepsilon) \to \infty,\ c(\varepsilon) = \mathrm{O}(p(\varepsilon)) \quad \text{as} \quad \varepsilon \to 0. \tag{15}$$

Theorem 2. *For ε small enough, there exists $\tilde{D} > 0$, independent of ε, so that,*

$$\left|\left|A_\varepsilon^{-1} - Q_\varepsilon^{-1} \oplus 0\right|\right| \leq p(\varepsilon)^{-1} + \tilde{D}\, q(\varepsilon) c(\varepsilon)^{-1}, \tag{16}$$

where 0 is the null operator on the subspace $\mathcal{H}^\varepsilon$.

Proof. Initially we are going to analyze the quadratic form

$$l_\varepsilon(\psi) := q_\varepsilon(\psi_\varepsilon) + b_\varepsilon(\psi^\varepsilon), \quad \psi \in \operatorname{dom} a_\varepsilon.$$

For each $\varepsilon > 0$, l_ε is a positive closed quadratic form. Let L_ε be the self-adjoint operator associated with l_ε. By conditions (12), (13) and (15), for ε small enough,

$$\left|\left|L_\varepsilon^{-1}\right|\right| \leq D_1\, c(\varepsilon)^{-1},$$

for some $D_1 > 0$. The condition (14) and the definition of l_ε implies that

$$|m_\varepsilon(\psi_\varepsilon, \psi^\varepsilon)| \leq q(\varepsilon)\, l_\varepsilon(\psi).$$

Consequently

$$|a_\varepsilon(\psi) - l_\varepsilon(\psi)| = 2\,|m_\varepsilon(\psi_\varepsilon, \psi^\varepsilon)| \leq 2\, q(\varepsilon)\, l_\varepsilon(\psi).$$

For ε small enough, so that $q(\varepsilon) \leq 1/4$, the above inequality implies that

$$1/2\, l_\varepsilon(\psi) \leq a_\varepsilon(\psi) \leq 3/2\, l_\varepsilon(\psi), \quad \forall \psi \in \operatorname{dom} a_\varepsilon.$$

Thus,

$$\left|\left|A_\varepsilon^{-1}\right|\right| \leq 2\, D_1\, c(\varepsilon)^{-1}.$$

Condition (13) implies that

$$\left|\left|B_\varepsilon^{-1}\right|\right| \leq p(\varepsilon)^{-1}. \tag{17}$$

For $\psi_1, \psi_2 \in \operatorname{dom} a_\varepsilon$ and ε small enough, we have

$$\begin{aligned}\left|\langle A_\varepsilon^{1/2}\psi_1, A_\varepsilon^{1/2}\psi_2\rangle - \langle L_\varepsilon^{1/2}\psi_1, L_\varepsilon^{1/2}\psi_2\rangle\right| &= |a_\varepsilon(\psi_1,\psi_2) - l_\varepsilon(\psi_1,\psi_2)| \\ \leq 2q(\varepsilon)\left(l_\varepsilon(\psi_1) l_\varepsilon(\psi_2)\right)^{1/2} &\leq 2\sqrt{2}\, q(\varepsilon)\left(l_\varepsilon(\psi_1) a_\varepsilon(\psi_2)\right)^{1/2}.\end{aligned}$$

Picking $\psi_1 = L_\varepsilon^{-1}\xi$, $\psi_2 = A_\varepsilon^{-1}\zeta$, where ξ, ζ are arbitrary elements of $\mathcal{H}$, we have

$$\begin{aligned}\left|\langle A_\varepsilon^{-1}\xi, \zeta\rangle - \langle L_\varepsilon^{-1}\xi, \zeta\rangle\right| &\leq 2\sqrt{2}\, q(\varepsilon)\left(\langle A_\varepsilon^{-1}\zeta, \zeta\rangle\ \langle L_\varepsilon^{-1}\xi, \xi\rangle\right)^{1/2} \\ &\leq 4\, D_1\, q(\varepsilon)\, c(\varepsilon)^{-1} ||\xi||\, ||\zeta||.\end{aligned}$$

Therefore,

$$\left|\left|A_\varepsilon^{-1} - L_\varepsilon^{-1}\right|\right| \leq 4\, D_1\, q(\varepsilon)\, c(\varepsilon)^{-1}. \tag{18}$$

Since $L_\varepsilon^{-1} = Q_\varepsilon^{-1} \oplus B_\varepsilon^{-1}$, we conclude that

$$\left|\left|L_\varepsilon^{-1} - Q_\varepsilon^{-1} \oplus 0\right|\right| = \left|\left|B_\varepsilon^{-1}\right|\right|,$$

where 0 is the null operator on the subspace $\mathcal{H}^\varepsilon$. Together with (17) and (18), this leads to (16). □

Remark 2. *There are versions of Theorems* 1 *and* 2 *for which the subspace $\mathcal{H}_\varepsilon$ and/or the operator Q_ε in fact do/does not depend on ε, say they are replaced by $\mathcal{H}_0$ and Q_0, respectively. The corresponding proofs are actually simpler than the one presented above.*

4.2. More about spatial tubes

The proposition below is a justification for considering the simpler action of t_ε instead of $\hat{t}_\varepsilon$, and it is a consequence of the fact that β_ε converges uniformly to 1 as $\varepsilon \to 0$. Its proof, along with the proofs of the other propositions in this section, will be the subject of Section 5.

Proposition 1. *Given $\mu > 0$, then for $\varepsilon > 0$ small enough, there exist $E_3, \tilde{E} > 0$, independent of ε, so that*

$$|\,\hat{t}_\varepsilon(\psi) - t_\varepsilon(\psi)\,| \leq E_3\,\varepsilon\,(t_\varepsilon + \mu)(\psi), \quad \psi \in \operatorname{dom} t_\varepsilon,$$

and

$$\left\|(\hat{T}_\varepsilon + \mu\mathbf{1})^{-1} - (T_\varepsilon + \mu\mathbf{1})^{-1}\right\|_{\mathrm{L}^2(I\times S)} \leq \tilde{E}\,\varepsilon.$$

Now we recall some results of [4] we shall use ahead. For each $\xi \in \mathbb{R}^2$, consider the problem

$$-\mathrm{div}[(1-\xi\cdot y)\nabla_y u] = \lambda(1-\xi\cdot y)u, \qquad u \in \mathcal{H}_0^1(S).$$

By picking $\xi = \varepsilon k(x) z_\alpha$, for ε small enough this operator is positive and with compact resolvent. Denote by $\lambda(\xi) > 0$ its first eigenvalue, i.e.,

$$\lambda(\xi) = \inf_{\{u\in\mathcal{H}_0^1(S):\, u\neq 0\}} \frac{\int_S (1-\xi\cdot y)|\nabla_y u|^2 dy}{\int_S (1-\xi\cdot y)|u|^2 dy}.$$

Thus, for $v \in \mathcal{H}_0^1(I\times S)$, for a.e.$[x]$ we have

$$\frac{1}{\varepsilon^2}\int_S \beta_\varepsilon(x,y)(|\nabla_y v|^2 - \lambda_0|v|^2)dy \geq \gamma_\varepsilon(x)\int_S \beta_\varepsilon(x,y)|v|^2 dy, \tag{19}$$

where

$$\gamma_\varepsilon(x) := \frac{\lambda\,(\varepsilon k(x) z_\alpha(x)) - \lambda_0}{\varepsilon^2}.$$

By taking into account that $k(x)$ is a bounded function, the following lemma was proven in [4]:

Lemma 1. *$\gamma_\varepsilon(x) \to -k(x)^2/4$ uniformly as $\varepsilon \to 0$.*

By (19), it is the clear that if we pick $c > \left\|k(x)^2/4\right\|_\infty$, then the quadratic forms t_ε and $\hat{t}_\varepsilon$ are (strictly) positive for $\varepsilon > 0$ small enough, and from now on we suppose that this inequality holds. Hence, $(-\infty, 0]$ is contained in the resolvent sets of both T_ε and $\hat{T}_\varepsilon$.

Again, for $\xi \in \mathbb{R}^2$ fixed, consider the problem [4]

$$-\Delta u_\xi - \lambda_0 u_\xi = -\xi\cdot\nabla_y u_0, \qquad u_\xi \perp u_0. \tag{20}$$

We recall that u_0 is the eigenfunction corresponding to the first eigenvalue λ_0 of the Dirichlet Laplacian in $\mathcal{H}_0^1(S)$. Denote by χ_1 and χ_2 the solutions to (20) for $\xi = (1,0)$ and $\xi = (0,1)$, respectively. By linearity, for $\xi = (\xi_1, \xi_2) \in \mathbb{R}^2$, the solution to (20) is given by

$$u_\xi = \xi_1\chi_1 + \xi_2\chi_2.$$

The following lemma will be useful ahead and it was also proven in [4].

Lemma 2. *For every $\xi \in \mathbb{R}^2$, we have*

$$\inf_{v \in H_0^1(S)} \int_S \Big[|\nabla_y v|^2 - \lambda_0 |v|^2 + 2(\xi \cdot \nabla_y u_0) v \Big] dy = -\frac{|\xi|^2}{4}. \tag{21}$$

Furthermore, the above infimum is reached for u_ξ given by (20).

Since (21) is a convex variational problem, its minimizer point u_ξ is unique. The function

$$\varphi_0(x,y) := k(x) \cos\alpha(x)\, \chi_1(y) - k(x) \sin\alpha(x)\, \chi_2(y) \tag{22}$$

is the solution to (20) for $\xi = k(x) z_\alpha$. We underline that both χ_1 and χ_2 are orthogonal to u_0 in $\mathrm{L}^2(S)$, thus φ_0 is orthogonal to u_0 as well. Such results from [4], that we have just reviewed, will be important for our considerations of the singular limit $\varepsilon \to 0$.

Therefore, for $\xi = k(x) z_\alpha$ the infimum in (21) is reached exactly at $\varphi_0(x,y)$ and such minimum value is $-k(x)^2/4$. Note that this function of curvature $k(x)$ is present in the operator (4) and also in the associated form (29), and this motivates our introduction of the specific subspaces $\mathcal{L}_0$ and $\mathcal{L}_\varepsilon$ below (and the different quadratic forms ahead as well).

First introduce the closed subspace $\mathcal{L}_0 := \{ w u_0 : w \in \mathrm{L}^2(I) \}$ of $\mathrm{L}^2(I \times S)$ and the orthogonal decomposition

$$\mathrm{L}^2(I \times S) = \mathcal{L}_0 \oplus \mathcal{L}_0^\perp. \tag{23}$$

Thus, given $\psi \in \mathrm{L}^2(I \times S)$, we can write

$$\psi(x,y) = w(x) u_0(y) + \eta(x,y), \tag{24}$$

for some unique $w \in \mathrm{L}^2(I)$ and unique $\eta \in \mathcal{L}_0^\perp$. Now, for each $\varepsilon > 0$, we introduce the subspace $\mathcal{L}_\varepsilon \subset \mathrm{L}^2(I \times S)$ of functions of the form

$$w(x) u_0(y) + \varepsilon w(x) \varphi_0(x,y), \qquad w \in \mathrm{L}^2(\mathbb{R}). \tag{25}$$

Using the characterization (24), we write each $\psi \in \mathrm{L}^2(I \times S)$ in the following form

$$\psi = (w u_0 + \varepsilon w \varphi_0) + (\eta - \varepsilon w \varphi_0), \tag{26}$$

with $(w u_0 + \varepsilon w \varphi_0) \in \mathcal{L}_\varepsilon$ and $(\eta - \varepsilon w \varphi_0) \in \mathcal{L}_0^\perp$; since $\mathcal{L}_\varepsilon \cap \mathcal{L}_0^\perp = \{0\}$, such decomposition is unique and so the Hilbert space $\mathrm{L}^2(I \times S)$ can be written as a (nonorthogonal) direct sum of the subspaces $\mathcal{L}_\varepsilon$ and $\mathcal{L}_0^\perp$.

For each $\varepsilon > 0$ define the quadratic form

$$l_\varepsilon(\psi) := t_\varepsilon(w u_0 + \varepsilon w \varphi_0) + t_\varepsilon(\eta - \varepsilon w \varphi_0), \tag{27}$$

$\mathrm{dom}\, l_\varepsilon = \mathcal{H}_0^1(I \times S)$, and denote by L_ε the associated self-adjoint operator.

Proposition 2. *Given $\mu > 0$, suppose that the derivatives of the functions $k(x), \tau(x)$ and $\alpha(x)$, up to second order, are continuous and bounded. Then, there exist $F_5, \tilde{F} > 0$ so that, for $\varepsilon > 0$ small enough,*

$$|t_\varepsilon(\psi) - l_\varepsilon(\psi)| \le F_5\, \varepsilon\, (l_\varepsilon + \mu)(\psi), \quad \psi \in \mathrm{dom}\, t_\varepsilon,$$

and

$$\left\| (T_\varepsilon + \mu \mathbf{1})^{-1} - (L_\varepsilon + \mu \mathbf{1})^{-1} \right\|_{\mathrm{L}^2(I\times S)} \leq \tilde{F}\, \varepsilon.$$

Now each space $\mathcal{L}_\varepsilon$ can be identified with $\mathcal{L}_0$ through the mapping

$$\omega(x)\,(u_0(y) + \varepsilon\varphi_0(x,y)) \longmapsto \omega(x)u_0(x),$$

and $\mathcal{L}_0$ with $\mathrm{L}^2(\mathbb{R})$ through

$$\omega(x)u_0(y) \mapsto \omega(x).$$

We have

$$\begin{aligned} \|\omega\,(u_0 + \varepsilon\varphi_0)\,\|^2_{\mathcal{L}_\varepsilon} &= \int_{\mathbb{R}\times S} |\omega(x)\,(u_0(y) + \varepsilon\varphi_0(x,y))\,|^2\, dydx \\ &= \int_{\mathbb{R}} (1 + \varepsilon^2 k(x)^2)|w(x)|^2 dx \\ &= \int_{\mathbb{R}\times S} (1 + \varepsilon^2 k(x)^2)|w(x)u_0(y)|^2 dydx, \end{aligned}$$

and thus

$$\|wu_0\|^2_{\mathcal{L}_0} \leq \|\omega\,(u_0 + \varepsilon\varphi_0)\,\|^2_{\mathcal{L}_\varepsilon} \leq (1 + \varepsilon^2\|k\|^2_\infty)\,\|wu_0\|^2_{\mathcal{L}_0},$$

as well as

$$\|w\|^2_{\mathrm{L}^2(I)} \leq \|\omega\,(u_0 + \varepsilon\varphi_0)\,\|^2_{\mathcal{L}_\varepsilon} \leq (1 + \varepsilon^2\|k\|^2_\infty)\,\|w\|^2_{\mathrm{L}^2(I)},$$

and by direct calculation,

$$\|w\|_{\mathrm{L}^2(I)} = \|wu_0\|_{\mathcal{L}_0}.$$

The subspaces $\mathcal{L}_\varepsilon$, $\mathcal{L}_0$ and $\mathrm{L}^2(I)$ are algebraically equivalent to each other, and also with equivalent norms; in addition, $(1 \pm \varepsilon^2\|k\|^2_\infty) \to 1$ uniformly as $\varepsilon \to 0$. Therefore it is possible to identify operators acting in $\mathcal{L}_\varepsilon$ with operators acting in $\mathcal{L}_0$, and then with operators acting in $\mathrm{L}^2(I)$. This is important in our dimensional reduction from the tube to the reference curve.

Restricted to $\mathcal{L}_\varepsilon$, that is, $\eta = \varepsilon w\varphi_0 \in \mathcal{L}_0^\perp$ (see (26)), we have

$$l_\varepsilon(\psi) = t_\varepsilon(wu_0 + \varepsilon w\varphi_0).$$

Due to the many identifications involved, it will be convenient to introduce the following sequence s_ε of quadratic forms in $\mathcal{L}_0$,

$$s_\varepsilon(wu_0) := t_\varepsilon(wu_0 + \varepsilon w\varphi_0), \quad w \in \mathcal{H}^1_0(I), \tag{28}$$

as well as the form t in $\mathcal{L}_0$, $\operatorname{dom} t = \{wu_0 : w \in \mathcal{H}^1_0(I)\}$,

$$\begin{aligned} t(wu_0) &:= \int_{I\times S} \left[|w'u_0|^2 + \left(C(S)(\tau + \alpha')(x) - \frac{k(x)^2}{4} + c \right) |wu_0|^2 \right] dydx \\ &= \int_I \left[|w'|^2 + \left(C(S)(\tau + \alpha')(x) - \frac{k(x)^2}{4} + c \right) |w|^2 \right] dx, \end{aligned} \tag{29}$$

whose associated self-adjoint operator is T described in (2) and (4), in case $I = [0, L]$ and $I = \mathbb{R}$, respectively, that can be thought of acting in either $\mathcal{L}_0$ or $\mathrm{L}^2(I)$.

We finish this subsection with a technical result that will be used ahead.

Lemma 3. *For $\eta \in \mathcal{H}_0^1(I \times S) \cap \mathcal{L}_0^\perp$, there exists $\tilde{G} > 0$ so that, for ε small enough,*

$$t_\varepsilon(\eta) \geq \frac{\tilde{G}}{\varepsilon^2}\|\eta\|^2.$$

Proof. Let λ_1 be the second eigenvalue of the Laplacian in $\mathcal{H}_0^1(S)$ and $\eta \in \mathcal{H}_0^1(I \times S) \cap \mathcal{L}_0^\perp$. It then follows that

$$\int_S \beta_\varepsilon(x,y)\left(\frac{|\nabla_y \eta|^2}{\varepsilon^2} - \lambda_1 \frac{|\eta|^2}{\varepsilon^2}\right) dy \geq \gamma_\varepsilon(x) \int_S \beta_\varepsilon(x,y)|\eta|^2 dy.$$

Since $\gamma_\varepsilon(x)$ converges uniformly to a bounded function as $\varepsilon \to 0$ (see Lemma 1), there exists $G_1 \in \mathbb{R}$ so that, for ε small enough,

$$\gamma_\varepsilon(x) \geq G_1, \qquad \forall x \in \mathbb{R}.$$

Thus,

$$\gamma_\varepsilon(x) \int_S \beta_\varepsilon(x,y)|\eta|^2 dy \geq G_1 \int_S \beta_\varepsilon(x,y)|\eta|^2 dy,$$

and so

$$\int_{I\times S} \beta_\varepsilon(x,y)\left(\frac{|\nabla_y \eta|^2}{\varepsilon^2} - \lambda_1 \frac{|\eta|^2}{\varepsilon^2}\right) dydx \geq G_1 \int_{I\times S} \beta_\varepsilon(x,y)|\eta|^2 dydx.$$

Adding and subtracting the term $\frac{\lambda_0}{\varepsilon^2}\int_{I\times S} \beta_\varepsilon(x,y)|\eta|^2 dydx$ on the left-hand side of the inequality above, we obtain

$$\begin{aligned}
&\int_{I\times S} \beta_\varepsilon(x,y)\left(\frac{|\nabla_y \eta|^2}{\varepsilon^2} - \lambda_0 \frac{|\eta|^2}{\varepsilon^2}\right) dydx \\
&\quad \geq G_1 \int_{I\times S} \beta_\varepsilon(x,y)|\eta|^2 dydx + \frac{(\lambda_1 - \lambda_0)}{\varepsilon^2} \int_{I\times S} \beta_\varepsilon(x,y)|\eta|^2 dydx.
\end{aligned}$$

Since $\beta_\varepsilon(x,y) \to 1$ uniformly as $\varepsilon \to 0$, for $\varepsilon > 0$ small enough, there exist numbers $\delta_1, \delta_2 \in \mathbb{R}$ so that $G_1\beta_\varepsilon(x,y) \geq \delta_1$ and $\beta_\varepsilon(x,y) \geq \delta_2 > 0$ for all $(x,y) \in I \times S$.

Therefore, for ε small enough, there exists $G_2 > 0$ so that

$$\begin{aligned}
t_\varepsilon(\eta) &\geq \int_{I\times S} \beta_\varepsilon(x,y)\left(\frac{|\nabla_y \eta|^2}{\varepsilon^2} - \lambda_0 \frac{|\eta|^2}{\varepsilon^2}\right) dydx + c\int_{\mathbb{R}\times S} |\eta|^2 dydx \\
&\geq \delta_1 \int_{I\times S} |\eta|^2 dydx + \frac{(\lambda_1 - \lambda_0)}{\varepsilon^2}\delta_2 \int_{I\times S} |\eta|^2 dydx + c\int_{I\times S} |\eta|^2 dydx \\
&\geq \frac{G_2}{\varepsilon^2} \int_{I\times S} |\eta|^2 dydx.
\end{aligned}$$

Lastly, it is enough to take $\tilde{G} = G_2$ to complete the proof of the lemma. □

In the next subsection a discussion of the main consequences of the above preparation is presented; in our opinion it is to be considered the main conclusions of this work.

4.3. Discussions

With respect to the results presented up to now, we discuss two points we have found compelling. The first one is a proof that if the reference curve has zero curvature, then the norm resolvent convergence of operators is in effect. The second one is a kind of counterexample to the converse of Theorems 1 and 2, a point of particular mathematical interest.

4.3.1. Norm convergence in case of zero curvature. The goal here is to apply Theorem 2 in order to prove norm resolvent convergence in case the curvature of the reference curve vanishes; it holds for bounded or unbounded tubes, but for definiteness we suppose that $I = \mathbb{R}$; in fact, for bounded tubes it was proven in [8] that such norm resolvent convergence holds for any curvature such that $k(x) \in \mathrm{L}^\infty[0, L]$. As already mentioned, a proof of norm convergence in case of unbounded tubes and nonvanishing curvature is still lacking.

Observe that if $k(x) \equiv 0$, then automatically $r(x)$ is a straight line (here it is then supposed to coincide with the x-axis) and the torsion $\tau(x)$ also vanishes. For fixed $\varepsilon > 0$, the asymptotic terms of the sequence of eigenvalues of the Laplacian in such tube was considered in [5].

Our norm resolvent convergence is as follows.

Theorem 3. *Suppose that $k(x) = 0$ for all $x \in \mathbb{R}$. Then, there exists $\tilde{J} > 0$ so that, for ε small enough,*

$$\left\| T_\varepsilon^{-1} - T^{-1} \oplus 0 \right\| \leq \tilde{J}\varepsilon,$$

where 0 denotes the null operator on the subspace $\mathcal{L}_0^\perp$.

Proof. By the orthogonal decomposition (23)–(24), $\psi \in \operatorname{dom} t_\varepsilon = \mathcal{H}_0^1(\mathbb{R} \times S)$ may be written in the form

$$\psi(x, y) = w(x)u_0(y) + \eta(x, y),$$

with $w \in \mathcal{H}^1(\mathbb{R})$ and $\eta \in \mathcal{H}_0^1(\mathbb{R} \times S) \cap \mathcal{L}_0^\perp$. Thus, the quadratic form $t_\varepsilon(\psi)$ can be rewritten as

$$t_\varepsilon(\psi) = t_\varepsilon(wu_0) + t_\varepsilon(\eta) + 2\, m_\varepsilon(wu_0, \eta),$$

where

$$m_\varepsilon(wu_0, \eta) = \int_{\mathbb{R}\times S} \Big[w'u_0 + w\,(\nabla_y u_0 \cdot Ry)\,\alpha'(x) \Big] \Big[\eta' + (\nabla_y \eta \cdot Ry)\,\alpha'(x) \Big] dxdy.$$

We are going to show that $t_\varepsilon(wu_0)$, $t_\varepsilon(\eta)$ and $m_\varepsilon(wu_0, \eta)$ satisfy the conditions (12)–(15), and then we apply Theorem 2.

A direct substitution shows that

$$\begin{aligned} t_\varepsilon(wu_0) &= \int_{\mathbb{R}} \Big[|w'|^2 + C(S)\alpha'(x)^2 |w|^2 + c|w|^2 \Big] dx \\ &\geq c \int_{\mathbb{R}} |w|^2 dx = c \int_{\mathbb{R}\times S} |wu_0|^2 dxdy. \end{aligned}$$

Lemma 3 guarantees that there exists $\tilde{G} > 0$ so that

$$t_\varepsilon(\eta) \geq \frac{\tilde{G}}{\varepsilon^2} \int_{\mathbb{R}\times S} |\eta|^2 dxdy.$$

Thus, the conditions (12), (13), (15) are satisfied. Now, we are going to show the condition (14). Since

$$\int_S \eta'(x,y) u_0(y)\, dy = 0, \qquad \text{a.e.[x]},$$

we have

$$\begin{aligned} m_\varepsilon(wu_0,\eta) = & \int_{\mathbb{R}\times S} w' u_0 \left(\nabla_y \eta \cdot Ry\right) \alpha'(x)\, dxdy \\ & + \int_{\mathbb{R}\times S} w \left(\nabla_y u_0 \cdot Ry\right) \eta' \alpha'(x)\, dxdy \\ & + \int_{\mathbb{R}\times S} w \left(\nabla_y u_0 \cdot Ry\right) \left(\nabla_y \eta \cdot Ry\right) \left(\alpha'(x)\right)^2 dxdy \end{aligned}$$

Upon integration by parts and Lemma 3, it follows that

$$\begin{aligned} \left| \int_{\mathbb{R}\times S} w' u_0 \left(\nabla_y \eta \cdot Ry\right) \alpha'(x)\, dxdy \right| &= \left| \int_{\mathbb{R}\times S} w' \left(\nabla_y u_0 \cdot Ry\right) \eta\, \alpha'(x)\, dxdy \right| \\ &\leq C_1 \left(\int_{\mathbb{R}\times S} |w' u_0|^2 dxdy \right)^2 \left(\int_{\mathbb{R}\times S} |\eta|^2\, dxdy \right)^2 \\ &\leq J_1\, \varepsilon\, t_\varepsilon(wu_0)^{1/2}\, t_\varepsilon(\eta)^{1/2}, \end{aligned}$$

for some $J_1 > 0$. Repeating this idea with the remaining integrals, we obtain

$$|m_\varepsilon(wu_0,\eta)| \leq J_2\, \varepsilon\, t_\varepsilon(wu_0)^{1/2}\, t_\varepsilon(\eta)^{1/2},$$

for some number $J_2 > 0$. Hence, the result follows by Theorem 2. □

4.3.2. Counterexample. In roughly terms, Theorems 1 and 2 tell us that a uniform convergence of positive quadratic forms implies a norm resolvent convergence of the corresponding (lower bounded) self-adjoint operators. A natural question is if the norm resolvent convergence of a sequence of positive (or uniformly lower bounded) operators implies the uniform convergence of the respective quadratic forms; we answer such question in the negative through an example.

For bounded tubes, that is, $I = [0, L]$, it was proven in [8] (see Theorem 7 and its proof therein) that $\hat{T}_\varepsilon$ converges to T (see (4) and (29)) in the norm resolvent sense; combined with Proposition 1, it follows that T_ε converges to T in the norm resolvent sense. Recall that t_ε and t denote the respective sesquilinear forms. Nevertheless, now we perform a study of the convergence of $t_\varepsilon(\psi)$ in the case of nonzero curvature of the reference curve; we will make use of the quadratic form s_ε, introduced in (28), and we have the following results:

Proposition 3. *For each $\psi \in \mathcal{H}_0^1(I \times S)$, take account of the decomposition* (26).

(i) *If ψ is so that $\eta \neq 0$ and $\eta \neq \varepsilon w\varphi_0$, for all $\varepsilon > 0$ small enough, that is, ψ has a nonzero component in $\mathcal{L}_\varepsilon^\perp$, then there is $\tilde{K} > 0$ with*

$$t_\varepsilon(\eta - \varepsilon\omega\varphi_0) \geq \frac{\tilde{K}}{\varepsilon^2} \|\eta - \varepsilon\omega\varphi_0\|^2,$$

and thus $\lim_{\varepsilon\to 0} t_\varepsilon(\psi) = +\infty$.

(ii) *If ψ is so that $\eta = 0$, that is $\psi = \omega u_0 \in \mathcal{L}_0$, then*

$$\begin{aligned}\lim_{\varepsilon\to 0} t_\varepsilon(\psi) &= \int_{I\times S} \left[|w'u_0|^2 + (C(S)(\tau+\alpha') + c)\,|wu_0|^2\right] dydx \\ &= \int_I \left[|w'|^2 + (C(S)(\tau+\alpha') + c)\,|w|^2\right] dx \\ &\neq t(\psi).\end{aligned}$$

Now we discuss a missing case in Proposition 3, that is, for nonzero curvature what happens with $t_\varepsilon(\psi_\varepsilon)$, for $\psi_\varepsilon \in \mathcal{L}_\varepsilon$, as $\varepsilon \to 0$.

Proposition 4. *Let $\mu > 0$ and suppose that the derivatives of the functions $k(x)$, $\tau(x)$ and $\alpha(x)$, up to second order, are continuous and bounded. Then, there is $\tilde{M} > 0$ so that for all $w \in \mathcal{H}_0^1(I)$ one has*

$$|s_\varepsilon(wu_0) - t(wu_0)| \leq \tilde{M}\,\varepsilon\,(t+\mu)(wu_0).$$

Therefore (see (29)*), for any vector $(wu_0 + \varepsilon w\varphi_0) \in \mathcal{L}_\varepsilon$ one has $\lim_{\varepsilon\to 0}(wu_0 + \varepsilon w\varphi_0) = wu_0$ in $\mathrm{L}^2(I \times S)$ and*

$$\lim_{\varepsilon\to 0} t_\varepsilon(wu_0 + \varepsilon w\varphi_0) = t(wu_0).$$

Hence, in this example the situation is more severe than just nonuniform convergence of quadratic forms, since by Propositions 3 and 4, there is a kind of discontinuity in the convergence to vectors in $\mathcal{L}_0$, in the sense that

$$t(\omega u_0) = \lim_{\varepsilon\to 0} t_\varepsilon(wu_0 + \varepsilon w\varphi_0) \neq \lim_{\varepsilon\to 0} t_\varepsilon(wu_0), \quad \forall w \in \mathcal{H}_0^1[0, L].$$

The missing term in $\lim_{\varepsilon\to 0} t_\varepsilon(wu_0)$, with respect to $t(\omega u_0)$, is directly related to the curvature $k(x)$, and when it is zero we have uniform convergence as previously discussed in Theorem 3. We think the possibility of this kind of phenomenon should not be discarded due to the singular nature of the involved limits, and it is also a way to take into account some subtle contributions of the "discarded dimensions." Otherwise it would be merely enough to write down the relevant ε-dependent quadratic form ($\hat{t}_\varepsilon$ in our case) and apply it to elements of $\mathcal{L}_0$ before taking $\varepsilon \to 0$, but sometimes this is not the case.

5. Proofs of the propositions

Proof of Proposition 1

Initially, observe that

$$(\hat{t}_\varepsilon + \mu)(\psi) \geq \mu\|\psi\|^2 \qquad \text{and} \qquad (t_\varepsilon + \mu)(\psi) \geq \mu\|\psi\|^2.$$

Consequently,

$$\|(\hat{T}_\varepsilon + \mu\mathbf{1})^{-1}\| \leq \frac{1}{\mu} \qquad \text{and} \qquad \|(T_\varepsilon + \mu\mathbf{1})^{-1}\| \leq \frac{1}{\mu}.$$

Since $\beta_\varepsilon \to 1$ uniformly as $\varepsilon \to 0$, for $\varepsilon > 0$ small enough, there exists $\sigma_1 > 0$ so that $\sigma_1 \leq \beta_\varepsilon$. Thus, since $k \in \mathrm{L}^\infty(\mathbb{R})$, $y \in S$ and S is a bounded region, there exist $E_1, E_2 > 0$ so that

$$\left|\left(\frac{1}{\beta_\varepsilon} - 1\right)\right| = \left|\frac{\varepsilon k(x)(y \cdot z_\alpha(x))}{\beta_\varepsilon}\right| \leq E_1\varepsilon,$$

and

$$c|(\beta_\varepsilon - 1)| \leq E_2\varepsilon,$$

for $\varepsilon > 0$ small enough. Under these conditions

$$\begin{aligned}
|\,\hat{t}_\varepsilon(\psi) - t_\varepsilon(\psi)\,| &= |\,(\hat{t}_\varepsilon + \mu)(\psi) - (t_\varepsilon + \mu)(\psi)\,| \\
&\leq \int_{\mathbb{R}\times S}\left|\left(\frac{1}{\beta_\varepsilon} - 1\right)\right| |\psi' + \nabla_y\psi \cdot Ry(\tau + \alpha')|^2 dydx \\
&\quad + \int_{\mathbb{R}\times S} c|(\beta_\varepsilon - 1)||\psi|^2 dydx \\
&\leq E_1\varepsilon \int_{\mathbb{R}\times S} |\psi' + \nabla_y\psi \cdot Ry(\tau + \alpha')|^2 dydx + E_2\varepsilon \int_{\mathbb{R}\times S} |\psi|^2 dydx \\
&\leq E_3\ \varepsilon\ (t_\varepsilon + \mu)(\psi)
\end{aligned}$$

for some $E_3 > 0$. Apply Theorem 1 to complete the proof of the proposition.

Proof of Proposition 2

Due to decomposition (23), each $\psi \in \mathcal{H}_0^1(\mathbb{R} \times S)$ can be written in the form

$$\psi = wu_0 + \eta, \qquad w \in \mathcal{H}^1(\mathbb{R}),\ \eta \in \mathcal{H}_0^1(\mathbb{R} \times S) \cap \mathcal{L}_0^\perp,$$

and consequently

$$\psi = wu_0 + \varepsilon w\varphi_0 + \eta_\varepsilon, \tag{30}$$

where $\eta_\varepsilon = \eta - \varepsilon w\varphi_0$.

By using (30), the quadratic form $(t_\varepsilon + \mu)(\psi)$ can be rewritten as

$$(t_\varepsilon + \mu)(\psi) = (t_\varepsilon + \mu)(wu_0 + \varepsilon w\varphi_0) + (t_\varepsilon + \mu)(\eta_\varepsilon) + 2\,m_\varepsilon(wu_0 + \varepsilon w\varphi_0, \eta_\varepsilon),$$

where

$$
\begin{aligned}
&m_\varepsilon(wu_0+\varepsilon w\varphi_0,\eta_\varepsilon)\\
&\quad=\int_{\mathbb{R}\times S} dydx\Big\{\,[(wu_0+\varepsilon w\varphi_0)'+\nabla_y(wu_0+\varepsilon w\varphi_0)\cdot Ry(\tau+\alpha')]\\
&\qquad\qquad\times[\eta_\varepsilon'+\nabla_y\eta_\varepsilon\cdot Ry(\tau+\alpha')]\,\Big\}\\
&\qquad+\int_{\mathbb{R}\times S}\frac{\beta_\varepsilon(x,y)}{\varepsilon^2}\,[\nabla_y(wu_0+\varepsilon w\varphi_0)\nabla_y\eta_\varepsilon-\lambda_0(wu_0+\varepsilon w\varphi_0)\eta_\varepsilon]\,dydx\\
&\qquad+\int_{\mathbb{R}\times S}(c+\mu)(wu_0+\varepsilon w\varphi_0)\eta_\varepsilon\,dydx.
\end{aligned}
$$

By definition

$$(l_\varepsilon+\mu)(\psi)=(t_\varepsilon+\mu)(wu_0+\varepsilon w\varphi_0)+(t_\varepsilon+\mu)(\eta_\varepsilon);$$

thus,

$$(t_\varepsilon+\mu)(\psi)-(l_\varepsilon+\mu)(\psi)=2\,m_\varepsilon(wu_0+\varepsilon w\varphi_0,\eta_\varepsilon).$$

Using integration by parts and the fact that all the derivatives of the functions $k(x),\tau(x),\alpha(x)$, up to second order, are defined and bounded functions, some calculations (rather long) show that there exist numbers $F_1,F_2,F_3,F_4>0$ so that

$$
\begin{aligned}
m_\varepsilon(wu_0+\varepsilon w\varphi_0,\eta_\varepsilon)\le F_1&\left(\int_{\mathbb{R}}|w'|^2dx\right)^{\frac12}\left(\int_{\mathbb{R}\times S}|\eta_\varepsilon|^2dydx\right)^{\frac12}\\
&+F_2\left(\int_{\mathbb{R}}|w|^2dx\right)^{\frac12}\left(\int_{\mathbb{R}\times S}|\eta_\varepsilon|^2dydx\right)^{\frac12},
\end{aligned}
$$

and, for $\varepsilon>0$ small enough,

$$(t_\varepsilon+\mu)(wu_0+\varepsilon w\varphi_0)\ge F_3\int_{\mathbb{R}}|w|^2dx, \tag{31}$$

$$(t_\varepsilon+\mu)(wu_0+\varepsilon w\varphi_0)\ge F_4\int_{\mathbb{R}}|w'|dx. \tag{32}$$

Since $\eta_\varepsilon\in\mathcal{H}_0^1(\mathbb{R}\times S)\cap\mathcal{L}_0^\perp$, we can apply Lemma 3 to get

$$(t_\varepsilon+\mu)(\eta_\varepsilon)\ge t_\varepsilon(\eta_\varepsilon)\ge\frac{\tilde G}{\varepsilon^2}\int_{\mathbb{R}\times S}|\eta_\varepsilon|^2\,dydx. \tag{33}$$

By (31), (32) and (33), it follows that

$$2\,|\,m_\varepsilon(wu_0+\varepsilon w\varphi_0,\eta_\varepsilon)|\le\ F_5\,\varepsilon\,(t_\varepsilon+\mu)(wu_0+\varepsilon w\varphi_0)^{1/2}\,(t_\varepsilon+\mu)(\eta_\varepsilon)^{1/2}, \tag{34}$$

for some number $F_5>0$.

Now, observe that

$$(t_\varepsilon+\mu)(wu_0+\varepsilon w\varphi_0)\le(l_\varepsilon+\mu)(\psi),$$

and

$$(t_\varepsilon+\mu)(\eta_\varepsilon)\le(l_\varepsilon+\mu)(\psi).$$

Thus, the inequality (34) can be rewritten as

$$|(t_\varepsilon + \mu)(\psi) - (l_\varepsilon + \mu)(\psi)| = 2\,|\,m_\varepsilon(wu_0 + \varepsilon w\varphi_0, \eta_\varepsilon)| \leq F_5\,\varepsilon\,(l_\varepsilon + \mu)(\psi). \tag{35}$$

An application of Theorem 1 completes the proof.

Proof of Proposition 3

For definiteness we assume that $I = \mathbb{R}$; the same proof applies if $I = [0, L]$. For $\psi \in \mathcal{H}_0^1(\mathbb{R} \times S) \cap \mathrm{L}^2(\mathbb{R} \times S)$ we shall use the decomposition (26). To prove (i), observe first that

$$l_\varepsilon(\psi) = t_\varepsilon(wu_0 + \varepsilon w\varphi_0) + t_\varepsilon(\eta - \varepsilon w\varphi_0) \geq t_\varepsilon(\eta - \varepsilon w\varphi_0).$$

By Lemma 3,

$$t_\varepsilon(\eta - \varepsilon w\varphi_0) \geq \frac{\tilde{G}}{\varepsilon^2} \int_{\mathbb{R}\times S} |\eta - \varepsilon w\varphi_0|^2 dydx.$$

Since it is supposed that $\eta \neq 0$ and $\eta \neq \varepsilon w\varphi_0$, we obtain

$$\lim_{\varepsilon\to 0} l_\varepsilon(\psi) \geq \lim_{\varepsilon\to 0} t_\varepsilon(\eta - \varepsilon w\varphi_0) = +\infty.$$

Now we are going to prove (ii). By Lemma 2,

$$\int_S \Big[|\nabla_y\varphi_0|^2 - \lambda_0|\varphi_0|^2 + 2k(x)(z_\alpha(x)\cdot\nabla_y u_0)\varphi_0\Big]dy = -\frac{k(x)^2}{4}. \tag{36}$$

This equality and some calculations imply that

$$\lim_{\varepsilon\to 0} t_\varepsilon(wu_0 + \varepsilon w\varphi_0) = t(wu_0).$$

On the other hand, the function φ_0 satisfy

$$-\Delta\varphi_0 - \lambda_0\varphi_0 = -k(x)(z_\alpha(x)\cdot\nabla_y u_0). \tag{37}$$

Equations (36) and (37) imply that

$$\int_S \left(|\nabla_y\varphi_0|^2 - \lambda_0|\varphi_0|^2\right) dydx = \frac{k(x)^2}{4}.$$

Again, this equality and some calculations imply that

$$\lim_{\varepsilon\to 0} t_\varepsilon(-\varepsilon w\varphi_0) = \int_{\mathbb{R}\times S} \frac{k(x)^2}{4}|w|^2|u_0|^2 dydx.$$

Therefore

$$\lim_{\varepsilon\to 0} l_\varepsilon(\psi) = \int_{\mathbb{R}\times S} \left[|w'u_0|^2 + (C(S)(\tau+\alpha') + c)\,|wu_0|^2\right] dydx.$$

Proof of Proposition 4

Since $\int_S |u_0|^2 dy = 1$ and $C(S) = \int_S |\nabla_y u_0 \cdot Ry|^2 dy$, one can rewrite $t(wu_0)$ in the following form

$$\begin{aligned} t(wu_0) &= \int_{\mathbb{R}} \left[|w'|^2 + \left((\tau(x) + \alpha'(x))^2 C(S) - \frac{k(x)^2}{4} + c \right) |w|^2 \right] dx \\ &= \int_{\mathbb{R}\times S} \left[|w'|^2 |u_0|^2 + |\nabla_y u_0 \cdot Ry|^2 (\tau(x) + \alpha'(x))^2 |w|^2 \right] dydx \\ &\quad + \int_{\mathbb{R}\times S} \left(-\frac{k(x)^2}{4} + c \right) |w|^2 |u_0|^2 dydx. \end{aligned}$$

Step 1. We begin with some observations. The Dirichlet condition at the boundary ∂S implies $\int_S \nabla_y |u_0|^2 dy = 0$. Consequently

$$\int_S u_0 \nabla_y u_0 \cdot Ry \, dy = 0.$$

By definition of $\varphi_0(x, y)$, one sees that

$$\int_S \varphi_0(x, y) u_0(y) dy = 0 \quad \text{and} \quad \int_S \varphi_0'(x, y) u_0(y) dy = 0 \quad \text{a.e.}[x].$$

Now, some calculations show that

$$\begin{aligned} &\Big| \int_{\mathbb{R}\times S} |(wu_0 + \varepsilon w\varphi_0)' + \nabla_y (wu_0 + \varepsilon w\varphi_0) \cdot Ry(\tau + \alpha')|^2 dydx \\ &\quad - \int_{\mathbb{R}\times S} \left[|w'|^2 |u_0|^2 + |\nabla_y u_0 \cdot Ry|^2 (\tau + \alpha')^2 |w|^2 \right] dydx \Big| \\ &= \Big| \int_{\mathbb{R}\times S} \varepsilon^2 |w'|^2 |\varphi_0|^2 \, dydx + \int_{\mathbb{R}\times S} \varepsilon^2 |w|^2 |\varphi_0'|^2 \, dydx \\ &\quad + \int_{\mathbb{R}\times S} \varepsilon^2 |w|^2 |\nabla_y \varphi_0 \cdot Ry|^2 (\tau + \alpha')^2 \, dydx \\ &\quad + \int_{\mathbb{R}\times S} 2\varepsilon w' w u_0 (\nabla_y \varphi_0 \cdot Ry)(\tau + \alpha') \, dydx \\ &\quad + \int_{\mathbb{R}\times S} 2\varepsilon^2 w' w \varphi_0 \varphi_0' \, dydx + \int_{\mathbb{R}\times S} 2\varepsilon w' w \varphi_0 (\nabla_y u_0 \cdot Ry)(\tau + \alpha') \, dydx \\ &\quad + \int_{\mathbb{R}\times S} 2\varepsilon^2 w' w \varphi_0 (\nabla_y \varphi_0 \cdot Ry)(\tau + \alpha') \, dydx \\ &\quad + \int_{\mathbb{R}\times S} 2\varepsilon |w|^2 \varphi_0' (\nabla_y u_0 \cdot Ry)(\tau + \alpha') \, dydx \\ &\quad + \int_{\mathbb{R}\times S} 2\varepsilon^2 |w|^2 \varphi_0' (\nabla_y \varphi_0 \cdot Ry)(\tau + \alpha') \, dydx \\ &\quad + \int_{\mathbb{R}\times S} 2\varepsilon |w|^2 (\nabla_y u_0 \cdot Ry)(\nabla_y \varphi_0 \cdot Ry)(\tau + \alpha')^2 \, dydx \Big| \end{aligned}$$

Observe that all the above integrals in the variable y are bounded functions of the variable x. For instance, the function

$$\begin{aligned} g(x) &:= \int_S \varphi_0(x,y)\nabla_y u_0 \cdot Ry\, dy \\ &= k(x)\cos\alpha(x)\int_S \chi_1(y)\left(\frac{\partial u_0}{\partial y_1}y_2 - \frac{\partial u_0}{\partial y_2}y_1\right)dy \\ &\quad - k(x)\sin\alpha(x)\int_S \chi_2(y)\left(\frac{\partial u_0}{\partial y_1}y_2 - \frac{\partial u_0}{\partial y_2}y_1\right)dy \end{aligned}$$

is bounded in $\mathbb{R}$ since $\|k\|_\infty < \infty$. Using these properties, there exist numbers $M_1, M_2, M_3 > 0$ so that

$$\begin{aligned} &\left|\int_{\mathbb{R}\times S} |(wu_0 + \varepsilon w\varphi_0)' + \nabla_y(wu_0 + \varepsilon w\varphi_0)\cdot Ry(\tau+\alpha')|^2 dydx \right. \\ &\qquad \left. - \int_{\mathbb{R}\times S}\Big[|w'|^2|u_0|^2 + |\nabla_y u_0 \cdot Ry|^2(\tau+\alpha')^2|w|^2\Big]dydx\right| \\ &\quad \le M_1\varepsilon\int_{\mathbb{R}}|w'|^2dx + M_2\varepsilon\int_{\mathbb{R}}|w|^2dx + M_3\varepsilon\left(\int_{\mathbb{R}}|w|^2dx\right)^{1/2}\left(\int_{\mathbb{R}}|w'|^2dx\right)^{1/2}. \end{aligned}$$

Step 2. We shall apply Lemma 2. A direct replacement, using the definition of $\varphi_0(x,y)$, shows that

$$\begin{aligned} &\int_{\mathbb{R}\times S}\Big[(|\nabla_y\varphi_0|^2 - \lambda_0|\varphi_0|^2) + 2k(x)(z_\alpha(x)\cdot\nabla_y u_0)\varphi_0\Big]|w|^2 dydx \\ &\qquad = -\int_{\mathbb{R}\times S}\frac{k(x)^2}{4}|w|^2|u_0|^2 dydx. \end{aligned}$$

Thus, one sees that there exists $M_4 > 0$ so that

$$\begin{aligned} &\left|\int_{\mathbb{R}\times S}\frac{\beta_\varepsilon}{\varepsilon^2}(|\nabla_y\psi|^2 - \lambda_0|\psi|^2)dydx + \int_{\mathbb{R}}\frac{k(x)^2}{4}|w|^2|u_0|^2 dydx\right| \\ &\quad = \left|\int_{\mathbb{R}\times S}\Big[\beta_\varepsilon(x,y)(|\nabla_y\varphi_0|^2 - \lambda_0|\varphi_0|^2) + 2k(x)(z_\alpha(x)\cdot\nabla_y u_0)\varphi_0\Big]|w|^2 dydx\right. \\ &\qquad \left. + \int_{\mathbb{R}\times S}\frac{k(x)^2}{4}|w|^2|u_0|^2 dydx\right| \\ &\quad = \left|\int_{\mathbb{R}\times S}\varepsilon k(x)(y\cdot z_\alpha(x))(|\nabla_y\varphi_0|^2 - \lambda_0|\varphi_0|^2)|w|^2 dydx\right| \\ &\quad \le M_4\,\varepsilon\int_{\mathbb{R}}|w|^2 dx. \end{aligned}$$

Again we have used the fact that

$$h(x) := k(x)\int_S (y\cdot z_\alpha(x))\,(|\nabla_y\varphi_0|^2 - \lambda_0|\varphi_0|^2)\,dy,$$

is a bounded function. With this we conclude step 2.

By Steps 1 and 2, there exist numbers $M_5, M_6, M_7 > 0$ so that

$$\begin{aligned}|s_\varepsilon(wu_0) - t(wu_0)| &= |(s_\varepsilon + \mu)(wu_0) - (t+\mu)(wu_0)| \\ &\leq M_5\,\varepsilon \int_{\mathbb{R}} |w'|^2 dx + M_6\,\varepsilon \int_{\mathbb{R}} |w|^2 dx \\ &\quad + M_7\,\varepsilon \left(\int_{\mathbb{R}} |w|^2 dx\right)^{1/2} \left(\int_{\mathbb{R}} |w'|^2 dx\right)^{1/2}.\end{aligned}$$

Observe that $\int_{\mathbb{R}} |w'|^2 dx \leq (t+\mu)(wu_0)$ and

$$\int_{\mathbb{R}} |w|^2 dx = \frac{1}{\mu}\int_{\mathbb{R}} \mu|w|^2 dx \leq \frac{1}{\mu}(t+\mu)(wu_0).$$

Thus, there exists $M_8 > 0$, so that

$$|(s_\varepsilon + \mu)(wu_0) - (t+\mu)(wu_0)| \leq$$

$$M_5\,\varepsilon\,(t+\mu)(wu_0) + \frac{M_6}{\mu}\,\varepsilon\,(t+\mu)(wu_0) + \frac{M_7}{\mu^{1/2}}\,\varepsilon\,((t+\mu)(wu_0))^{1/2}((t+\mu)(wu_0))^{1/2}$$

$$\leq M_8\,\varepsilon\,(t+\mu)(wu_0)$$

This completes the proof of Proposition 4.

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Equilibrium Analysis of a Dissipative Fermion System

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Abstract. A model of an open system of fermion particles submitted to a constant magnetic field and immersed in a reservoir of phonons is considered within this article. The focus is set on the large time behavior of this system, the purpose being to illustrate the methods of Quantum Markov Semigroup Theory. After providing sufficient conditions to ensure the existence of the semigroup, this report goes through the construction of stationary states, the analysis of the equilibrium via detailed balance conditions. Ergodic behavior of the system is obtained as a byproduct of the above.

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1. Introduction

This paper provides a mathematical model of transport phenomena for a class of open quantum systems where the main part is made of fermion particles in a magnetic field. The above system is immersed in a reservoir of phonons (boson particles) which induces dissipation. The goal is to apply the methods of the qualitative analysis of Quantum Markov Theory as developed in a series of recent researches (see [18], [19], [33], [24], [34], [22], [23], [21], [17], [36]). More precisely, the following issues are investigated:

- Construction of the Quantum Markov Semigroup describing the open system dynamics;
- The existence of invariant states;
- Equilibrium and the convergence towards the equilibrium (ergodicity);
- Analysis of the decoherence.

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A *Quantum Markov Semigroup* (QMS) arises as the natural non commutative extension of the well-known concept of Markov semigroup defined on a classical probability space and represents the loss-memory evolution of a microscopic system in accordance with the quantum uncertainty principle. The roots of the theory go back to the first researches on the so-called *open quantum systems* (for an account see [2]), and have found its main non commutative tools in much older abstract results like the characterization of *completely positive* maps due to Stinespring (see [38]).

Definition 1. Let $\mathfrak{A}$ be a *-algebra and $\mathcal{P} : \mathfrak{A} \to \mathfrak{A}$ a linear map. $\mathcal{P}$ is *completely positive* if for any finite collection $a_1, \ldots, a_n,\ b_1, \ldots, b_n$ of elements of $\mathfrak{A}$ the element

$$\sum_{i,j} {a_i}^* \mathcal{P}({b_i}^* b_j) a_j$$

is positive.

Throughout this paper, we will restrict our *-algebras to the significant cases of C^*algebras and von Neumann algebras of operators on a complex separable Hilbert space $\mathfrak{h}$. The symbol $\mathfrak{M}$ will be used to denote a generic von Neumann algebra, while $\mathfrak{B}$ will be assigned to a C^*-algebra. Moreover, we always assume that our C^*-algebra $\mathfrak{B}$ contains a unit $\mathbf{1}$. In this case states are elements of the dual $\mathfrak{B}^*$ of $\mathfrak{B}$. A state φ is *pure* if the only positive linear functionals majorized by φ are of the form $\lambda\varphi$ with $0 \leq \lambda \leq 1$. For an abelian C^*-algebra, the set of pure states coincides with that of all *characters*, also called spectrum of the algebra (see [8], Prop. 2.3.27, p. 62). A character φ of an abelian C^*-algebra $\mathfrak{A}$ is a state which satisfies $\varphi(ab) = \varphi(a)\varphi(b)$, for all $a, b \in \mathfrak{A}$; the set of all these elements is usually denoted $\sigma(\mathfrak{A})$ (for *spectrum*) or $P_{\mathfrak{A}}$ (for *pure states*).

If $\mathfrak{M}$ is a von Neumann algebra, its predual is denoted $\mathfrak{M}_*$. The predual contains in particular all the normal states. As a rule, we will only deal with *normal states* φ for which there exists a density matrix ρ, that is, a positive trace-class operator of $\mathfrak{h}$ with unit trace, such that $\varphi(a) = \mathrm{tr}\,(\rho\, a)$ for all $a \in \mathcal{A}$.

Definition 2. A quantum *sub-Markov semigroup, or quantum dynamical semigroup* (QDS) on a *-algebra $\mathfrak{A}$ which has a unit $\mathbf{1}$, is a one-parameter family $\mathcal{T} = (\mathcal{T}_t)_{t \in \mathbb{R}_+}$ of linear maps of $\mathfrak{A}$ into itself satisfying

(M1) $\mathcal{T}_0(x) = x$, for all $x \in \mathfrak{A}$;
(M2) Each $\mathcal{T}_t(\cdot)$ is completely positive;
(M3) $\mathcal{T}_t(\mathcal{T}_s(x)) = \mathcal{T}_{t+s}(x)$, for all $t, s \geq 0$, $x \in \mathfrak{A}$;
(M4) $\mathcal{T}_t(\mathbf{1}) \leq \mathbf{1}$ for all $t \geq 0$.

A quantum dynamical semigroup is called *quantum Markov* (QMS) if $\mathcal{T}_t(\mathbf{1}) = \mathbf{1}$ for all $t \geq 0$.

We state now different topological conditions on the above semigroups.

If $\mathfrak{A}$ is a C^*-algebra, a quantum Markov semigroup defined on $\mathfrak{A}$ is called a *quantum Feller semigroup* if

(M5s) For each $x \in \mathfrak{A}$, the map $t \mapsto \mathcal{T}_t(x)$ is strongly continuous.

A general quantum dynamical semigroup is *uniformly* (*or norm*) *continuous* if it additionally satisfies

(M5u) $\lim_{t\to 0} \sup_{\|x\|\leq 1} \|\mathcal{T}_t(x) - x\| = 0$.

If $\mathfrak{A}$ is a von Neumann algebra, (M5s) is usually replaced by the weaker condition

(M5σ) For each $x \in \mathfrak{A}$, the map $t \mapsto \mathcal{T}_t(x)$ is σ-weak continuous on $\mathfrak{A}$, and $\mathcal{T}_t(\cdot)$ is normal or σ-weak continuous.

The generator $\mathcal{L}$ of the semigroup $\mathcal{T}$ is then defined in the w^* or σ-weak sense. That is, its domain $D(\mathcal{L})$ consists of elements x of the algebra for which the w^*-limit of $t^{-1}(\mathcal{T}_t(x) - x)$ exists as $t \to 0$. This limit is denoted then $\mathcal{L}(x)$.

The *predual semigroup* $\mathcal{T}_*$ is defined on $\mathfrak{M}_*$ as $\mathcal{T}_{*t}(\varphi)(x) = \varphi(\mathcal{T}_t(x))$ for all $t \geq 0,\ x \in \mathfrak{M},\ \varphi \in \mathfrak{M}_*$. Its generator is denoted $\mathcal{L}_*$.

2. Landau levels

We follow [3] to introduce Landau levels for a single electron submitted to a magnetic field. Further on, a whole system of electrons will be considered and subsequently, perturbations due to the action of a boson reservoir will be introduced.

Consider the Hilbert space $\mathfrak{h} = L^2(\mathbb{R}^2)$, which will be used to represent an electron subject to a constant magnetic field. On the above space we take the orthonormal basis of Hermite functions,

$$e_n(x) = \frac{1}{\pi^{1/4}\sqrt{2^n n!}} e^{-\frac{x^2}{2}} h_n(x), \tag{1}$$

where h_n denotes the nth Hermite polynomial which is characterized by

$$h_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}. \tag{2}$$

The argument which justifies the choice of this particular orthonormal basis is that each e_n is an eigenvector of the harmonic oscillator Hamiltonian $H_0 = \frac{1}{2}\left(P^2 + Q^2\right)$, where P denotes the momentum operator and Q, the position operator.

$$H_0 e_n = \left(n + \frac{1}{2}\right) e_n. \tag{3}$$

We consider now the action of a magnetic field pointing along the positive direction of the z-axis. By choosing the gauge adequately, one may suppose that this field is produced by a vector potential $V^{\uparrow} = \frac{1}{2}(-y, x, 0)$, so that the magnetic field is given by $\overrightarrow{B} = \nabla \times V^{\uparrow} = (0, 0, 1)$. Define

$$Q_- = -i\frac{\partial}{\partial x} + \frac{y}{2} \tag{4}$$

$$P_- = -i\frac{\partial}{\partial y} - \frac{x}{2}, \tag{5}$$

and a new Hamiltonian

$$H^{\uparrow} = \frac{1}{2}\left(P_-^2 + Q_-^2\right). \tag{6}$$

Now, suppose the magnetic field being oriented along the negative z-axis, which means a vector potential $V^{\downarrow} = \frac{1}{2}(y, -x, 0)$ and $\overrightarrow{B} = \nabla \times V^{\downarrow} = (0, 0, -1)$. Consequently, introduce the operators

$$Q_+ = -i\frac{\partial}{\partial y} + \frac{x}{2}, \tag{7}$$

$$P_+ = -i\frac{\partial}{\partial x} - \frac{y}{2}, \tag{8}$$

$$H^{\downarrow} = \frac{1}{2}\left(P_+^2 + Q_+^2\right). \tag{9}$$

One obtains the following commutativity relations

$$[Q_+, Q_-] = [P_+, Q_-] = [Q_+, P_-] = [P_+, P_-] = 0$$

So that $[H^{\uparrow}, H^{\downarrow}] = 0$ and one can choose a family of orthonormal vectors $\psi_{m,\ell}$ such that

$$H^{\downarrow}\psi_{m,\ell} = \left(m + \frac{1}{2}\right)\psi_{m,\ell} \tag{10}$$

$$H^{\uparrow}\psi_{m,\ell} = \left(\ell + \frac{1}{2}\right)\psi_{m,\ell}. \tag{11}$$

These two Hamiltonians are both degenerate. To summarize, let define $S = \{\uparrow, \downarrow\}$ and consider two maps $E, d : S \times \mathbb{N}^2 \to \mathbb{N}$ such that for any $s \in S$, and $\mathbf{n} = (m, \ell)$, they are given by

$$E(s, \mathbf{n}) = \begin{cases} \left(m + \frac{1}{2}\right) & \text{if } s = \downarrow, \\ \left(\ell + \frac{1}{2}\right) & \text{if } s = \uparrow. \end{cases} \tag{12}$$

$$d(s, \mathbf{n}) = \begin{cases} \ell & \text{if } s = \downarrow, \\ m & \text{if } s = \uparrow. \end{cases} \tag{13}$$

That is, $E(s, \mathbf{n})$ is the eigenvalue of H^s, and $d(s, \mathbf{n})$ its index of *degeneracy*.

Each unbounded Hamiltonian H^s has a domain

$$D(H^s) = \left\{ u = \sum_{\mathbf{n}\in\mathbb{N}^2} \alpha(\mathbf{n})\psi_{\mathbf{n}} \in \mathfrak{h}_0 : \sum_{\mathbf{n}\in\mathbb{N}^2} \left(\alpha(\mathbf{n})E(s, \mathbf{n})\right)^2 < \infty \right\}.$$

Under the action of the field, it has been experimentally observed that the available states clump together into Landau levels separated by the cyclotron energy. As the magnetic field is swept, the Landau levels move relative to the Fermi energy.

These considerations will determine the definition of a connectivity matrix between "sites" (m, ℓ) in a further section of this report.

3. A representation of a magnetic fermion system

Now, a Fermi–Fock space will be used to represent a system of particles like the electrons above. On the other hand, the dynamics of this system requires to be written through the second quantization of the single particle Hamiltonian.

3.1. The Fermi–Fock space

Let denote $\mathfrak{h}_0 = L^2(\mathbb{R}^2)$. Assume $(\psi_{m,\ell})_{m,\ell\in\mathbb{N}^2}$ to be the orthonormal basis constructed in the previous section. We denote by a boldface character vectors $\mathbf{n} = (m,\ell) \in \mathbb{N}^2$.

The set of all finite subsets of $\mathbb{N}^2$ is denoted $\mathfrak{P}_f\left(\mathbb{N}^2\right)$ and for any $\Lambda \in \mathfrak{P}_f\left(\mathbb{N}^2\right)$, we denote $\mathfrak{h}_0^\Lambda$ the finite-dimensional Hilbert subspace of $\mathfrak{h}_0$ generated by the vectors $(\psi_{m,\ell};\ (m,\ell) \in \Lambda)$.

We introduce the fermionic Fock space $\mathfrak{h} = \Gamma_f(\mathfrak{h}_0)$ associated to $\mathfrak{h}_0$. Call first $\Gamma(\mathfrak{h}_0) = \bigoplus_{n\in\mathbb{N}} \mathfrak{h}_0^{\otimes n}$, the Fock space, and $e(u) = \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} u^{\otimes n}$, for any $u \in \mathfrak{h}_0$. The family of vectors $(e(u);\ u \in \mathfrak{h}_0)$ generates the Fock space. These vectors are usually referred to as *coherent* (*pure*) *states*.

Define an operator $\mathbf{P}_\mathrm{a}$ on the Fock space as follows,

$$\mathbf{P}_\mathrm{a}(f_1 \otimes f_2 \otimes \cdots \otimes f_n) = \frac{1}{n!} \sum_\pi \varepsilon_\pi f_{\pi_1} \otimes \cdots \otimes f_{\pi_n}.$$

The sum is over all permutations $\pi : \{1,\ldots,n\} \to \{\pi_1,\ldots,\pi_n\}$ of the indices and ε_π is 1 if π is even and -1 if π is odd. Define the anti-symmetric tensor product on the Fock space as $f_1 \wedge \cdots \wedge f_n = \mathbf{P}_\mathrm{a}(f_1 \otimes f_2 \otimes \cdots \otimes f_n)$. In this manner, the Fermi–Fock space $\mathfrak{h}$ is obtained as

$$\mathfrak{h} = \Gamma_f(\mathfrak{h}_0) = \mathbf{P}_\mathrm{a}\left(\bigoplus_{n\in\mathbb{N}} \mathfrak{h}_0^{\otimes n}\right) = \bigoplus_{n\in\mathbb{N}} \mathfrak{h}_0^{\wedge n}.$$

3.2. Creation and annihilation operators

Define on $\Gamma(\mathfrak{h}_0)$, $a(f)$ and $a^\dagger(f)$ by initially setting $a(f)\psi^{(0)} = 0$, $a^\dagger(f)\psi^{(0)} = f$, for $\psi = (\psi^{(0)}, \psi^{(1)}, \ldots) \in \Gamma(\mathfrak{h}_0)$ with $\psi^{(j)} = 0$ for all $j \geq 1$, and

$$a^\dagger(f)(f_1 \otimes \cdots \otimes f_n) = \sqrt{n+1} f \otimes f_1 \otimes \cdots \otimes f_n. \tag{14}$$

$$a(f)(f_1 \otimes \cdots \otimes f_n) = \sqrt{n} \langle f, f_1\rangle f_2 \otimes f_3 \otimes \cdots \otimes f_n. \tag{15}$$

Finally, define annihilation and creation on $\Gamma_f(\mathfrak{h}_0)$ as $b(f) = \mathbf{P}_\mathrm{a} a(f) \mathbf{P}_\mathrm{a}$ and $b^\dagger(f) = \mathbf{P}_\mathrm{a} a^\dagger(f) \mathbf{P}_\mathrm{a}$.

These operators satisfy the Canonical Anti-commutation Relations (CAR).

$$\{b(f), b(g)\} = 0 = \{b^\dagger(f), b^\dagger(g)\} \tag{16}$$

$$\{b(f), b^\dagger(g)\} = \langle f, g\rangle \mathbf{1}, \tag{17}$$

for all $f, g \in \mathfrak{h}_0$, where we use the notation $\{A, B\} = AB + BA$ for two operators A and B.

$b(f)$ and $b^\dagger(g)$ have bounded extensions to the whole space $\mathfrak{h}$ since $\|b(f)\| = \|f\| = \|b^\dagger(f)\|$.

The C^*-algebra generated by $\mathbf{1}$ and all the $b(f)$, $f \in \mathfrak{h}_0$, is denoted $\mathfrak{A}(\mathfrak{h}_0)$. It is known as the canonical *CAR* algebra.

We write $b^\dagger_{\mathbf{n}} = b^\dagger(\psi_{\mathbf{n}})$ (respectively $b_{\mathbf{n}} = b(\psi_{\mathbf{n}})$) the creation (respectively annihilation) operator associated with $\psi_{\mathbf{n}} \in \mathfrak{h}_0$, ($\mathbf{n} = (m, \ell) \in \mathbb{N}^2$). Within this framework, the number operator is given by $N_{\mathbf{n}} = b^\dagger_{\mathbf{n}} b_{\mathbf{n}}$.

Remark 1. The algebra $\mathfrak{A}(\mathfrak{h}_0)$ is the unique, up to *-isomorphism, C^*-algebra generated by elements $b(f)$ satisfying the CAR over $\mathfrak{h}_0$. The family

$$(b(f), b^\dagger(g);\ f, g \in \mathfrak{h}_0)$$

is **irreducible** on $\mathfrak{h}$: the only operators which commute with this family are the scalar multiples of the identity. The same property is satisfied by $(b_{\mathbf{n}}, b^\dagger_{\mathbf{n}};\ \mathbf{n} \in \mathbb{N}^2)$, since $(\psi_{\mathbf{n}})_{\mathbf{n}\in\mathbb{N}^2}$ is an orthonormal basis of $\mathfrak{h}_0$.

The algebra $\mathfrak{A}(\mathfrak{h}_0)$ is the strong closure of $\mathfrak{D} = \bigcup_{\Lambda\in\mathfrak{P}_f(\mathbb{N}^2)} \mathfrak{A}(\mathfrak{h}_0^\Lambda)$, (**quasi-local property**). Moreover, the finite-dimensional algebras $\mathfrak{A}(\mathfrak{h}_0^\Lambda)$ are isomorphic to algebras of matrices with complex components.

3.3. Second quantization of Hamiltonians

For each $s \in S$, the second quantization of the Hamiltonian H^s on the Fock space $\Gamma(\mathfrak{h}_0)$ is denoted $\mathbf{H}^s_0 = \Gamma(H^s)$, which is defined as usual as

$$\mathbf{H}^s_0 e(u) = e(H^s u),\ (u \in D(H^s)). \tag{18}$$

Thus, the Hamiltonian on the Fermi–Fock space is given by

$$\mathbf{H}^s = \mathbf{P}_{\mathrm{a}} \mathbf{H}^s_0 \mathbf{P}_{\mathrm{a}} = \sum_{\mathbf{i}} E(s, \mathbf{i}) b^\dagger_{\mathbf{i}} b_{\mathbf{i}}. \tag{19}$$

3.4. Configuration of particles

Since $\mathbb{N}^2$ is a countable set, from now on we choose a fixed enumeration, that is we write

$$\mathbb{N}^2 = \{\mathbf{n}_0, \mathbf{n}_1, \ldots, \mathbf{n}_k, \ldots\},$$

where $\mathbf{n}_0 = (0, 0)$, $\mathbf{n}_k = (m_k, \ell_k)$. Though the choice of an enumeration is worthless to mathematics, it is particularly meaningful in physics. We will come back on this question later, after introducing some concepts of Graph Theory. At this stage, we simply need to refer to a given order to pick up points in $\mathbb{N}^2$.

For each $F \in \mathfrak{P}_f\left(\mathbb{N}^2\right)$, we write 1_F the characteristic function of this set. Thus, $1_F : \mathbb{N}^2 \to \{0, 1\}$ and we call this function $\eta = 1_F$ a *configuration*. We denote $\mathfrak{C}$ the set of all configurations, that is

$$\mathfrak{C} = \left\{\eta : \mathbb{N}^2 \to \{0, 1\};\ \eta(\mathbf{n}) = 1 \text{ for a finite number of points } \mathbf{n}\right\}.$$

Notice that this set is contained in each space $\ell^p(\mathbb{N}^2)$, for $p \in [1, \infty]$.

Given $\eta \in \mathfrak{C}$, its *support* is the smallest finite set $\Lambda \subset \mathbb{N}^2$ such that $\eta(\mathbf{k}) = 0$ for all $\mathbf{k} \in \Lambda^c$. Let denote $\mathfrak{C}(\Lambda)$ the set of all configurations with support contained in a finite set $\Lambda \subset \mathbb{N}^2$.

Let $1_{\mathbf{k}}$ be the configuration $1_{\{\mathbf{k}\}}$, $(\mathbf{k} \in \mathbb{N}^2)$ and for all $\eta = 1_{\{\mathbf{n}_1,\ldots,\mathbf{n}_m\}}$.

$$\mathbf{b}^\dagger(\eta) = b^\dagger_{\mathbf{n}_m} b^\dagger_{\mathbf{n}_{m-1}} \ldots b^\dagger_{\mathbf{n}_1} \tag{20}$$

$$\mathbf{b}(\eta) = b_{\mathbf{n}_m} b_{\mathbf{n}_{m-1}} \ldots b_{\mathbf{n}_1}, \tag{21}$$

To obtain a cyclic representation of $\mathfrak{A}(\mathfrak{h}_0)$ call $|0\rangle$ the vacuum vector in $\mathfrak{h}$, and

$$|\eta\rangle = \mathbf{b}^\dagger(\eta)\,|0\rangle,\ (\eta \in \mathfrak{C}).$$

Then $(|\eta\rangle;\ \eta \in \mathfrak{C})$ is an orthonormal basis of $\mathfrak{h}$. So, any $x \in \mathfrak{A}(\mathfrak{h}_0)$ can be represented as an operator in $\mathfrak{L}(\mathfrak{h})$ in the form

$$x = \sum_{\eta,\zeta \in \mathfrak{C}} x(\eta,\zeta)|\eta\rangle\langle\zeta|.$$

Moreover, for each $x \in \mathfrak{D}$, there exists a finite set $\Lambda \subset \mathbb{N}^2$ such that the sum above can be reduced to $\eta, \zeta \in \mathfrak{C}(\Lambda)$.

The domain $D(\mathbf{H}^s)$ includes $\mathfrak{v}$, the vector space spanned by $(|\eta\rangle,\ \eta \in \mathfrak{C})$. Given $\eta = 1_{\{\mathbf{n}_1,\ldots,\mathbf{n}_m\}}$, let denote

$$E(s,\eta) := \sum_{i=1}^{m} E(s,\mathbf{n}_i) = \sum_{\mathbf{k}} \eta(\mathbf{k}) E(s,\mathbf{k}), \tag{22}$$

so that

$$\mathbf{H}^s|\eta\rangle = E(s,\eta)|\eta\rangle, \tag{23}$$

and this Hamiltonian can formally be written as

$$\mathbf{H}^s = \sum_{\eta \in \mathfrak{C}} E(s,\eta)|\eta\rangle\langle\eta|. \tag{24}$$

The restriction

$$\mathbf{H}^{s,\Lambda} = \sum_{\text{support } \eta \,\subset\, \Lambda} E(s,\eta)|\eta\rangle\langle\eta|$$

of $\mathbf{H}^s$ to each space $\Gamma_f(\mathfrak{h}_0^\Lambda)$ is an element of $\mathfrak{A}(\mathfrak{h}_0^\Lambda)$, $\Lambda \in \mathfrak{P}_f\left(\mathbb{N}^2\right)$, so that $\mathbf{H}^{s,\Lambda}$ is a bounded operator. Moreover, for each fixed $\eta \in \mathfrak{C}$ it holds

$$\left\|\mathbf{H}^s|\eta\rangle - \mathbf{H}^{s,\Lambda}|\eta\rangle\right\| = E(s,\eta)(1 - 1_\Lambda(\eta)) \to 0,$$

as Λ increases to $\mathbb{N}^2$.

4. The open system dynamics

The interaction of the main system with a reservoir of phonons is now considered. This will be reflected through a Quantum Markov Semigroup, that is, a generator of the semigroup will be proposed. As it is well known, the Markovian approach to open system dynamics is usually obtained by limiting procedures involving a rescaling of both time and space (e.g., the so-called *stochastic limit* introduced by Accardi et al. in [1], which includes the weak coupling limit). Here, we use the general form obtained for the generator in such approaches. This form has been

rigorously studied by Gorini, Kossakowski and Sudharshan in [28], Lindblad [30], Christensen and Evans [11]. Moreover, the case of fermions systems submitted to perturbations due to phonons has been firstly studied in [35] and extended as an example of a decoherent system in [36]. No magnetic field has been considered up to now. Here below, we partially rephrase the construction given in [36], adapted to the current main dynamics which includes the action of a magnetic field.

We start noticing that elementary computations based on the C.A.R. yield

$$b_{\mathbf{j}}^{\dagger}|\eta\rangle = (1-\eta(\mathbf{j}))|\eta + 1_{\mathbf{j}}\rangle, \tag{25}$$

$$b_{\mathbf{i}}|\eta\rangle = \eta(\mathbf{i})|\eta - 1_{\mathbf{i}}\rangle,\ (\mathbf{i},\mathbf{j}\in\mathbb{N}^2), \tag{26}$$

$$N_{\mathbf{i}}|\eta\rangle := b_{\mathbf{i}}^{\dagger}b_{\mathbf{i}}|\eta\rangle = \eta(\mathbf{i})|\eta\rangle, \tag{27}$$

for any $\eta \in \mathfrak{C}$.

The *transport* of a particle from a site $\mathbf{i}$ to a site $\mathbf{j}$, is characterized by a *connectivity matrix* $C(s) = (c_{\mathbf{i},\mathbf{j}}(s))$ for all $s \in S$, and operators $L_{\mathbf{i},\mathbf{j}}(s)$ defined as

$$L_{\mathbf{i},\mathbf{j}}(s) = \sqrt{c_{\mathbf{i},\mathbf{j}}(s)}\ b_{\mathbf{j}}^{\dagger}b_{\mathbf{i}}. \tag{28}$$

This corresponds to the action of a boson reservoir (phonons) on the system of fermions. Each fermion is pushed to jump between different sites of $\mathbb{N}^2$, following the connectivity matrix. That is, the connectivity matrix defines a *graph* which characterizes the transition between different Landau levels and different energies inside them. Following the customary notions on graphs, the set of vertices here is $V = \mathbb{N}^2$ and the set of edges or arcs is a subset $A = \{\{\mathbf{n},\mathbf{k}\} :\ \text{for } \mathbf{n}\neq\mathbf{k}\}$. We say that two vertices are adjacent if $\{\mathbf{n},\mathbf{k}\}\in A$ and $\mathbf{n}\sim\mathbf{k}$. And $c_{\mathbf{n},\mathbf{k}}(s) > 0$ represent the necessary energy to push an electron from the vertex $\mathbf{n}$ to $\mathbf{k}$ if $\mathbf{n}\sim\mathbf{k}$ and $c_{\mathbf{n},\mathbf{k}}(s) = 0$ otherwise.

A finite sequence $\mathbf{n}_0, \mathbf{n}_1, \ldots, \mathbf{n}_k$ of vertices is said a *walk* of *length* k if $\mathbf{n}_j \sim \mathbf{n}_{j+1}$ for $j = 0, 1, \ldots, k-1$. Thus, for instance, a configuration η as introduced in the previous section, is the characteristic function of a walk. A graph is called *connected* if any pair of distinct vertices is connected by a walk. Given two vertices $\mathbf{n},\mathbf{k}$ the notation $\partial(\mathbf{n},\mathbf{k})$ is the length of the shortest walk connecting $\mathbf{n}$ and $\mathbf{k}$. The *degree* or *valency* of a vertex $\mathbf{n}\in V$ is defined by

$$\kappa(\mathbf{n}) = |\{\mathbf{k}\in V :\ \mathbf{n}\sim\mathbf{k}\}|, \tag{29}$$

where $|\cdot|$ denotes the cardinality.

To fix the origin o of the stratified graph, we notice that

$$(d(\uparrow,\mathbf{0}), E(\uparrow,\mathbf{0})) = (d(\downarrow,\mathbf{0}), E(\downarrow,\mathbf{0})) = (0,\frac{1}{2}).$$

Thus, this origin o will be associated to $\mathbf{0} = (0,0)\in\mathbb{N}^2$.

The stratification is defined then through the sets

$$V_j = \{\mathbf{n}\in V :\ \partial(o,\mathbf{n}) = j\},\ V = \mathbb{N}^2 = \bigcup_{j=1}^{\infty} V_j.$$

Thus, the definition of the connectivity matrix contains the physical data of the model. One has to consider that for each Landau level, the electron energies should be stratified according to Fermi levels. Accordingly, we additionally assume that for any $s \in S$,

$$\sup_{\mathbf{i}} \sum_{\mathbf{j}\in\mathbb{N}^2} c_{\mathbf{i},\mathbf{j}}(s) < \infty. \tag{30}$$

Each operator $L_{\mathbf{i},\mathbf{j}}(s)$ is an element of $\mathfrak{A}(\mathfrak{h}_0)$ and $\|L_{\mathbf{i},\mathbf{j}}(s)\| = \sqrt{c_{\mathbf{i},\mathbf{j}}(s)}$. Now, for each $\Lambda \in \mathfrak{P}_f(\mathbb{N})$, $s \in S$ and $x \in \mathfrak{A}(\mathfrak{h}_0)$, define

$$\varphi_\Lambda(x) = \sum_{i,\mathbf{j}\in\Lambda} L_{\mathbf{i},\mathbf{j}}(s)^* x L_{\mathbf{i},\mathbf{j}}(s).$$

$\varphi_\Lambda : \mathfrak{A}(\mathfrak{h}_0) \to \mathfrak{A}(\mathfrak{h}_0)$ is a completely positive map.

For each vector $|\eta\rangle$ of the orthonormal basis in $\mathfrak{h}$,

$$\begin{aligned}
\|\varphi_\Lambda(x)|\eta\rangle\| &\le \sum_{\mathbf{i},\mathbf{j}\in\Lambda} \left\|L_{\mathbf{i},\mathbf{j}}(s)^* x L_{\mathbf{i},\mathbf{j}}(s)|\eta\rangle\right\| \\
&= \sum_{\mathbf{i},\mathbf{j}\in\Lambda} \eta(\mathbf{i})(1-\eta(\mathbf{j}))\sqrt{c_{\mathbf{i},\mathbf{j}}(s)}\left\|L_{\mathbf{i},\mathbf{j}}(s)^* x|\eta - 1_i + 1_j\rangle\right\| \\
&\le \sum_{\mathbf{i},\mathbf{j}\in\Lambda} \eta(\mathbf{i})(1-\eta(\mathbf{j}))c_{\mathbf{i},\mathbf{j}}(s)\,\|x\| \le \left(\sum_{\mathbf{i}\in\Lambda}\eta(\mathbf{i})\right)\left(\sup_{\mathbf{i}}\sum_{\mathbf{j}} c_{\mathbf{i},\mathbf{j}}(s)\right)\|x\| \\
&\le \left(\sum_{\mathbf{i}\in\mathbb{N}^2}\eta(\mathbf{i})\right)\left(\sup_{\mathbf{i}}\sum_{\mathbf{j}} c_{\mathbf{i},\mathbf{j}}(s)\right)\|x\|
\end{aligned}$$

So that $\|\varphi_\Lambda(x)|\eta\rangle\|$ is uniformly bounded as Λ run over $\mathfrak{P}_f(\mathbb{N})$. Moreover,

$$\sum_{\mathbf{i},\mathbf{j}} \left\|L_{\mathbf{i},\mathbf{j}}(s)^* x L_{\mathbf{i},\mathbf{j}}(s)|\eta\rangle\right\| < \infty$$

so that $\|(\varphi_\Lambda(x) - \varphi(x))u\| \to 0$ for all $u \in \mathfrak{v}$ as $\Lambda \uparrow \mathbb{N}$, where the operator

$$\varphi(x) = \sum_{\mathbf{i},\mathbf{j}} L_{\mathbf{i},\mathbf{j}}(s)^* x L_{\mathbf{i},\mathbf{j}}(s),$$

is defined on the dense manifold $\mathfrak{v}$ for all $x \in \mathfrak{A}(\mathfrak{h}_0)$.

As a result, $\varphi_\Lambda(\mathbf{1})$ converges in the same sense to

$$\varphi(\mathbf{1}) = \sum_{\mathbf{i},\mathbf{j}} L_{\mathbf{i},\mathbf{j}}(s)^* L_{\mathbf{i},\mathbf{j}}(s).$$

Moreover, notice that $\mathcal{L}^s(|\eta\rangle\langle\zeta|) \in \mathfrak{A}(\mathfrak{h}_0)$ for any $\eta, \zeta \in \mathfrak{C}$. Thus, for all element

$$x = \sum_{\eta,\zeta\in\mathfrak{C}(\Lambda)} x(\eta,\zeta)|\eta\rangle\langle\zeta| \in \mathfrak{D},$$

(for some Λ finite), it holds that $\mathcal{L}^s(x) \in \mathfrak{A}(\mathfrak{h}_0)$.

Let denote $W^*(\mathbf{H}^s)$ (respectively $C^*(\mathbf{H}^s)$) the von Neumann (resp. C^*) algebra generated by $\mathbf{H}^s$. To summarize,

Theorem 1. *Under the hypotheses on the operators* $\mathbf{H}^s$ *and* (30)*, for each* $x \in \mathfrak{A}(\mathfrak{h}_0)$ *the unbounded operator*

$$\mathcal{L}^s(x) = i[\mathbf{H}^s, x] - \frac{1}{2}\sum_{\mathbf{i},\mathbf{j}} \left(L_{\mathbf{i},\mathbf{j}}(s)^* L_{\mathbf{i},\mathbf{j}}(s) x - 2L_{\mathbf{i},\mathbf{j}}(s)^* x L_{\mathbf{i},\mathbf{j}}(s) + x L_{\mathbf{i},\mathbf{j}}(s)^* L_{\mathbf{i},\mathbf{j}}(s) \right), \tag{31}$$

whose domain contains the dense manifold $\mathfrak{v}$*, is the generator of a quantum Feller semigroup* $\mathcal{T}$ *on the* C^**-algebra* $\mathfrak{A}(\mathfrak{h}_0)$*. This semigroup is extended into a* σ*-weak continuous quantum Markov semigroup defined on the whole algebra* $\mathfrak{L}(\mathfrak{h})$*.*

Moreover, the semigroup leaves the algebra $W^*(\mathbf{H}^s)$ *invariant, that is* $\mathcal{T}_t(W^*(\mathbf{H}^s)) \subset W^*(\mathbf{H}^s)$*. The generator* L *of the reduced semigroup* $T_t = \mathcal{T}_t|_{W^*(\mathbf{H}^s)}$ *corresponds to that of a classical exclusion:*

$$Lf(\eta) = \sum_{\mathbf{i},\mathbf{j}} \gamma_{\mathbf{i},\mathbf{j}}(s,\eta)\left(f(\eta + 1_{\mathbf{j}} - 1_{\mathbf{i}}) - f(\eta)\right), \tag{32}$$

for all bounded cylindrical function $f : \mathfrak{C} \to \mathbb{R}$*, and* $\gamma_{\mathbf{i},\mathbf{j}}(s,\eta) = \eta(\mathbf{i})(1-\eta(\mathbf{j}))c_{\mathbf{i},\mathbf{j}}(s)$*.*

Proof. We first notice that there exists the minimal quantum Markov semigroup associated with the generator (31). Indeed this holds since $\mathfrak{v}$ is dense in $\mathfrak{h} = \Gamma_f(\mathfrak{h}_0)$, and it is a core for $G = -i\mathbf{H}^s - \frac{1}{2}\sum_{\mathbf{i},\mathbf{j}} L_{\mathbf{i},\mathbf{j}}(s)^* L_{\mathbf{i},\mathbf{j}}(s)$, which is the generator of a contraction semigroup, and the Markovian property is guaranteed by $\mathcal{L}^s(\mathbf{1}) = 0$. Let $\mathcal{T}$ denote this minimal semigroup (Davies, 1977) which is defined through the use of the σ-weak topology in all of $\mathfrak{L}(\mathfrak{h})$. It satisfies the equation

$$\langle v, \mathcal{T}_t(x)u\rangle = \langle v, xu\rangle + \int_0^t \langle v, \mathcal{L}^s\left(\mathcal{T}_r(x)\right)u\rangle dr, \tag{33}$$

where $u, v \in \mathfrak{v}$, $x \in \mathfrak{L}(\mathfrak{h})$.

Take $x \in \mathfrak{A}(\mathfrak{h}_0)$ and $\Lambda \in \mathfrak{P}_f(\mathbb{N})$. Call P_Λ the projection of $\mathfrak{h} = \Gamma_f(\mathfrak{h}_0)$ onto $\mathfrak{h}^\Lambda = \Gamma_f(\mathfrak{h}_0^\Lambda)$. Notice that for all $a \in \mathfrak{A}(\mathfrak{h}_0)$, the net of projected operators $P_\Lambda a P_\Lambda \in \mathfrak{A}(\mathfrak{h}_0^\Lambda)$ converges strongly to a, as $\Lambda \uparrow \mathbb{N}^2$ since $\mathfrak{A}(\mathfrak{h}_0)$ is the strong closure of $\mathfrak{D} = \bigcup \mathfrak{A}(\mathfrak{h}_0^\Lambda)$. Call $\mathbf{P}_\Lambda(a) = P_\Lambda a P_\Lambda$ the projection of an element of the algebra $\mathfrak{A}(\mathfrak{h}_0)$ and $\mathcal{T}_t^\Lambda(x) = P_\Lambda \mathcal{T}_t(x) P_\Lambda$, $x \in \mathfrak{A}(\mathfrak{h}_0^\Lambda)$, $t \geq 0$. This is a semigroup acting on $\mathfrak{A}(\mathfrak{h}_0^\Lambda)$ whose generator, determined by (33), is $\mathcal{L}^{s,\Lambda}(x) = P_\Lambda \mathcal{L}^s(x) P_\Lambda$, for each $x \in \mathfrak{A}(\mathfrak{h}_0^\Lambda)$. $\mathcal{L}^{s,\Lambda}(x)$ is a matrix in a finite-dimensional space, so that it is a bounded operator. As a result, each $\mathcal{T}^\Lambda$ is a norm-continuous semigroup.

To prove that the minimal semigroup $\mathcal{T}$ satisfies the Feller property on the algebra $\mathfrak{A}(\mathfrak{h}_0)$, we first consider $x \in \mathfrak{D}$. So that there is $\Lambda_0 \in \mathfrak{P}_f\left(\mathbb{N}^2\right)$ such that $x \in \mathfrak{A}(\mathfrak{h}_0^\Lambda)$, which yields $\mathbf{P}_\Lambda(x) = x$ for all $\Lambda \in \mathfrak{P}_f\left(\mathbb{N}^2\right)$ containing Λ_0. Moreover, $\mathcal{T}_t(x) \in \mathfrak{A}(\mathfrak{h}_0)$ since $\mathcal{L}^s(x) \in \mathfrak{A}(\mathfrak{h}_0)$. Then, for all such Λ, and any $u \in \mathfrak{h}$

$$\|(\mathcal{T}_t(x) - x)u\| \leq \left\|(\mathcal{T}_t(x) - \mathcal{T}_t^\Lambda(x))u\right\| + \left\|\mathcal{T}_t^\Lambda(x) - x\right\| \|u\|.$$

Since $\mathbf{P}_\Lambda \circ \mathcal{T}_t(x)$ strongly converges to $\mathcal{T}_t(x)$ as Λ increases, given any $\epsilon > 0$ we can choose $\Lambda \in \mathfrak{P}_f(\mathbb{N})$ to have the first right-hand term in the previous inequality

less than $\epsilon/2$. On the other hand, for this Λ we also have $\lim_{t\to 0}\left\|\mathcal{T}_t^{\Lambda}-\mathbf{1}\right\|=0$ and t_0 may be selected to have the second right-hand term in the inequality less than $\epsilon/2$ too for any $t<t_0$. This proves Feller property for $x\in\mathfrak{D}$.

If $x\in\mathfrak{A}(\mathfrak{h}_0)$, we pick a net $x_\Lambda\in\mathfrak{A}(\mathfrak{h}_0^\Lambda)$ which strongly converges to x, use the fact that $\mathcal{T}_t(\cdot)$ is a contraction and the property (M5s) proved for elements in $\mathfrak{D}$ to conclude. $\mathcal{T}$ is thus a quantum Feller semigroup on the algebra $\mathfrak{A}(\mathfrak{h}_0)$.

To study the classical reduction, it suffices to use the C.A.R. Indeed,

$$[b_{\mathbf{k}}^\dagger b_{\mathbf{k}}, b_{\mathbf{j}}^\dagger b_{\mathbf{i}}]=(\delta_{kj}-\delta_{ki})b_{\mathbf{j}}^\dagger b_{\mathbf{i}}.$$

Moreover, since each operator $L_{\mathbf{i},\mathbf{j}}(s)$ is bounded and $L_{\mathbf{i},\mathbf{j}}(s)\mathfrak{v}\subset\mathfrak{v}\subset D(\mathbf{H}^s)$, the commutator $[\mathbf{H}^s,L_{\mathbf{i},\mathbf{j}}(s)]$ is well defined on $\mathfrak{v}$ and can be extended to all of $\mathfrak{h}$ as a bounded operator and the following important equation holds

$$[\mathbf{H}^s,L_{\mathbf{i},\mathbf{j}}(s)]=\sum_k E(s,\mathbf{k})\sqrt{c_{\mathbf{i},\mathbf{j}}(s)}[b_{\mathbf{k}}^\dagger b_{\mathbf{k}},b_{\mathbf{j}}^\dagger b_{\mathbf{i}}]=(E(s,\mathbf{j})-E(s,\mathbf{i}))L_{\mathbf{i},\mathbf{j}}(s). \tag{34}$$

This property implies that $\mathbf{H}^s$ reduces the semigroup (see, e.g., [36]), that is, the algebra generated by this operator remains invariant under the action of the semigroup.

The algebra $\mathbf{Cyl}(\mathbf{H}^s)$ of operators of the form

$$x=\sum_\eta f(\eta)|\eta\rangle\langle\eta|,$$

where $f:\mathfrak{C}\to\mathbb{C}$ is a bounded cylindrical function, form a dense subalgebra of $C^*(\mathbf{H}^s)$.

We compute $\mathcal{L}^s(x)$ for $x\in\mathbf{Cyl}(\mathbf{H}^s)$.

The following additional notation will be used: $\mathbf{i}\to_\eta\mathbf{j}$, means that $\eta(\mathbf{i})=1$ and $\eta(\mathbf{j})=0$ (under the configuration η a particle occupying the site $\mathbf{i}$ can move to the free site $\mathbf{j}$).

An elementary computation yields

$$\begin{aligned}
&L_{\mathbf{i},\mathbf{j}}(s)^*L_{\mathbf{i},\mathbf{j}}(s)|\eta\rangle\langle\eta|=c_{\mathbf{i},\mathbf{j}}(s)\eta(\mathbf{i})(1-\eta(\mathbf{j}))|\eta\rangle\langle\eta|\\
&|\eta\rangle\langle\eta|L_{\mathbf{i},\mathbf{j}}(s)^*L_{\mathbf{i},\mathbf{j}}(s)=c_{\mathbf{i},\mathbf{j}}(s)\eta(\mathbf{i})(1-\eta(\mathbf{j}))|\eta\rangle\langle\eta|\\
&L_{\mathbf{i},\mathbf{j}}(s)^*|\eta\rangle\langle\eta|L_{\mathbf{i},\mathbf{j}}(s)=c_{\mathbf{i},\mathbf{j}}(s)(1-\eta(\mathbf{i}))\eta(\mathbf{j})|\eta-1_{\mathbf{j}}+1_{\mathbf{i}}\rangle\langle\eta-1_{\mathbf{j}}+1_{\mathbf{i}}|.
\end{aligned}$$

$$\begin{aligned}
&\mathcal{L}^s(|\eta\rangle\langle\eta|)\\
&\quad=-\frac{1}{2}\sum_{\mathbf{i},\mathbf{j}}\left(L_{\mathbf{i},\mathbf{j}}(s)^*L_{\mathbf{i},\mathbf{j}}(s)|\eta\rangle\langle\eta|-2L_{\mathbf{i},\mathbf{j}}(s)^*|\eta\rangle\langle\eta|L_{\mathbf{i},\mathbf{j}}(s)+|\eta\rangle\langle\eta|L_{\mathbf{i},\mathbf{j}}(s)^*L_{\mathbf{i},\mathbf{j}}(s)\right)\\
&\quad=\sum_{\mathbf{i},\mathbf{j}:\mathbf{j}\to_\eta\mathbf{i}}c_{\mathbf{i},\mathbf{j}}(s)|\eta-1_j+1_i\rangle\langle\eta-1_j+1_i|-\sum_{\mathbf{i},\mathbf{j}:\mathbf{i}\to_\eta\mathbf{j}}c_{\mathbf{i},\mathbf{j}}(s)|\eta\rangle\langle\eta|.
\end{aligned}$$

Now, for any $x = \sum_\eta f(\eta)|\eta\rangle\langle\eta| \in \mathbf{Cyl}(\mathbf{H}^s)$,

$$\mathcal{L}^s(x) = \sum_\eta \left(\sum_{\mathbf{i},\mathbf{j}:\mathbf{j}\to_\eta\mathbf{i}} c_{\mathbf{i},\mathbf{j}}(s) f(\eta)|\eta - 1_j + 1_i\rangle\langle\eta - 1_j + 1_i| - \sum_{\mathbf{i},\mathbf{j}:\mathbf{i}\to_\eta\mathbf{j}} c_{\mathbf{i},\mathbf{j}}(s) f(\eta)|\eta\rangle\langle\eta| \right),$$

and notice that a change of variables $\eta \mapsto \eta - 1_\mathbf{j} + 1_\mathbf{i}$ yields

$$\begin{aligned} &\sum_\eta \sum_{\mathbf{i},\mathbf{j}:\mathbf{j}\to_\eta\mathbf{i}} c_{\mathbf{i},\mathbf{j}}(s) f(\eta)|\eta - 1_j + 1_i\rangle\langle\eta - 1_j + 1_i| \\ &\quad = \sum_\eta \sum_{\mathbf{i},\mathbf{j}:\mathbf{i}\to_\eta\mathbf{j}} c_{\mathbf{i},\mathbf{j}}(s) f(\eta - 1_i + 1_j)|\eta\rangle\langle\eta|. \end{aligned}$$

Therefore, we finally obtain

$$\mathcal{L}^s(x) = \sum_\eta \sum_{\mathbf{i},\mathbf{j}:\mathbf{i}\to_\eta\mathbf{j}} c_{\mathbf{i},\mathbf{j}}(s) \left(f(\eta - 1_i + 1_j) - f(\eta) \right) |\eta\rangle\langle\eta|,$$

from which (32) follows.

The above expression gives the generator of the semigroup restricted to $W^*(\mathbf{H}^s)$. $C^*(\mathbf{H}^s)$ is isomorphic to the algebra $C(\sigma(\mathbf{H}^s))$ of continuous complex-valued functions on the spectrum $\sigma(\mathbf{H}^s)$ and contains continuous cylindrical functions as a uniformly dense sub-algebra. It is clear that L given by (32) leaves the above dense subalgebra invariant, thus the reduced semigroup applies $C(\sigma(\mathbf{H}^s))$ into itself, moreover, the Feller continuity property is inherited from the quantum Markov semigroup. □

5. Stationary states

To start the analysis of stationary states, a first question to answer is about their possible existence. One way to answer this question in our setting, without additional hypotheses is the following. Theorem IV.1 in [19] is easily applicable here, since the coefficients $L_{\mathbf{i},\mathbf{j}}$ are bounded, so that the following Corollary holds.

Corollary 1. *Under the hypotheses of Theorem* 1*, there exists two self-adjoint operators X and Y, where X is positive, Y is bounded from below and with finite-dimensional spectral projections associated with bounded intervals, such that*

$$\langle u, \mathcal{L}^s(X)\, u\rangle \leq -\langle u, Yu\rangle, \tag{35}$$

for all $u \in \mathfrak{V}$.

As a result, the semigroup $\mathcal{T}^s$ has a normal stationary state.

Proof. The reader is referred to [19] Theorem IV.1 or [24] for the proof of the second part of this corollary, that is, a normal stationary state exists as soon as one finds operators X and Y according to the hypothesis here above.

Now, to prove the first part, let $\mathbf{k} \in \mathbb{N}^2$ be fixed and consider $X = |1_{\mathbf{k}}\rangle\langle 1_{\mathbf{k}}|$. This is clearly a positive operator. And let define

$$Y = -\sum_{\mathbf{i}\neq\mathbf{k}} c_{\mathbf{i},\mathbf{k}}(s)|1_{\mathbf{i}}\rangle\langle 1_{\mathbf{i}}|.$$

To prove the inequality (35), it suffices to check it for all $u = |\eta\rangle$, ($\eta \in \mathfrak{C}$). Let $|\eta\rangle$ be one of those vectors.

$$\begin{aligned}\langle \eta, \mathcal{L}^s\left(|1_{\mathbf{k}}\rangle\langle 1_{\mathbf{k}}|\right)\eta\rangle &= \sum_{\mathbf{i}\neq\mathbf{k}} c_{\mathbf{i},\mathbf{k}}(s)\eta(\mathbf{i})^2 - \left(\sum_{\mathbf{j}\neq\mathbf{k}} c_{\mathbf{k},\mathbf{j}}(s)\right)\eta(\mathbf{k})^2 \\ &\leq \sum_{\mathbf{i}\neq\mathbf{k}} c_{\mathbf{i},\mathbf{k}}(s)\eta(\mathbf{i})^2 \leq -\langle \eta, Y\eta\rangle.\end{aligned}$$

This concludes the proof. □

So, our QMS has at least an invariant state. Moreover, a straightforward computation allows to check that the operator

$$G = -i\mathbf{H}^s - \frac{1}{2}\sum_{\mathbf{k},\ell} L_{\mathbf{k},\ell}(s)^* L_{\mathbf{k},\ell}(s), \tag{36}$$

and the operators $L_{\mathbf{k},\ell}$ have no common invariant subspace. This fact implies that there exists a *faithful* normal stationary state as proved in [21].

We turn now to construct explicit stationary states under some additional hypotheses.

It worths noticing that the coefficients $L_{\mathbf{i},\mathbf{j}}(s)$ of the dissipative part of the generator depend of s only through the matrix $C(s)$. As a result, $[L_{\mathbf{i},\mathbf{j}}(\uparrow), L_{\mathbf{i},\mathbf{j}}(\downarrow)] = 0$ and since $[\mathbf{H}^{\uparrow}, \mathbf{H}^{\downarrow}] = 0$ it follows that for all $x \in \mathfrak{A}(\mathfrak{h}_0)$ the operators $\mathcal{L}^{\uparrow}(x)$ and $\mathcal{L}^{\downarrow}(x)$ commute.

Consider $s \in S$ fixed and let

$$\rho = \sum_{\eta\in\mathfrak{C}} p(\eta)|\eta\rangle\langle\eta| \tag{37}$$

be a density matrix, where $\sum_\eta p(\eta) = 1$. Then $[\mathbf{H}^s, \rho] = 0$, for both, $s = \uparrow$ and $s = \downarrow$. That is, ρ is a stationary state for both **closed (or non dissipative) dynamics**, defined by the generator $-i[\mathbf{H}^s, \bullet]$ over trace-class operators. However, this situation dramatically changes in the presence of dissipation, that is, for the open system dynamics. For such a density matrix ρ, the action of the predual generator $\mathcal{L}^s_*$ on it reduces to

$$\mathcal{L}^s_*(\rho) = -\frac{1}{2}\sum_{\mathbf{i},\mathbf{j}} \left(L_{\mathbf{i},\mathbf{j}}(s)^* L_{\mathbf{i},\mathbf{j}}(s)\rho - 2L_{\mathbf{i},\mathbf{j}}(s)\rho L_{\mathbf{i},\mathbf{j}}(s)^* + \rho L_{\mathbf{i},\mathbf{j}}(s)^* L_{\mathbf{i},\mathbf{j}}(s)\right). \tag{38}$$

And the condition $\mathcal{L}^s_*(\rho) = 0$ yields the equation

$$\sum_{\mathbf{i},\mathbf{j}} \gamma_{\mathbf{i},\mathbf{j}}(s,\eta)\left(p(\eta + 1_{\mathbf{j}} - 1_{\mathbf{i}}) - p(\eta)\right) = 0, \tag{39}$$

which will depend on $s \in S$.

In the next theorem we give a sufficient condition to construct a stationary state based on the above computation.

Theorem 2. *Let assume that*

$$\pi(\mathbf{i})c_{\mathbf{i},\mathbf{j}}(s) = \pi(\mathbf{j})c_{\mathbf{j},\mathbf{i}}(s),\ (\mathbf{i},\mathbf{j} \in \mathbb{N}^2) \tag{40}$$

where $(\pi(\mathbf{i}))_{\mathbf{i}\in\mathbb{N}^2}$ *is any sequence of positive numbers. Then a normal state with density matrix* ρ *given by* (37) *is stationary for the dynamics* $\uparrow$ *and* $\downarrow$ *if*

$$p(\eta) = \prod_{\mathbf{i}\in\mathbb{N}^2} \alpha_{\mathbf{i}}(\eta(\mathbf{i})),$$

for all $\eta \in \mathfrak{C}$*, where* $\alpha_{\mathbf{i}} : \{0,1\} \to [0,1]$ *is, for each* $\mathbf{i} \in \mathbb{N}^2$*, a probability measure given by*

$$\alpha_{\mathbf{i}}(x) = \frac{(\pi(\mathbf{i}))^x}{1+\pi(\mathbf{i})}, \quad (\mathbf{i} \in \mathbb{N}^2, x \in \{0,1\}). \tag{41}$$

Proof. Notice that given the probabilities $\alpha_{\mathbf{i}}$ on $\{0,1\}$, by Kolmogorov's Theorem there is a unique probability measure $\mathbf{P}_\alpha$ on the set of configurations $\mathfrak{C}$ with marginals

$$\mathbf{P}_\alpha(\{\eta \in \mathfrak{C} :\ \eta(\mathbf{i}) = 1,\ \text{for all } \mathbf{i} \in I;\ \eta(\mathbf{j}) = 0,\ \text{for all } \mathbf{j} \in J\})$$

$$= \prod_{\mathbf{i}\in I} \alpha_{\mathbf{i}}(1) \prod_{\mathbf{j}\in J} \alpha_{\mathbf{j}}(0).$$

And $p(\eta) = \mathbf{P}_\alpha(\{\eta\})$.

Let ρ be given by (37). Then $\mathcal{L}^s_*(\rho) = 0$ if and only if $\mathrm{tr}\,(\mathcal{L}^s_*(\rho)|\eta\rangle\langle\eta|) = 0$ for all $\eta \in \mathfrak{C}$. Notice that $\zeta - 1_{\mathbf{j}} + 1_{\mathbf{i}} = \eta$ if and only if $\zeta = \eta - 1_{\mathbf{i}} + 1_{\mathbf{j}}$, for $\eta, \zeta \in \mathfrak{C}$, $\mathbf{i},\mathbf{j} \in \mathbb{N}^2$. Thus, if we write

$$\rho = \sum_\zeta p(\zeta)|\zeta\rangle\langle\zeta|,$$

the previous theorem yields

$$\mathcal{L}^s_*(\rho) = \sum_\zeta \sum_{\mathbf{i},\mathbf{j}:\mathbf{i}\to_\zeta\mathbf{j}} c_{\mathbf{i},\mathbf{j}}(s)p(\zeta)\left(|\zeta - 1_{\mathbf{i}} + 1_{\mathbf{j}}\rangle\langle\zeta - 1_{\mathbf{i}} + 1_{\mathbf{j}}| - |\zeta\rangle\langle\zeta|\right).$$

Now, $\mathrm{tr}\,(|\zeta - 1_{\mathbf{i}} + 1_{\mathbf{j}}\rangle\langle\zeta - 1_{\mathbf{i}} + 1_{\mathbf{j}}||\eta\rangle\langle\eta|) = 1$ if and only if $\zeta = \eta - 1_{\mathbf{j}} + 1_{\mathbf{i}}$. Thus, $\mathrm{tr}\,(\mathcal{L}_*(\rho)|\eta\rangle\langle\eta|) = 0$ if and only if

$$\sum_{\mathbf{i},\mathbf{j}} (1 - \eta(\mathbf{i}))\eta(\mathbf{j})\left(c_{\mathbf{i},\mathbf{j}}(s)p(\eta - 1_j + 1_i) - c_{\mathbf{j},\mathbf{i}}(s)p(\eta)\right) = 0.$$

Notice that $\alpha_{\mathbf{i}}(0)p(\eta + 1_{\mathbf{i}}) = p(\eta)\alpha_{\mathbf{i}}(1)$ and $\alpha_{\mathbf{j}}(1)p(\eta - 1_{\mathbf{j}}) = p(\eta)\alpha_{\mathbf{j}}(0)$. These equations yields

$$c_{\mathbf{i},\mathbf{j}}(s)p(\eta - 1_{\mathbf{j}} + 1_{\mathbf{i}}) - c_{\mathbf{j},\mathbf{i}}(s)p(\eta) = \left(c_{\mathbf{i},\mathbf{j}}(s)\frac{\pi(\mathbf{i})}{\pi(\mathbf{j})} - c_{\mathbf{j},\mathbf{i}}(s)\right)p(\eta),$$

and the last term between brackets is zero, by the hypothesis (40). The last expression implies that $Lp(\eta) = 0$. Moreover the above computations yield

$$\mathcal{L}_*^s(|\eta\rangle\langle\eta|) = \sum_{\mathbf{i},\mathbf{j}} \gamma_{\mathbf{i},\mathbf{j}}(s,\eta)\left(|\eta - 1_i + 1_j\rangle\langle\eta - 1_i + 1_j| - |\eta\rangle\langle\eta|\right),$$

which commutes with $\mathbf{H}^s$ and the proof is complete. □

The hypothesis (40) corresponds to a reversibility condition for the classical exclusion semigroup as shown in [29], also known as a *detailed balance condition* in physics. This question is related to the concept of an *equilibrium state*, defined as one that has zero entropy production.

6. Analysis of the equilibrium

Assume that ρ is the density matrix of a normal, faithful, stationary state. We denote J the usual modular conjugation operator introduced by Tomita–Takesaki, which is anti unitary and satisfies $J^* = J$, $J^2 = \mathbf{1}$. In our framework, a cyclic vector is $\xi = |0\rangle$, and J is given as $Ja\xi = a^*\xi$, $\mathrm{tr}\,(\rho a) = \langle\xi, a\xi\rangle$. Denote $\theta(a) = JaJ$, for any $a \in \mathfrak{L}(\mathfrak{h})$. Notice that for each $u, v \in \mathfrak{h}$, $\theta(|u\rangle\langle v|) = |v\rangle\langle u|$. Moreover, $\theta(a)b\xi = JaJb\xi = Jab^*\xi = ba^*\xi = b\theta(a)\xi$. This is a well-known fact of Tomita–Takesaki's theory: JaJ is an element of the generalized commutant algebra.

As a result, the following functional is easily seen to be positive and defines a normal state on the algebra $\mathfrak{L}(\mathfrak{h}) \otimes \mathfrak{L}(\mathfrak{h})$

$$\Omega(a \otimes b) = \mathrm{tr}\left(\rho^{1/2}\theta(a)\rho^{1/2}b\right). \tag{42}$$

6.1. Entropy production and detailed balance

Inspired in the classical Markov theory, we introduce two dynamics associated to $\mathcal{T}^s$.

Definition 3. The *forward* (respectively *backward*) semigroup is defined on the tensor product algebra $\mathfrak{L}(\mathfrak{h}) \otimes \mathfrak{L}(\mathfrak{h})$ like

$$\overrightarrow{\Phi}_t^s = \mathbf{1} \otimes \mathcal{T}_t^s, \text{ (respectively, } \overleftarrow{\Phi}_t^s = \mathcal{T}_t^s \otimes \mathbf{1}), \tag{43}$$

for all $t \geq 0$.

By duality, $\overrightarrow{\Phi_{*t}^s}(\Omega)$ (resp. $\overleftarrow{\Phi_{*t}^s}(\Omega)$) is defined as

$$\overrightarrow{\Phi_{*t}^s}(\Omega)(a \otimes b) = \Omega(\overrightarrow{\Phi_t^s}(a \otimes b)) = \mathrm{tr}\left(\rho^{1/2}\theta(a)\rho^{1/2}\mathcal{T}_t(b)\right). \tag{44}$$

$$\left(\text{resp. } \overleftarrow{\Phi_{*t}^s}(\Omega)(a \otimes b) = \Omega(\overleftarrow{\Phi_t^s}(a \otimes b)) = \mathrm{tr}\left(\rho^{1/2}\theta(\mathcal{T}_t(a))\rho^{1/2}b\right)\right). \tag{45}$$

Here we adopt a definition of a detailed balance like in Ref.[26] .

Definition 4. We say that the QMS $\mathcal{T}^s$ satisfies the Standard Quantum Detailed Balance (SQDB) condition with respect to ρ on $\mathfrak{L}(\mathfrak{h})$ if $\overrightarrow{\Phi_{*t}^s}(\Omega) = \overleftarrow{\Phi_{*t}^s}(\Omega)$, for all $t \geq 0$.

This condition is equivalent to

$$\mathrm{tr}\left(\rho^{1/2}\theta(a)\rho^{1/2}\mathcal{L}^s\left(b\right)\right) = \mathrm{tr}\left(\rho^{1/2}\theta(\mathcal{L}^s\left(a\right))\rho^{1/2}b\right), \tag{46}$$

for all $a, b \in \mathfrak{L}(\mathfrak{h})$.

Remark 2. The state Ω has a density matrix with respect to the trace $\mathrm{Tr}\left(\cdot\right)$ defined on trace-class operators of $\mathfrak{h}\otimes\mathfrak{h}$, that is

$$\Omega(a\otimes b) = \mathrm{Tr}\left(D\, a\otimes b\right),$$

for $a\otimes b \in \mathfrak{L}(\mathfrak{h})\otimes\mathfrak{L}(\mathfrak{h})$.

Indeed, denote $(e_n)_{n\in N}$ an orthonormal basis of $\mathfrak{h}$ which gives a **diagonal representation** of ρ. That is,

$$\rho = \sum_{n\in\mathbb{N}} \rho(n)|e_n\rangle\langle e_n|.$$

Now, consider $a = |e_k\rangle\langle e_\ell|$, $b = |e_i\rangle\langle e_j|$. So that $a\otimes b = |e_k\rangle\langle e_\ell|\otimes|e_i\rangle\langle e_j|$ and

$$\begin{aligned}\Omega(|e_k\otimes e_i\rangle\langle e_\ell\otimes e_j|) &= \mathrm{tr}\left(\rho^{1/2}|e_\ell\rangle\langle e_k|\rho^{1/2}|e_i\rangle\langle e_j|\right)\\ &= \delta_{k,i}\delta_{\ell,j}\rho^{1/2}(k)\rho^{1/2}(\ell).\end{aligned}$$

So that, if one introduces the trace-class operator

$$D = \sum_{k',\ell'\in\mathbb{N}} \rho^{1/2}(k')\rho^{1/2}(\ell')|e_{k'}\otimes e_{k'}\rangle\langle e_{\ell'}\otimes e_{\ell'}|, \tag{47}$$

one obtains

$$\mathrm{Tr}\left(D|e_k\otimes e_i\rangle\langle e_\ell\otimes e_j|\right) = \delta_{k,i}\delta_{\ell,j}\rho^{1/2}(k)\rho^{1/2}(\ell). \tag{48}$$

From this equation it follows that D defined in (47) is the density of Ω.

Furthermore, the densities of $\overrightarrow{\Omega}_t = \overrightarrow{\Phi^s_{*t}}(\Omega)$ and $\overleftarrow{\Omega}_t = \overleftarrow{\Phi^s_{*t}}(\Omega)$ are respectively

$$\begin{aligned}\overrightarrow{D}_t &= \left(\mathbf{1}\otimes\mathcal{T}_{*t}\right)(D)\\ \overleftarrow{D}_t &= \left(\mathcal{T}_{*t}\otimes\mathbf{1}\right)(D).\end{aligned}$$

Finally, the detailed balance condition (46) is equivalent to each one of the following dual expressions

$$\mathrm{Tr}\left(D(\mathbf{1}\otimes\mathcal{L}^s)(a\otimes b)\right) = \mathrm{Tr}\left(D(\mathcal{L}^s\otimes\mathbf{1})(a\otimes b)\right). \tag{49}$$

$$\mathrm{Tr}\left((\mathbf{1}\otimes\mathcal{L}^s_*)(D)(a\otimes b)\right) = \mathrm{Tr}\left((\mathcal{L}^s_*\otimes\mathbf{1})(D)(a\otimes b)\right). \tag{50}$$

Definition 5. The *entropy* between $\overrightarrow{\Omega}_t$ and $\overleftarrow{\Omega}_t$ is given by

$$S(\overrightarrow{\Omega}_t, \overleftarrow{\Omega}_t) = \overrightarrow{\Omega}_t(\log\overrightarrow{D}_t - \log\overleftarrow{D}_t) = \mathrm{Tr}\left(\overrightarrow{D}_t(\log\overrightarrow{D}_t - \log\overleftarrow{D}_t)\right).$$

And, consequently, the **entropy production** of the initial density matrix ρ is given through

$$\mathbf{e}(\rho) = \frac{d}{dt}S(\overrightarrow{\Omega}_t, \overleftarrow{\Omega}_t)|_{t=0} = \lim_{t\to 0+}\frac{S(\overrightarrow{\Omega}_t, \overleftarrow{\Omega}_t)}{t}. \tag{51}$$

The following result has been proven in [25] to where the reader is referred for further details.

Theorem 3. *A quantum Markov semigroup has zero entropy production if and only if* $S(\overrightarrow{\Omega}_t, \overleftarrow{\Omega}_t) = 0$ *for all* $t \geq 0$. *In particular, it has zero entropy production if and only if it satisfies the detailed balance condition* (46).

To check (50), it suffices to show that for all $\alpha,\ \alpha',\ \beta,\ \beta' \in \mathbb{N}$,

$$\begin{aligned} &\mathrm{Tr}\left((\mathbf{1}\otimes\mathcal{L}_*^s)(D)|e_\alpha\rangle\langle e_\beta|\otimes|e_{\alpha'}\rangle\langle e_{\beta'}|\right) \\ &\quad = \mathrm{Tr}\left((\mathcal{L}_*^s\otimes\mathbf{1})(D)|e_\alpha\rangle\langle e_\beta|\otimes|e_{\alpha'}\rangle\langle e_{\beta'}|\right). \end{aligned} \tag{52}$$

Or, expanding the above equation, one needs to prove that

$$\begin{aligned} &\sum_{k,\ell}\rho^{1/2}(k)\rho^{1/2}(\ell)\mathrm{Tr}\left((\mathbf{1}\otimes\mathcal{L}_*^s)\left(|e_k\otimes e_k\rangle\langle e_\ell\otimes e_\ell|\right)|e_\alpha\rangle\langle e_\beta|\otimes|e_{\alpha'}\rangle\langle e_{\beta'}|\right) \\ &\quad = \sum_{k,\ell}\rho^{1/2}(k)\rho^{1/2}(\ell)\mathrm{Tr}\left((\mathcal{L}_*^s\otimes\mathbf{1})\left(|e_k\otimes e_k\rangle\langle e_\ell\otimes e_\ell|\right)|e_\alpha\rangle\langle e_\beta|\otimes|e_{\alpha'}\rangle\langle e_{\beta'}|\right) \end{aligned}$$

To perform the above computation, we write the pre dual generator in the form:

$$\mathcal{L}_*^s(\sigma) = G\sigma + \Phi_*(\sigma) + \sigma G^*,$$

for any trace-class operator σ, where G is given by (36) and

$$\Phi_*(\sigma) = \sum_{\mathbf{k},\ell} L_{\mathbf{k},\ell}(s)\sigma L_{\mathbf{k},\ell}(s)^* \tag{53}$$

One has first

$$\begin{aligned} (\mathbf{1}\otimes\mathcal{L}_*^s)\left(|e_k\otimes e_k\rangle\langle e_\ell\otimes e_\ell|\right) &= |e_k\otimes Ge_k\rangle\langle e_\ell\otimes e_\ell| \\ &\quad + |e_k\rangle\langle e_\ell|\otimes\Phi_*(|e_k\rangle\langle e_\ell|) \\ &\quad + |e_k\otimes e_k\rangle\langle e_\ell\otimes Ge_\ell|. \end{aligned}$$

So that,

$$\begin{aligned} &\mathrm{Tr}\left((\mathbf{1}\otimes\mathcal{L}_*^s)\left(|e_k\otimes e_k\rangle\langle e_\ell\otimes e_\ell|\right)|e_\alpha\rangle\langle e_\beta|\otimes|e_{\alpha'}\rangle\langle e_{\beta'}|\right) \\ &\quad = \delta_{\ell,\alpha}\delta_{k,\alpha'}\delta_{\alpha,\beta}\langle e_{\beta'}, Ge_k\rangle + \delta_{\ell,\alpha}\delta_{k,\alpha'}\langle e_{\beta'}, \Phi_*(|e_k\rangle\langle e_\ell|)e_\beta\rangle \\ &\qquad + \delta_{\ell,\alpha}\delta_{k,\alpha'}\delta_{\alpha',\beta'}\langle Ge_\ell, e_\alpha\rangle. \end{aligned} \tag{54}$$

A similar computation yields

$$\begin{aligned} &\mathrm{Tr}\left((\mathcal{L}_*^s\otimes\mathbf{1})\left(|e_k\otimes e_k\rangle\langle e_\ell\otimes e_\ell|\right)|e_\alpha\rangle\langle e_\beta|\otimes|e_{\alpha'}\rangle\langle e_{\beta'}|\right) \\ &\quad = \delta_{\ell,\alpha}\delta_{k,\beta'}\delta_{\alpha,\beta}\langle e_{\alpha'}, Ge_k\rangle + \delta_{\ell,\beta}\delta_{k,\beta'}\langle e_{\alpha'}, \Phi_*(|e_k\rangle\langle e_\ell|)e_\alpha\rangle \\ &\qquad + \delta_{\ell,\beta}\delta_{k,\beta'}\delta_{\alpha',\beta'}\langle Ge_\ell, e_\alpha\rangle. \end{aligned} \tag{55}$$

Replacing (54) in the left-hand side of the expanded version of (52), yields

$$\begin{aligned} &\mathrm{Tr}\left((\mathbf{1}\otimes\mathcal{L}_*^s)\left(D\right)|e_\alpha\rangle\langle e_\beta|\otimes|e_{\alpha'}\rangle\langle e_{\beta'}|\right) \\ &\quad = \rho^{1/2}(\alpha)\rho^{1/2}(\alpha')\left[\delta_{\alpha,\beta}\langle e_{\beta'}, Ge_{\alpha'}\rangle + \langle e_{\beta'}, \Phi_*(|e_{\alpha'}\rangle\langle e_\alpha|)e_\beta\rangle + \delta_{\alpha',\beta'}\langle Ge_\alpha, e_\beta\rangle\right] \end{aligned} \tag{56}$$

Similarly, replacing (55) in the right-hand side of the expanded version of (52) gives

$$\mathrm{Tr}\left((\mathcal{L}_*^s \otimes \mathbf{1})(D)\,|e_\alpha\rangle\langle e_\beta| \otimes |e_{\alpha'}\rangle\langle e_{\beta'}|\right) \tag{57}$$
$$= \rho^{1/2}(\beta)\rho^{1/2}(\beta')\left[\delta_{\alpha,\beta}\langle e_{\alpha'}, Ge_{\beta'}\rangle + \langle e_{\alpha'}, \Phi_*(|e_{\beta'}\rangle\langle e_\beta|)e_\alpha\rangle + \delta_{\alpha',\beta'}\langle Ge_\beta, e_\alpha\rangle\right].$$

To summarize, we obtain the following corollary, where we keep the above notations. Recall that $\Re G = -\frac{1}{2}\sum_{\mathbf{i},\mathbf{j}} L_{\mathbf{i},\mathbf{j}}(s)^* L_{\mathbf{i},\mathbf{j}}(s)$, $\Im G = -\mathbf{H}^s$.

Corollary 2. *Let ρ be the density matrix of a normal, faithful, stationary state. Assume that ρ is diagonalized by the orthonormal basis $(e_n)_{n\in\mathbb{N}}$, as well as G. Then, the quantum Markov semigroup satisfies the detailed balance condition if and only if*

$$\rho(\alpha)\phi(\alpha,\beta) = \rho(\beta)\phi(\beta,\alpha), \tag{58}$$

for all $\alpha, \beta \in \mathbb{N}$, where $\phi : \mathbb{N}\times\mathbb{N} \to \mathbb{C}$ is defined as

$$\phi(\alpha,\beta) = \langle e_\beta, \Phi_*(|e_\alpha\rangle\langle e_\alpha|)e_\beta\rangle = \langle e_\alpha, \Phi(_*|e_\beta\rangle\langle e_\beta|)e_\alpha\rangle, \tag{59}$$

for all $\alpha, \beta \in \mathbb{N}$.

Proof. Let us write $Ge_r = G(r)e_r$, for all $r \in \mathbb{N}$, and compare (56) with (57). One notices that $\langle e_{\beta'}, Ge_{\alpha'}\rangle = G(\alpha')\delta_{\alpha',\beta'} = \langle e_{\alpha'}, Ge_{\beta'}\rangle$, $\langle Ge_\alpha, e_\beta\rangle = \overline{G(\alpha)}\delta_{\alpha,\beta} = \langle Ge_\beta, e_\alpha\rangle$. So that, (50) is satisfied if and only if for all $\alpha, \alpha', \beta, \beta' \in \mathbb{N}$,

$$\rho^{1/2}(\alpha)\rho^{1/2}(\alpha')\langle e_{\beta'}, \Phi_*(|e_{\alpha'}\rangle\langle e_\alpha|)e_\beta\rangle = \rho^{1/2}(\beta)\rho^{1/2}(\beta')\langle e_{\alpha'}, \Phi_*(|e_{\beta'}\rangle\langle e_\beta|)e_\alpha\rangle.$$

The above condition is equivalent to

$$\langle e_{\beta'}, \Phi_*(|\rho^{1/2}e_{\alpha'}\rangle\langle\rho^{1/2}e_\alpha|)e_\beta\rangle = \langle e_{\alpha'}, \Phi_*(|\rho^{1/2}e_{\beta'}\rangle\langle\rho^{1/2}e_\beta|)e_\alpha\rangle. \tag{60}$$

Consider the algebraic tensor product $\mathcal{V} = \mathfrak{I}_1(\mathfrak{h}) \otimes_a \mathfrak{h}$ of trace-class operators with the Hilbert space $\mathfrak{h}$. For each couple of elements $\sum_p \sigma_p \otimes_a u_p$, $\sum_q \sigma'_q \otimes_a u'_q \in \mathcal{V}$, consider

$$\langle\langle \sum_p \sigma_p \otimes_a u_p, \sum_q \sigma'_q \otimes_a u'_q\rangle\rangle = \sum_{p,q}\langle u_p, \Phi_*({a_p}^* a_q)u'_q\rangle.$$

This defines a scalar product on $\mathcal{V}$ since Φ_* is completely positive.

Now, (60) becomes

$$\langle\langle |e_r\rangle\langle\rho^{1/2}e_{\alpha'}| \otimes e_{\beta'}, |e_r\rangle\langle\rho^{1/2}e_\alpha| \otimes e_\beta\rangle\rangle = \langle\langle |e_r\rangle\langle\rho^{1/2}e_{\beta'}| \otimes e_{\alpha'}, |e_r\rangle\langle\rho^{1/2}e_\beta| \otimes e_\alpha\rangle\rangle,$$

for any $r \in \mathbb{N}$. Thus, using polarization on the scalar product $\langle\langle\cdot\rangle\rangle$, this condition holds if and only if (60) is satisfied for any $\alpha, \beta \in \mathbb{N}$ and $\alpha' = \alpha$, $\beta' = \beta$. □

Let us apply this result to our model. Here, the so-called *classical reduction* of the semigroup by $\mathbf{H}^s$ follows from the relation $[\, H^s, L_{\mathbf{i},\mathbf{j}}(s)] = (E(s,\mathbf{j}) - E(s,\mathbf{i}))L_{\mathbf{i},\mathbf{j}}(s)$, for all $\mathbf{i},\mathbf{j}$ (see [36], [33], [37]). This implies that $(|\eta\rangle,\ \eta \in \mathfrak{C})$ diagonalizes both, $\Re G = -\frac{1}{2}\sum_{\mathbf{k},\ell} L_{\mathbf{k},\ell}(s)^* L_{\mathbf{k},\ell}(s)$ and $\Im G = -\mathbf{H}^s$. Thus, we consider ρ given by

$$\rho = \sum_{\eta\in\mathfrak{C}} \rho(\eta)|\eta\rangle\langle\eta|.$$

A straightforward computation gives

$$\phi(\eta,\zeta)=\sum_{\mathbf{i},\mathbf{j}}|\langle\zeta,L_{\mathbf{i},\mathbf{j}}(s)\eta\rangle|^2.$$

Notice that the above sum is indeed reduced to indexes $\mathbf{i},\mathbf{j}$ such that $L_{\mathbf{i},\mathbf{j}}(s)|\eta\rangle$ is colinear with $|\zeta\rangle$. Moreover,

$$|\langle\zeta,L_{\mathbf{i},\mathbf{j}}(s)\eta\rangle|^2=|\langle b_{\mathbf{j}}\zeta,b_{\mathbf{i}}\eta\rangle|^2c_{\mathbf{i},\mathbf{j}}(s)=\langle b_{\mathbf{j}}\zeta,b_{\mathbf{i}}\eta\rangle c_{\mathbf{i},\mathbf{j}}(s)$$

So, that $\phi(\eta,\zeta)=\sum_{\mathbf{i},\mathbf{j}}\langle b_{\mathbf{j}}\zeta,b_{\mathbf{i}}\eta\rangle c_{\mathbf{i},\mathbf{j}}(s)$, and (58) becomes

$$\rho(\eta)\sum_{\mathbf{i},\mathbf{j}}\langle b_{\mathbf{j}}\zeta,b_{\mathbf{i}}\eta\rangle c_{\mathbf{i},\mathbf{j}}(s)=\rho(\zeta)\sum_{\mathbf{i},\mathbf{j}}\langle b_{\mathbf{i}}\eta,b_{\mathbf{j}}\zeta\rangle c_{\mathbf{j},\mathbf{i}}(s) \tag{61}$$

The above equation reveals that the balance depends on the exchange of two components of the configurations only. Let $\pi(\mathbf{i})$ denote $\rho(1_{\mathbf{i}})$. Therefore, (61) reduces to

$$\pi(\mathbf{i})c_{\mathbf{i},\mathbf{j}}(s)=\pi(\mathbf{j})c_{\mathbf{j},\mathbf{i}}(s). \tag{62}$$

This is exactly the reversibility condition which has been discovered in the commutative case and was used, without normalization, in Theorem 2 (see equation (40)) to construct a stationary state. To recover $\rho(\eta)$ from (62) for any configuration η, it suffices to notice that (61) is satisfied by

$$\rho(\eta)=\prod_{\mathbf{i}\in\mathbb{N}^2}\pi(\mathbf{i})^{\eta(\mathbf{i})} \tag{63}$$

To summarize, we have the following conclusion.

Corollary 3. *Under the hypotheses of Theorem* 1*, a density matrix which is diagonal in the orthonormal basis* $(|\eta\rangle;\ \eta\in\mathfrak{C})$*, with components* $(\rho(\eta);\eta\in\mathfrak{C})$*, corresponds to an equilibrium state if and only if the detailed balance condition* (62) *is satisfied.*

The above result will be rephrased in a slightly different manner in the next subsection to recover a unique faithful stationary state in the Gibbs form.

6.2. Ergodicity: the convergence towards the equilibrium

Once determined an equilibrium state, one wants to know whether the dynamics drives any other state towards the above as time increases. As we shall see, this question is deeply related to *connectivity* of the graph determined by the matrix $(c_{\mathbf{i},\mathbf{j}}(s))$.

Here, one can easily check that the following relation holds on generalized commutator algebras:

$$\left\{\mathbf{H}^s,L_{\mathbf{i},\mathbf{j}}(s)^*,L_{\mathbf{i},\mathbf{j}}(s);\ \mathbf{i},\mathbf{j}\in\mathbb{N}^2\right\}'=\left\{L_{\mathbf{i},\mathbf{j}}(s)^*,L_{\mathbf{i},\mathbf{j}}(s);\ i,j\in\mathbb{N}\right\}'. \tag{64}$$

As it has been proved in [18], (see also [20]), if the algebras above are trivial, that is equal to $\mathbb{C}\mathbf{1}$, then the QMS is ergodic, that is, for any other state σ, one has $\mathcal{T}_{*t}(\sigma)\to\rho$ in the w^*-topology as $t\to\infty$, where ρ is supposed to be the equilibrium state.

To have a connected graph, we add a cemetery to our system by completing $\mathbb{N}^2$ with a point $\partial \notin \mathbb{N}^2$. We assume that $c_{\mathbf{i},\partial}(s), c_{\partial,\mathbf{j}}(s) > 0$ but $c_{\partial,\partial} = 0$. On the other hand, we put $L_{\mathbf{i},\partial} = \sqrt{c_{\mathbf{i},\partial}(s)}\ b_{\mathbf{i}}$, $L_{\partial,\mathbf{j}} = \sqrt{c_{\partial,\mathbf{j}}(s)}\ b_{\mathbf{j}}^\dagger$, for all $\mathbf{i},\mathbf{j} \in \mathbb{N}^2$, and $L_{\partial,\partial} = 0$. Configurations are now defined on $\overline{\mathbb{N}^2} = \mathbb{N}^2 \cup \{\partial\}$. Finally define $E_\partial = \mu > 0$, which we call the *chemical potential*. The generator $\mathcal{L}^s(\cdot)$ is naturally extended taking the sum in (31) running over all indexes $(\mathbf{i},\mathbf{j}) \in \overline{\mathbb{N}^2} \times \overline{\mathbb{N}^2}$. Moreover, this time the set $\left\{ L_{\mathbf{i},\mathbf{j}}(s), L_{\mathbf{i},\mathbf{j}}^*;\ \mathbf{i},\mathbf{j} \in \overline{\mathbb{N}^2} \right\}$ includes all the operators $b_{\mathbf{k}}^\dagger, b_{\mathbf{k}}$ generating the CAR algebra, so that its generalized commutant algebra is trivial. Thus, in this case we have

$$\left\{ L_{\mathbf{i},\mathbf{j}}(s)^*, L_{\mathbf{i},\mathbf{j}}(s);\ i,j \in \mathbb{N} \right\}' = \left\{ b_{\mathbf{k}}^\dagger, b_{\mathbf{k}},\ \mathbf{k} \in \mathbb{N}^2 \right\}',$$

and the semigroup is ergodic as soon as we provide a faithful stationary state.

In the following we assume $\beta > 0$. A straightforward computation yields

$$\mathrm{tr}\left(e^{-\beta(\mathbf{H}^s - \mu N)} \right) = \prod\nolimits_{\mathbf{i}\in\mathbb{N}^2} \left(1 + e^{-\beta(E(s,\mathbf{i})-\mu)} \right) < \infty,$$

where $N = \sum_{\mathbf{k}\in\mathbb{N}^2} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}$ is the total number (unbounded) operator.

Corollary 4. *Suppose that the transport coefficients satisfy the detailed balance condition*

$$e^{-\beta(E(s,\mathbf{i})-\mu)} c_{\mathbf{i},\mathbf{j}}(s) = e^{-\beta(E(s,\mathbf{j})-\mu)} c_{\mathbf{j},\mathbf{i}}(s),\ (\mathbf{i},\mathbf{j} \in \overline{\mathbb{N}^2}) \tag{65}$$

where $\beta > 0$. Denote

$$Z(s,\beta,\mu) = \left(e^{-\beta(\mathbf{H}^s - \mu N)} \right).$$

Then

$$\rho = \frac{1}{Z(s,\beta,\mu)} e^{-\beta(\mathbf{H}^s - \mu N)},$$

is a faithful equilibrium state of the quantum Markov semigroup $\mathcal{T}^s$. The semigroup is ergodic and decoherent along the basis $(|\eta\rangle, \eta \in \mathfrak{C})$, that is, for all $\eta \neq \zeta$ and all state σ, it holds:

$$\langle \eta | \mathcal{T}_{*t}(\sigma) | \zeta \rangle \to 0, \tag{66}$$

as $t \to \infty$.

Proof. The equilibrium follows straightforward from Corollary 3 before, since

$$\pi(\mathbf{i}) = e^{-\beta(E(s,\mathbf{i})-\mu)},\ (\mathbf{i} \in \mathbb{N}^2)$$

satisfies (62), though it is not normalized. Thus, $\rho(\eta)$ is given here as

$$\rho(\eta) = \frac{1}{Z(s,\beta,\mu)} \prod_{\mathbf{i}\in\mathbb{N}^2} \pi(\mathbf{i})^{\eta(\mathbf{i})} = \frac{e^{-\beta(E(s,\eta)-\mu N(\eta))}}{Z(s,\beta,\mu)},\ (\eta \in \mathfrak{C}),$$

where $N|\eta\rangle = N(\eta)|\eta\rangle$. That is,

$$\rho = \frac{1}{Z(s,\beta,\mu)} e^{-\beta(\mathbf{H}^s - \mu N)}.$$

Moreover, the previous remarks based on the main results of [18] imply the convergence towards the equilibrium. Indeed, by construction, the state is faithful. The decoherent behavior is a simply consequence of the convergence to the equilibrium, since ρ is diagonal in the basis $(|\eta\rangle, \eta \in \mathfrak{C})$. □

Conclusions and outlook

Here, we have illustrated a number of applications of the Markov theory of quantum interacting particles to transport problems. Particles are supposed to satisfy the Pauli exclusion principle, and are immersed in a phonon reservoir. The model uses a representation of energy levels through labels in $\mathbb{N}^2$. That requires to introduce a connectivity matrix or a graph, which contains the information about physical meaningful energy transitions. This graph crucially determines the coefficients of the semigroup generator. Moreover, they play a fundamental role in the study of conductivity, a subject which we did not cover in the current report.

The analysis of conductivity is a subject currently under study as part of a research program on non equilibrium dynamics.

Finally, we didn't touch here the derivation of the generator through any class of limit (weak coupling or stochastic). The reader interested in such a class of problems is referred to [1]. That is, we adopted as the outset the Markov approach and proposed a (phenomenological) form of the semigroup generator. Even though, an interesting open question is the derivation of a master equation for interacting particle systems with memory, that is, non Markovian.

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A New Formula Relating Localisation Operators to Time Operators

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Abstract. We consider in a Hilbert space a self-adjoint operator H and a family $\Phi \equiv (\Phi_1, \dots, \Phi_d)$ of mutually commuting self-adjoint operators. Under some regularity properties of H with respect to Φ, we propose two new formulae for a time operator for H and prove their equality. One of the expressions is based on the time evolution of an abstract localisation operator defined in terms of Φ while the other one corresponds to a stationary formula. Under the same assumptions, we also conduct the spectral analysis of H by using the method of the conjugate operator.

Among other examples, our theory applies to Friedrichs Hamiltonians, Stark Hamiltonians, some Jacobi operators, the Dirac operator, convolution operators on locally compact groups, pseudodifferential operators, adjacency operators on graphs and direct integral operators.

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1. Introduction and main results

Let H be a self-adjoint operator in a Hilbert space $\mathcal{H}$ and let T be a linear operator in $\mathcal{H}$. Generally speaking, the operator T is called a time operator for H if it satisfies the canonical commutation relation

$$[T, H] = i, \tag{1.1}$$

or, alternatively, the relation

$$T\,\mathrm{e}^{-itH} = \mathrm{e}^{-itH}(T + t), \quad t \in \mathbb{R}. \tag{1.2}$$

Obviously, these two equations are very formal and not equivalent. So many authors have proposed various sets of conditions in order to give a precise meaning to them. For instance, one has introduced the concept of infinitesimal Weyl relation in the weak or in the strong sense [18], the T-weak Weyl relation [21] or various generalised versions of the Weyl relation (see, *e.g.*, [6, 17]). However, in most of these publications the pair $\{H, T\}$ is a priori given and the authors are mainly interested in the properties of H and T that can be deduced from a relation like (1.2). In particular, the self-adjointness of T, the spectral nature of H and T, the connection with the survival probability, the form of T in the spectral representation of H, the relation with the theory of irreversibility and many other properties have been extensively discussed in the literature (see [23, Sec. 8], [24, Sec. 3], [5, 12, 15, 16, 38] and references therein).

Our approach is radically different. Starting from a self-adjoint operator H, one wonders if there exists a linear operator T such that (1.1) holds in a suitable sense. And can we find a universal procedure to construct such an operator? This paper is a first attempt to answer these questions.

Our interest in these questions has been recently aroused by a formula put into evidence in [37]. Along the proof of the existence of time delay for hypoelliptic pseudodifferential operators $H := h(P)$ in $\mathsf{L}^2(\mathbb{R}^d)$, the author derives an integral formula linking the time evolution of localisation operators to the derivative with respect to the spectral parameter of H. The formula reads as follows: if Q stands for the family of position operators in $\mathsf{L}^2(\mathbb{R}^d)$ and $f : \mathbb{R}^d \to \mathbb{C}$ is some appropriate function with $f = 1$ in a neighbourhood of 0, then one has on suitable elements $\varphi \in \mathsf{L}^2(\mathbb{R}^d)$

$$\lim_{r\to\infty} \tfrac{1}{2} \int_0^\infty \mathrm{d}t \, \big\langle \varphi, \big[\, \mathrm{e}^{-itH} \, f(Q/r) \, \mathrm{e}^{itH} - \mathrm{e}^{itH} \, f(Q/r) \, \mathrm{e}^{-itH} \, \big] \varphi \big\rangle = \big\langle \varphi, i \tfrac{\mathrm{d}}{\mathrm{d}H} \, \varphi \big\rangle, \tag{1.3}$$

where $\frac{\mathrm{d}}{\mathrm{d}H}$ stands for the operator acting as $\frac{\mathrm{d}}{\mathrm{d}\lambda}$ in the spectral representation of H. Accordingly, this formula furnishes a preliminary procedure to obtain a time operator T only constructed in terms of H, the position operators Q and the function f.

A review of the methods used in [37] suggested to us that Equation (1.3) could be extended to the case of an abstract pair of operator H and position operators Φ acting in a Hilbert space $\mathcal{H}$, as soon as H and Φ satisfy two appropriate commutation relations. Namely, suppose that you are given a self-adjoint operator H and a family $\Phi \equiv (\Phi_1, \ldots, \Phi_d)$ of mutually commuting self-adjoint operators in $\mathcal{H}$. Then, roughly speaking, the first condition requires that for some $\omega \in \mathbb{C} \setminus \mathbb{R}$ the map

$$\mathbb{R}^d \ni x \mapsto \mathrm{e}^{-ix\cdot\Phi} (H - \omega)^{-1} \, \mathrm{e}^{ix\cdot\Phi} \in \mathscr{B}(\mathcal{H})$$

is 3-times strongly differentiable (see Assumption 2.2 for a precise statement). The second condition, Assumption 2.3, requires that the operators $\mathrm{e}^{-ix\cdot\Phi} \, H \, \mathrm{e}^{ix\cdot\Phi}$, $x \in \mathbb{R}^d$, define a family of mutually commuting operators. Given this, our main result reads as follows (see Theorem 5.5 for a precise statement):

Theorem 1.1. *Let H and Φ be as above. Let f be a Schwartz function on $\mathbb{R}^d$ such that $f = 1$ on a neighbourhood of 0 and $f(x) = f(-x)$ for each $x \in \mathbb{R}^d$. Then, for each φ in some suitable subset of $\mathcal{H}$ one has*

$$\lim_{r\to\infty} \tfrac{1}{2} \int_0^\infty \mathrm{d}t \, \big\langle \varphi, \big[\, \mathrm{e}^{-itH} \, f(\Phi/r) \, \mathrm{e}^{itH} - \mathrm{e}^{itH} \, f(\Phi/r) \, \mathrm{e}^{-itH} \, \big] \varphi \big\rangle = \langle \varphi, T_f \varphi \rangle, \quad (1.4)$$

where the operator T_f acts, in an appropriate sense, as $i\frac{\mathrm{d}}{\mathrm{d}\lambda}$ in the spectral representation of H.

One infers from this result that the operator T_f is a time operator. Furthermore, an explicit description of T_f is also available: if H'_j denotes the self-adjoint operator associated with the commutator $i[H, \Phi_j]$ and $H' := (H'_1, \ldots, H'_d)$, then T_f is formally given by

$$T_f = -\tfrac{1}{2}\big(\Phi \cdot R'_f(H') + R'_f(H') \cdot \Phi\big), \quad (1.5)$$

where $R'_f : \mathbb{R}^d \to \mathbb{C}^d$ is some explicit function (see Section 4 and Proposition 5.2).

In summary, once a family of mutually commuting self-adjoint operators $(\Phi_1, \ldots, \Phi_d)$ satisfying Assumptions 2.2 and 2.3 has been given, then a time operator can be defined either in terms of the l.h.s. of (1.4) or in terms of (1.5). When suitably defined, both expressions lead to the same operator. We also mention that the equality (1.4), with r.h.s. defined by (1.5), provides a crucial preliminary step for the proof of the existence of quantum time delay and Eisenbud-Wigner Formula for abstract scattering pairs $\{H, H+V\}$. In addition, Theorem 1.1 establishes a new relation between time dependent scattering theory (l.h.s.) and stationary scattering theory (r.h.s.) for a general class of operators. We refer to the discussion in Section 6 for more information on these issues.

Let us now describe more precisely the content of this paper. In Section 2 we recall the necessary definitions from the theory of the conjugate operator and define a critical set $\kappa(H)$ for the operator H. In the more usual setup where $H = h(P)$ is a function of the momentum vector operator P and Φ is the position vector operator Q in $\mathsf{L}^2(\mathbb{R}^d)$, it is known that the critical values of h

$$\kappa_h := \big\{ \lambda \in \mathbb{R} \mid \exists x \in \mathbb{R}^d \text{ such that } h(x) = \lambda \text{ and } h'(x) = 0 \big\}$$

plays an important role (see, *e.g.*, [1, Sec. 7]). For instance, one cannot obtain a simple Mourre estimate at these values. Such phenomena also occur in the abstract setup. Since the operator H is a priori not a function of an auxiliary operator as $h(P)$, the derivative appearing in the definition of κ_h does not have a direct counterpart. However, the identities $(\partial_j h)(P) = i[h(P), Q_j]$ suggest to define the set of critical values $\kappa(H)$ in terms of the vector operator $H' := \big(i[H, \Phi_1], \ldots, i[H, \Phi_d]\big)$. This is the content of Definition 2.5. In Lemma 2.6 and Theorem 3.6, we show that $\kappa(H)$ is closed, contains the set of eigenvalues of H, and that the spectrum of H in $\sigma(H) \setminus \kappa(H)$ is purely absolutely continuous. The proof of the latter result relies on the construction, described in Section 3, of an appropriate conjugate operator for H.

In Section 4, we recall some definitions in relation with the function f that appear in Theorem 1.1. The function R_f is introduced and some of its properties are presented. Section 5 is the core of the paper and its most technical part. It contains the definition of T_f and the proof of the precise version of Theorem 1.1. Suitable subspaces of $\mathcal{H}$ on which the operators are well defined and on which the equalities hold are introduced.

An interpretation of our results is proposed in Section 6. The relation with the theory of time operators is explained, and various cases are presented. The importance of Theorem 5.5 for the proof of the existence of the quantum time delay and Eisenbud-Wigner Formula is also sketched.

In Section 7, we show that our results apply to many operators H appearing in physics and mathematics literature. Among other examples, we treat Friedrichs Hamiltonians, Stark Hamiltonians, some Jacobi operators, the Dirac operator, convolution operators on locally compact groups, pseudodifferential operators, adjacency operators on graphs and direct integral operators. In each case, we are able to exhibit a natural family of nontrivial position operators Φ satisfying our assumptions. The diversity of the examples covered by our theory make us strongly believe that Formula (1.4) is of natural character. Moreover it also suggests that the existence of time delay is a very common feature of quantum scattering theory. We also point out that one by-product of our study is an efficient algorithm for the choice of a conjugate operator for a given self-adjoint operator H (see Section 3). This allows us to obtain (or reobtain) non trivial spectral results for various important classes of self-adjoint operators H.

As a final comment, we would like to emphasize that one of the main interest of our study comes from the fact that we do not restrict ourselves to the standard position operators Q and to operators H which are functions of P. Due to this generality, we cannot rely on the usual canonical commutation relation of Q and P and on the subjacent Fourier analysis. This explains the constant use of abstract commutators methods throughout the paper.

2. Critical values

In this section, we recall some standard notions on the conjugate operator theory and introduce our general framework. The set of critical values is defined and some of its properties are outlined. This subset of the spectrum of the operator under investigation plays an essential role in the sequel.

We first recall some facts principally borrowed from [1]. Let H and A be two self-adjoint operators in a Hilbert space $\mathcal{H}$. Their respective domain are denoted by $\mathcal{D}(H)$ and $\mathcal{D}(A)$, and for suitable $\omega \in \mathbb{C}$ we write R_ω for $(H-\omega)^{-1}$. The operator H is of class $C^1(A)$ if there exists $\omega \in \mathbb{C} \setminus \sigma(H)$ such that the map

$$\mathbb{R} \ni t \mapsto \mathrm{e}^{-itA} R_\omega \mathrm{e}^{itA} \in \mathscr{B}(\mathcal{H}) \tag{2.1}$$

is strongly differentiable. In that case, the quadratic form

$$\mathcal{D}(A) \ni \varphi \mapsto \langle A\varphi, R_\omega\varphi\rangle - \langle R_\omega^*\varphi, A\varphi\rangle \in \mathbb{C}$$

extends continuously to a bounded operator denoted by $[A, R_\omega] \in \mathscr{B}(\mathcal{H})$. It also follows from the $C^1(A)$-condition that $\mathcal{D}(H) \cap \mathcal{D}(A)$ is a core for H and that the quadratic form $\mathcal{D}(H) \cap \mathcal{D}(A) \ni \varphi \mapsto \langle H\varphi, A\varphi\rangle - \langle A\varphi, H\varphi\rangle$ is continuous in the topology of $\mathcal{D}(H)$. This form extends then uniquely to a continuous quadratic form $[H, A]$ on $\mathcal{D}(H)$, which can be identified with a continuous operator from $\mathcal{D}(H)$ to the adjoint space $\mathcal{D}(H)^*$. Finally, the following equality holds:

$$[A, R_\omega] = R_\omega [H, A] R_\omega. \tag{2.2}$$

It is also proved in [13, Lemma 2] that if $[H, A]\mathcal{D}(H) \subset \mathcal{H}$, then the unitary group $\{\mathrm{e}^{itA}\}_{t\in\mathbb{R}}$ preserves the domain of H, *i.e.*, $\mathrm{e}^{itA}\,\mathcal{D}(H) \subset \mathcal{D}(H)$ for all $t \in \mathbb{R}$. In the sequel, we shall say that $i[H, A]$ is essentially self-adjoint on $\mathcal{D}(H)$ if $[H, A]\mathcal{D}(H) \subset \mathcal{H}$ and if $i[H, A]$ is essentially self-adjoint on $\mathcal{D}(H)$ in the usual sense.

We now extend this framework in two directions: in the number of conjugate operators and in the degree of regularity with respect to these operators. So, let us consider a family $\Phi \equiv (\Phi_1, \ldots, \Phi_d)$ of mutually commuting self-adjoint operators in $\mathcal{H}$ (throughout the paper, we use the term "commute" for operators commuting in the sense of [26, Sec. VIII.5]). Then we know from [7, Sec. 6.5] that any measurable function $f \in \mathsf{L}^\infty(\mathbb{R}^d)$ defines a bounded operator $f(\Phi)$ in $\mathcal{H}$. In particular, the operator $\mathrm{e}^{ix\cdot\Phi}$, with $x \cdot \Phi \equiv \sum_{j=1}^d x_j\Phi_j$, is unitary for each $x \in \mathbb{R}^d$. Note also that the conjugation

$$C_x : \mathscr{B}(\mathcal{H}) \to \mathscr{B}(\mathcal{H}), \quad B \mapsto \mathrm{e}^{-ix\cdot\Phi}\, B\, \mathrm{e}^{ix\cdot\Phi}$$

defines an automorphism of $\mathscr{B}(\mathcal{H})$.

Within this framework, the operator H is said to be of class $C^m(\Phi)$ for $m = 1, 2, \ldots$ if there exists $\omega \in \mathbb{C} \setminus \sigma(H)$ such that the map

$$\mathbb{R}^d \ni x \mapsto \mathrm{e}^{-ix\cdot\Phi}\, R_\omega\, \mathrm{e}^{ix\cdot\Phi} \in \mathscr{B}(\mathcal{H}) \tag{2.3}$$

is strongly of class C^m in $\mathcal{H}$. One easily observes that if H is of class $C^m(\Phi)$, then the operator H is of class $C^m(\Phi_j)$ for each j (the class $C^m(\Phi_j)$ being defined similarly).

Remark 2.1. A bounded operator $S \in \mathscr{B}(\mathcal{H})$ belongs to $C^1(A)$ if the map (2.1), with R_ω replaced by S, is strongly differentiable. Similarly, $S \in \mathscr{B}(\mathcal{H})$ belongs to $C^m(\Phi)$ if the map (2.3), with R_ω replaced by S, is strongly C^m.

In the sequel, we assume that H is regular with respect to unitary group $\{\mathrm{e}^{ix\cdot\Phi}\}_{x\in\mathbb{R}^d}$ in the following sense.

Assumption 2.2. The operator H is of class $C^1(\Phi)$, and for each $j \in \{1, \ldots, d\}$, $i[H, \Phi_j]$ is essentially self-adjoint on $\mathcal{D}(H)$, with its self-adjoint extension denoted by H'_j. The operator H'_j is of class $C^1(\Phi)$, and for each $k \in \{1, \ldots, d\}$, $i[H'_j, \Phi_k]$ is essentially self-adjoint on $\mathcal{D}(H'_j)$, with its self-adjoint extension denoted by H''_{jk}.

The operator H''_{jk} is of class $C^1(\Phi)$, and for each $\ell \in \{1, \ldots, d\}$, $i[H''_{jk}, \Phi_\ell]$ is essentially self-adjoint on $\mathcal{D}(H''_{jk})$, with its self-adjoint extension denoted by $H'''_{jk\ell}$.

This assumption implies the invariance of $\mathcal{D}(H)$ under the action of the unitary group $\{\mathrm{e}^{ix\cdot\Phi}\}_{x\in\mathbb{R}^d}$. Indeed, this follows from the condition $[H, \Phi_j]\mathcal{D}(H) \subset \mathcal{H}$ and from [13, Lemma 2] that $\mathrm{e}^{it\Phi_j}\,\mathcal{D}(H) \subset \mathcal{D}(H)$ for all $t \in \mathbb{R}$. In fact, one easily obtains that $\mathrm{e}^{it\Phi_j}\,\mathcal{D}(H) = \mathcal{D}(H)$, and since this property holds for each j one also has $\mathrm{e}^{ix\cdot\Phi}\,\mathcal{D}(H) = \mathcal{D}(H)$ for all $x \in \mathbb{R}^d$. As a consequence, we obtain in particular that each self-adjoint operator

$$H(x) := \mathrm{e}^{-ix\cdot\Phi}\,H\,\mathrm{e}^{ix\cdot\Phi} \tag{2.4}$$

(with $H(0) = H$) has domain $\mathcal{D}[H(x)] = \mathcal{D}(H)$.

Similarly, the domains $\mathcal{D}(H'_j)$ and $\mathcal{D}(H''_{jk})$ are left invariant by the action of the unitary group $\{\mathrm{e}^{ix\cdot\Phi}\}_{x\in\mathbb{R}^d}$, and the operators $H'_j(x) := \mathrm{e}^{-ix\cdot\Phi}\,H'_j\,\mathrm{e}^{ix\cdot\Phi}$ and $H''_{jk}(x) := \mathrm{e}^{-ix\cdot\Phi}\,H''_{jk}\,\mathrm{e}^{ix\cdot\Phi}$ are self-adjoint operators with domains $\mathcal{D}(H'_j)$ and $\mathcal{D}(H''_{jk})$ respectively.

Our second main assumption concerns the family of operators $H(x)$.

Assumption 2.3. The operators $\{H(x)\}_{x\in\mathbb{R}^d}$ mutually commute.

Using the fact that the map $\mathbb{R}^d \ni x \mapsto C_x \in \mathsf{Aut}[\mathscr{B}(\mathcal{H})]$ is a group morphism, one easily shows that Assumption 2.3 is equivalent the commutativity of each $H(x)$ with H. Furthermore, Assumptions 2.2 and 2.3 imply additional commutation relations:

Lemma 2.4. *The operators $H(x)$, $H'_j(y)$, $H''_{k\ell}(z)$ mutually commute for each j, k, $\ell \in \{1, \ldots, d\}$ and each $x, y, z \in \mathbb{R}^d$.*

Proof. Let $\omega \in \mathbb{C} \setminus \mathbb{R}$, $x, y, z \in \mathbb{R}^d$, $j, k, \ell, m \in \{1, \ldots, d\}$, and set $R(x) := [H(x) - \omega]^{-1}$, $R'_j(x) := [H'_j(x) - \omega]^{-1}$ and $R''_{jk}(x) := [H''_{jk}(x) - \omega]^{-1}$. By assumption, one has the equality

$$R(x)\,\tfrac{R(\varepsilon e_j)-R(0)}{\varepsilon} = \tfrac{R(\varepsilon e_j)-R(0)}{\varepsilon}\,R(x)$$

for each $\varepsilon \in \mathbb{R} \setminus \{0\}$. Taking the strong limit as $\varepsilon \to 0$, and using (2.2) and Assumption 2.3, one obtains

$$R(0)\,\big[R(x)H'_j - H'_jR(x)\big]\,R(0) = 0.$$

Since the resolvent $R(0)$ on the left is injective, this implies that $R(x)H'_j - H'_jR(x) = 0$ on $\mathcal{D}(H)$. Furthermore, since $\mathcal{D}(H)$ is a core for H'_j the last equality can be extended to $\mathcal{D}(H'_j)$. So, one gets

$$R'_j(0)R(x) = R'_j(0)R(x)\big(H'_j - \omega\big)R'_j(0) = R(x)R'_j(0).$$

One infers from this that $H(x)$ and $H'_j(y)$ commute by using the morphism property of the map $\mathbb{R}^d \ni x \mapsto C_x \in \mathsf{Aut}[\mathscr{B}(\mathcal{H})]$.

A similar argument leads to the commutativity of the operators $H'_j(x)$ and $H'_k(y)$ by considering the operators $R'_j(x)\frac{R(\varepsilon e_k)-R(0)}{\varepsilon}$ and $\frac{R(\varepsilon e_k)-R(0)}{\varepsilon}R'_j(x)$. The commutativity of $H(x)$ and $H''_{jk}(z)$ is obtained by considering the operators

$R(x)\frac{R'_j(\varepsilon e_k)-R'_j(0)}{\varepsilon}$ and $\frac{R'_j(\varepsilon e_k)-R'_j(0)}{\varepsilon}R(x)$, and the commutativity of $H'_j(y)$ and $H''_{k\ell}(z)$ by considering the operators $R'_j(y)\frac{R'_k(\varepsilon e_\ell)-R'_k(0)}{\varepsilon}$ and $\frac{R'_k(\varepsilon e_\ell)-R'_k(0)}{\varepsilon}R'_j(y)$. Finally, the commutation between $H''_{jk}(x)$ and $H''_{\ell m}(y)$ is obtained by considering the operators $R''_{jk}(x)\frac{R'_\ell(\varepsilon e_m)-R'_\ell(0)}{\varepsilon}$ and $\frac{R'_\ell(\varepsilon e_m)-R'_\ell(0)}{\varepsilon}R''_{jk}(x)$. Details are left to the reader. □

For simplicity, we write H' for the vector operator $(H'_1,\dots,H'_d)$, and define for each measurable function $f:\mathbb{R}^d\to\mathbb{C}$ the operator $f(H')$ by using the d-variables functional calculus. The symbol $E^H(\cdot)$ denotes the spectral measure of H.

Definition 2.5. A number $\lambda\in\mathbb{R}$ is called a regular value of H if there exists $\delta>0$ such that

$$\lim_{\varepsilon\searrow 0}\left\|\left[(H')^2+\varepsilon\right]^{-1}E^H\big((\lambda-\delta,\lambda+\delta)\big)\right\|<\infty. \tag{2.5}$$

A number $\lambda\in\mathbb{R}$ that is not a regular value of H is called a critical value of H. We denote by $\kappa(H)$ the set of critical values of H.

From now on, we shall use the shorter notation $E^H(\lambda;\delta)$ for $E^H\big((\lambda-\delta,\lambda+\delta)\big)$. In the next lemma we put into evidence some useful properties of the set $\kappa(H)$.

Lemma 2.6. *Let Assumptions* 2.2 *and* 2.3 *be verified. Then the set* $\kappa(H)$ *possesses the following properties:*

(a) $\kappa(H)$ *is closed.*
(b) $\kappa(H)$ *contains the set of eigenvalues of* H.
(c) *The limit* $\lim_{\varepsilon\searrow 0}\left\|\left[(H')^2+\varepsilon\right]^{-1}E^H(J)\right\|$ *is finite for each compact set* $J\subset\mathbb{R}\setminus\kappa(H)$.
(d) *For each compact set* $J\subset\mathbb{R}\setminus\kappa(H)$, *there exists a compact set* $U\subset(0,\infty)$ *such that* $E^H(J)=E^{|H'|}(U)E^H(J)$.

Proof. (a) Let λ_0 be a regular value for H, *i.e.*, there exists $\delta_0>0$ such that (2.5) holds with λ replaced by λ_0. Let $\lambda\in(\lambda_0-\delta_0,\lambda_0+\delta_0)$ and let $\delta>0$ such that

$$(\lambda-\delta,\lambda+\delta)\subset(\lambda_0-\delta_0,\lambda_0+\delta_0).$$

Then, since $E^H(\lambda;\delta)=E^H(\lambda_0;\delta_0)E^H(\lambda;\delta)$, one has

$$\lim_{\varepsilon\searrow 0}\left\|\left[(H')^2+\varepsilon\right]^{-1}E^H(\lambda;\delta)\right\|\le\lim_{\varepsilon\searrow 0}\left\|\left[(H')^2+\varepsilon\right]^{-1}E^H(\lambda_0;\delta_0)\right\|<\infty.$$

But this means exactly that λ is a regular value for any $\lambda\in(\lambda_0-\delta_0,\lambda_0+\delta_0)$. So the set of regular values is open, and $\kappa(H)$ is closed.

(b) Let $\lambda\in\mathbb{R}$ be an eigenvalue of H, and let φ_λ be an associated eigenvector with norm one. Since H is of class $C^1(\Phi_j)$ for each j, we know from the Virial theorem [1, Prop. 7.2.10] that $E^H(\{\lambda\})H'_jE^H(\{\lambda\})=0$ for each j. This, together with Lemma 2.4, implies that

$$E^H(\{\lambda\})\left[(H')^2+\varepsilon\right]^{-1}E^H(\{\lambda\})=\varepsilon^{-1}E^H(\{\lambda\})$$

for each $\varepsilon > 0$. In particular, we obtain for each $\delta > 0$ the equalities

$$\big[(H')^2 + \varepsilon\big]^{-1} E^H(\lambda;\delta)\varphi_\lambda = E^H(\{\lambda\})\big[(H')^2 + \varepsilon\big]^{-1} E^H(\{\lambda\})\varphi_\lambda = \varepsilon^{-1}\varphi_\lambda,$$

and

$$\begin{aligned}\lim_{\varepsilon\searrow 0} \big\|\big[(H')^2 + \varepsilon\big]^{-1} E^H(\lambda;\delta)\big\| &\geq \lim_{\varepsilon\searrow 0} \big\|\big[(H')^2 + \varepsilon\big]^{-1} E^H(\lambda;\delta)\varphi_\lambda\big\| \\ &= \lim_{\varepsilon\searrow 0} \varepsilon^{-1}\|\varphi_\lambda\| = \infty.\end{aligned}$$

Since δ has been chosen arbitrarily, this implies that λ is not a regular value of H.

(c) This follows easily by using a compacity argument.

(d) Let us concentrate first on the lower bound of U. Clearly, if $|H'|$ is strictly positive, then U can be chosen in $(0,\infty)$ and thus is bounded from below by a strictly positive number. So assume now that $|H'|$ is not strictly positive, that is $0 \in \sigma(|H'|)$. By absurd, suppose that U is not bounded from below by a strictly positive number, *i.e.*, there does not exist $a > 0$ such that $U \subset (a,\infty)$. Then for $n = 1, 2, \ldots$, there exists $\psi_n \in \mathcal{H}$ such that $E^{|H'|}\big([0,1/n)\big)E^H(J)\psi_n \neq 0$, and the vectors

$$\varphi_n := \frac{E^{|H'|}\big([0,1/n)\big)E^H(J)\psi_n}{\|E^{|H'|}\big([0,1/n)\big)E^H(J)\psi_n\|}$$

satisfy $\|\varphi_n\| = 1$, and $E^H(J)\varphi_n = E^{|H'|}\big([0,1/n)\big)\varphi_n = \varphi_n$. It follows by point (c) that

$$\begin{aligned}\text{Const.} \geq \lim_{\varepsilon\searrow 0} \big\|\big[(H')^2 + \varepsilon\big]^{-1} E^H(J)\big\| &\geq \lim_{\varepsilon\searrow 0} \big\|\big[(H')^2 + \varepsilon\big]^{-1} E^H(J)\varphi_n\big\| \\ &= \lim_{\varepsilon\searrow 0} \big\|\big[(H')^2 + \varepsilon\big]^{-1} E^{|H'|}\big([0,1/n)\big)\varphi_n\big\| \\ &\geq \lim_{\varepsilon\searrow 0} \big(n^{-2} + \varepsilon\big)^{-1}\|\varphi_n\| \\ &= n^2,\end{aligned}$$

which leads to a contradiction when $n \to \infty$.

Let us now concentrate on the upper bound of U. Clearly, if $|H'|$ is a bounded operator, one can choose a bounded subset U of $\mathbb{R}$ and thus U is upper bounded. So assume now that $|H'|$ is not a bounded operator. By absurd, suppose that U is not bounded from above, *i.e.*, there does not exist $b < \infty$ such that $U \subset (0,b)$. Then for $n = 1, 2, \ldots$, there exists $\psi_n \in \mathcal{H}$ such that $E^{|H'|}\big([n,\infty)\big)E^H(J)\psi_n \neq 0$, and the vectors

$$\varphi_n := \frac{E^{|H'|}\big([n,\infty)\big)E^H(J)\psi_n}{\|E^{|H'|}\big([n,\infty)\big)E^H(J)\psi_n\|}$$

satisfy $\|\varphi_n\| = 1$, and $E^H(J)\varphi_n = E^{|H'|}\big([n,\infty)\big)\varphi_n = \varphi_n$. It follows by Assumption 2.2 and Lemma 2.4 that $|H'|E^H(J)$ is a bounded operator, and

$$\text{Const.} \geq \big\||H'|E^H(J)\big\| \geq \big\||H'|E^H(J)\varphi_n\big\| = \big\||H'|E^{|H'|}\big([n,\infty)\big)\varphi_n\big\| \geq n\|\varphi_n\|$$

which leads to a contradiction when $n \to \infty$. □

3. Locally smooth operators and absolute continuity

In this section we exhibit a large class of locally H-smooth operators. We also show that the operator H is purely absolutely continuous in $\sigma(H) \setminus \kappa(H)$. These results are obtained by using commutators methods as presented in [1].

In order to motivate our choice of conjugate operator for H, we present first a formal calculation. Let A_η be given by

$$A_\eta := \tfrac{1}{2}\big\{\eta(H)H' \cdot \Phi + \Phi \cdot H'\eta(H)\big\},$$

where η is some real function with a sufficiently rapid decrease to 0 at infinity. Then A_η satisfies with H the commutation relation

$$i[H, A_\eta] = \tfrac{i}{2}\sum_{j=1}^{d}\big\{\eta(H)H'_j\,[H, \Phi_j] + [H, \Phi_j]\,H'_j\eta(H)\big\} = (H')^2\eta(H),$$

which provides (in a sense to be specified) a Mourre estimate. So, in the sequel, one only has to justify these formal manipulations and to determinate an appropriate function η.

First of all, one observes that for each $j \in \{1, \dots, d\}$ and each $\omega \in \mathbb{C} \setminus \sigma(H)$ the operator $H'_j R_\omega \equiv H'_j(H-\omega)^{-1}$ is a bounded operator. Indeed, one has $(H-\omega)^{-1}\mathcal{H} = \mathcal{D}(H) \subset \mathcal{D}(H'_j)$ by Assumption 2.2. In the following lemmas, Assumptions 2.2 and 2.3 are tacitly assumed, and we set $\langle x\rangle := (1+x^2)^{1/2}$ for any $x \in \mathbb{R}^n$.

Lemma 3.1.

(a) *For each $j,k \in \{1,\dots,d\}$ and each $\gamma,\omega \in \mathbb{C}\setminus\sigma(H)$, the bounded operator $R_\gamma H'_j R_\omega$ belongs to $C^1(\Phi_k)$.*

(b) *For each $j,k \in \{1,\dots,d\}$ the bounded self-adjoint operator $\langle H\rangle^{-2}H'_j\langle H\rangle^{-2}$ belongs to $C^1(\Phi_k)$.*

(c) *For each $j,k,\ell \in \{1,\dots,d\}$, the bounded self-adjoint operator $i\big[\langle H\rangle^{-2}H'_j\langle H\rangle^{-2}, \Phi_k\big]$ belongs to $C^1(\Phi_\ell)$.*

(d) *The operator H is of class $C^3(\Phi)$.*

Proof. (a) Due to Assumption 2.2 one has for each $\varphi \in \mathcal{D}(\Phi_k)$

$$\begin{aligned}
&\big\langle \Phi_k\varphi, R_\gamma H'_j R_\omega\varphi\big\rangle - \big\langle R_{\bar\omega}H'_j R_{\bar\gamma}\varphi, \Phi_k\varphi\big\rangle\\
&\quad= \big\langle \Phi_k\varphi, R_\gamma H'_j R_\omega\varphi\big\rangle - \big\langle \Phi_k R_{\bar\gamma}\varphi, H'_j R_\omega\varphi\big\rangle\\
&\qquad+ \big\langle \Phi_k R_{\bar\gamma}\varphi, H'_j R_\omega\varphi\big\rangle - \big\langle R_{\bar\omega}H'_j R_{\bar\gamma}\varphi, \Phi_k\varphi\big\rangle\\
&\quad= \big\langle [R_{\bar\gamma}, \Phi_k]\varphi, H'_j R_\omega\varphi\big\rangle + \big\langle \Phi_k R_{\bar\gamma}\varphi, H'_j R_\omega\varphi\big\rangle - \big\langle H'_j R_{\bar\gamma}\varphi, \Phi_k R_\omega\varphi\big\rangle\\
&\qquad+ \big\langle H'_j R_{\bar\gamma}\varphi, \Phi_k R_\omega\varphi\big\rangle - \big\langle R_{\bar\omega}H'_j R_{\bar\gamma}\varphi, \Phi_k\varphi\big\rangle\\
&\quad= \big\langle [R_{\bar\gamma}, \Phi_k]\varphi, H'_j R_\omega\varphi\big\rangle + \big\langle [H'_j, \Phi_k]R_{\bar\gamma}\varphi, R_\omega\varphi\big\rangle + \big\langle H'_j R_{\bar\gamma}\varphi, [\Phi_k, R_\omega]\varphi\big\rangle.
\end{aligned}$$

This implies that there exists $\mathrm{c} < \infty$ such that

$$\big|\big\langle \Phi_k\varphi, R_\gamma H'_j R_\omega\varphi\big\rangle - \big\langle R_{\bar\omega}H'_j R_{\bar\gamma}\varphi, \Phi_k\varphi\big\rangle\big| \le \mathrm{c}\,\|\varphi\|^2.$$

for each $\varphi \in \mathcal{D}(\Phi_k)$, and thus the statement follows from [1, Lemma 6.2.9].

(b) Since $\langle H\rangle^{-2} = R_{-i}R_i$, the operator $\langle H\rangle^{-2}H'_j\langle H\rangle^{-2}$ is clearly bounded and self-adjoint. Furthermore, by observing that

$$\langle H\rangle^{-2}H'_j\langle H\rangle^{-2} = R_i\big(R_{-i}H'_jR_i\big)R_{-i}$$

one concludes from (a) that $\langle H\rangle^{-2}H'_j\langle H\rangle^{-2}$ is the product of three operators belonging to $C^1(\Phi_k)$, and thus belongs to $C^1(\Phi_k)$ due to [1, Prop. 5.1.5].

(c) Taking Lemma 2.4 into account, one gets

$$i\big[\langle H\rangle^{-2}H'_j\langle H\rangle^{-2},\Phi_k\big] = -2(R_iH'_kR_i)(R_{-i}H'_jR_{-i})(R_i+R_{-i}) + \langle H\rangle^{-2}H''_{jk}\langle H\rangle^{-2}.$$

The first term is a product of operators which belong to $C^1(\Phi_\ell)$, and thus it belongs to $C^1(\Phi_\ell)$. For the second term, a calculation similar to the one presented in (a) using Assumption 2.2 shows that this term also belongs to $C^1(\Phi_\ell)$, and so the claim is proved.

(d) In this part of the proof, we freely use the notations of [1] for some regularity classes with respect to the group generated by Φ_ℓ. Let us set $\mathcal{G} := \mathcal{D}(H)$, and consider $z \in \mathbb{C}\setminus\sigma(H)$ and $j,k,\ell \in \{1,\dots,d\}$. We know from the proof of (a) that the equality

$$i\big[i[R_z,\Phi_j],\Phi_k\big] = -i[R_z,\Phi_k]H'_jR_z - R_zH''_{jk}R_z - H'_jR_zi[R_z,\Phi_k] \tag{3.1}$$

holds on $\mathcal{H}$. We also know from Assumption 2.2 and [1, Lemma 5.1.2.(b)] that $R_z \in C^1(\Phi_\ell;\mathcal{H},\mathcal{G})$, that H'_j belongs to $C^1(\Phi_\ell;\mathcal{G},\mathcal{H})$ and that H''_{jk} belongs to $C^1(\Phi_\ell;\mathcal{G},\mathcal{H})$. So, each term of the r.h.s. of (3.1) belongs to $C^1(\Phi_\ell)$, due to [1, Lemma 5.1.5]. This implies that $i\big[i[R_z,\Phi_j],\Phi_k\big] \in C^1(\Phi_\ell)$, which proves the claim. □

We can now give a precise definition of the conjugate operator A we will use, and prove its self-adjointness. For that purpose, we consider the family

$$\Pi_j := \langle H\rangle^{-2}\,H'_j\,\langle H\rangle^{-2}\,, \qquad j=1,\dots,d,$$

of mutually commuting bounded self-adjoint operators, and we write

$$\Pi := (\Pi_1,\dots,\Pi_d)$$

for the associated vector operator. Due to Lemma 3.1.(b), each operator Π_j belongs to $C^1(\Phi_j)$. Therefore the operator

$$A := \tfrac{1}{2}\big(\Pi\cdot\Phi + \Phi\cdot\Pi\big)$$

is well defined and symmetric on $\bigcap_{j=1}^d \mathcal{D}(\Phi_j)$. For the next lemma, we note that this set contains the domain $\mathcal{D}(\Phi^2)$ of Φ^2.

Lemma 3.2. *The operator A is essentially self-adjoint on $\mathcal{D}(\Phi^2)$.*

Proof. We use the criterion of essential self-adjointness [27, Thm. X.37].

Given $a > 1$, we define the self-adjoint operator $N := \Phi^2 + \Pi^2 + a$ with domain $\mathcal{D}(N) \equiv \mathcal{D}(\Phi^2)$ and observe that in the form sense on $\mathcal{D}(N)$ one has

$$\begin{aligned} N^2 &= \Phi^4 + \Pi^4 + a^2 + 2a\Phi^2 + 2a\Pi^2 + \Phi^2\Pi^2 + \Pi^2\Phi^2 \\ &= \Phi^4 + \Pi^4 + a^2 + 2a\Phi^2 + 2a\Pi^2 + \sum_{j,k} \big\{ \Phi_j \Pi_k^2 \Phi_j + \Pi_k \Phi_j^2 \Pi_k \big\} + R \end{aligned}$$

with $R := \sum_{j,k} \big\{ \Pi_k [\Pi_k, \Phi_j] \Phi_j + \Phi_j [\Phi_j, \Pi_k] \Pi_k + [\Pi_k, \Phi_j]^2 \big\}$. Now, the following inequality holds

$$\sum_{j,k} \big\{ \Pi_k [\Pi_k, \Phi_j] \Phi_j + \Phi_j [\Phi_j, \Pi_k] \Pi_k \big\} \geq -d\Phi^2 - \sum_{j,k} \big(\Pi_k [\Pi_k, \Phi_j] \big)^2.$$

Thus there exists $c > 0$ such that $R \geq -d\Phi^2 - c$. Altogether, we have shown that in the form sense on $\mathcal{D}(N)$

$$N^2 \geq \Phi^4 + \Pi^4 + (a^2 - c) + (2a - d)\Phi^2 + 2a\Pi^2 + \sum_{j,k} \big\{ \Phi_j \Pi_k^2 \Phi_j + \Pi_k \Phi_j^2 \Pi_k \big\},$$

where the r.h.s. is a sum of positive terms for a large enough. In particular, one has for $\varphi \in \mathcal{D}(N)$

$$\|N\varphi\|^2 \geq \big\| \Pi_j \Phi_j \varphi \big\|^2 + \big\| \Phi_j \Pi_j \varphi \big\|^2,$$

which implies that

$$\|A\varphi\| \leq \tfrac{1}{2} \sum_j \big\{ \big\| \Pi_j \Phi_j \varphi \big\| + \big\| \Phi_j \Pi_j \varphi \big\| \big\} \leq d \|N\varphi\|.$$

It remains to estimate the commutator $[A, N]$. In the form sense on $\mathcal{D}(N)$, one has

$$\begin{aligned} 2[A, N] = \sum_{j,k} \big\{ & [\Pi_j, \Phi_k] \Phi_j \Phi_k + \Phi_k [\Pi_j, \Phi_k] \Phi_j + \Phi_j [\Pi_j, \Phi_k] \Phi_k + \Phi_j \Phi_k [\Pi_j, \Phi_k] \\ & + \Pi_j [\Phi_j, \Pi_k] \Pi_k + \Pi_j \Pi_k [\Phi_j, \Pi_k] + [\Phi_j, \Pi_k] \Pi_j \Pi_k + \Pi_k [\Phi_j, \Pi_k] \Pi_j \big\}. \end{aligned}$$

The last four terms are bounded. For the other terms, Lemma 3.1.(c), together with the bound

$$|\langle \Phi_j \varphi, B \Phi_k \varphi \rangle| \leq \|B\| \, \langle \varphi, \Phi^2 \varphi \rangle \leq \|B\| \, \langle \varphi, N\varphi \rangle, \quad \varphi \in \mathcal{D}(N), \ B \in \mathscr{B}(\mathcal{H}),$$

leads to the desired estimate, *i.e.*, $\langle \varphi, [A, N] \varphi \rangle \leq \text{Const.} \, \langle \varphi, N\varphi \rangle$. □

Lemma 3.3. *The operator H is of class $C^2(A)$ and the sesquilinear form $i[H, A]$ on $\mathcal{D}(H)$ extends to the bounded positive operator $\langle H \rangle^{-2} (H')^2 \langle H \rangle^{-2}$.*

Proof. One has for each $\varphi \in \mathcal{D}(\Phi^2)$ and each $\omega \in \mathbb{C} \setminus \sigma(H)$

$$\begin{aligned} & 2\big\{ \big\langle R_{\bar{\omega}} \varphi, A\varphi \big\rangle - \big\langle A\varphi, R_\omega \varphi \big\rangle \big\} \qquad (3.2) \\ & \quad = \sum_j \big\{ \big\langle R_{\bar{\omega}} \varphi, \big(\Pi_j \Phi_j + \Phi_j \Pi_j \big) \varphi \big\rangle - \big\langle \big(\Pi_j \Phi_j + \Phi_j \Pi_j \big) \varphi, R_\omega \varphi \big\rangle \big\} \\ & \quad = \sum_j \big\{ \big\langle \Pi_j \varphi, [R_\omega, \Phi_j] \, \varphi \big\rangle + \big\langle \, [\Phi_j, R_{\bar{\omega}}] \, \varphi, \Pi_j \varphi \big\rangle \big\}. \end{aligned}$$

Since all operators in the last equality are bounded and since $\mathcal{D}(\Phi^2)$ is a core for A, this implies that H is of class $C^1(A)$ [1, Lemma 6.2.9].

Now observe that the following equalities hold on $\mathcal{H}$

$$i[R_\omega, A] = \tfrac{i}{2} \textstyle\sum_j \left\{ \Pi_j [R_\omega, \Phi_j] + [R_\omega, \Phi_j] \Pi_j \right\} = -R_\omega \langle H \rangle^{-2} (H')^2 \langle H \rangle^{-2} R_\omega.$$

Therefore the sesquilinear form $i[H, A]$ on $\mathcal{D}(H)$ extends to the bounded positive operator $\langle H \rangle^{-2} (H')^2 \langle H \rangle^{-2}$. Finally, the operator $i[R_\omega, A]$ can be written as a product of factors in $C^1(\Phi_\ell)$ for each ℓ, namely

$$i[R_\omega, A] = - \textstyle\sum_j R_\omega \left(R_{-i} H_j' R_i \right) \left(R_{-i} H_j' R_i \right) R_\omega.$$

So $i[R_\omega, A]$ also belongs to $C^1(\Phi_\ell)$ for each ℓ, and thus a calculation similar to the one of (3.2) shows that $i[R_\omega, A]$ belongs to $C^1(A)$. This implies that H is of class $C^2(A)$. □

Definition 3.4. A number $\lambda \in \mathbb{R}$ is called a A-regular value of H if there exist numbers $a, \delta > 0$ such that $(H')^2 E^H(\lambda; \delta) \geq a\, E^H(\lambda; \delta)$. The complement of this set in $\mathbb{R}$ is denoted by $\kappa^A(H)$.

The set of A-regular values corresponds to the Mourre set with respect to A. Indeed, if λ is a A-regular value, then $(H')^2 E^H(\lambda; \delta) \geq a\, E^H(\lambda; \delta)$ for some $a, \delta > 0$ and

$$E^H(\lambda; \delta) i[H, A] E^H(\lambda; \delta) = E^H(\lambda; \delta) \langle H \rangle^{-2} (H')^2 \langle H \rangle^{-2} E^H(\lambda; \delta) \geq a' E^H(\lambda; \delta),$$

where $a' := a \cdot \inf_{\mu \in (\lambda - \delta, \lambda + \delta)} \langle \mu \rangle^{-4}$. In the framework of Mourre theory, this means that the operator A is strictly conjugate to H at the point λ [1, Sec. 7.2.2].

Lemma 3.5. *The sets $\kappa(H)$ and $\kappa^A(H)$ are equal.*

Proof. Let λ be a A-regular value of H. Then there exist $a, \delta > 0$ such that

$$E^H(\lambda; \delta) \leq a^{-1} (H')^2 E^H(\lambda; \delta),$$

and we obtain for $\varepsilon > 0$:

$$\begin{aligned}
&\left\| \left[(H')^2 + \varepsilon \right]^{-1} E^H(\lambda; \delta) \right\|^2 \\
&\quad = \sup_{\varphi \in \mathcal{H},\, \|\varphi\| = 1} \left\langle \left[(H')^2 + \varepsilon \right]^{-1} \varphi, E^H(\lambda; \delta) \left[(H')^2 + \varepsilon^2 \right]^{-1} \varphi \right\rangle \\
&\quad \leq a^{-2} \sup_{\varphi \in \mathcal{H},\, \|\varphi\| = 1} \left\langle \left[(H')^2 + \varepsilon \right]^{-1} \varphi, E^H(\lambda; \delta) (H')^4 [(H')^2 + \varepsilon]^{-1} \varphi \right\rangle \\
&\quad \leq a^{-2} \left\| (H')^2 [(H')^2 + \varepsilon]^{-1} \right\|^2 \\
&\quad \leq a^{-2},
\end{aligned}$$

which implies, by taking the limit $\lim_{\varepsilon \searrow 0}$, that λ is a regular value.

Now, let λ be a regular value of H. Then there exists $\delta > 0$ such that

$$\begin{aligned}\text{Const.} &\geq \lim_{\varepsilon \searrow 0} \left\| \left[(H')^2 + \varepsilon \right]^{-1} E^H(\lambda;\delta) \right\| \\ &= \lim_{\varepsilon \searrow 0} \left\| E^H(\lambda;\delta) \left[(H')^2 E^H(\lambda;\delta) + \varepsilon \right]^{-1} E^H(\lambda;\delta) \right\| \\ &= \lim_{\varepsilon \searrow 0} \left\| \left[(H')^2 E^H(\lambda;\delta) + \varepsilon \right]^{-1} \right\|_{\mathscr{B}(\mathcal{H}_{\lambda,\delta})}, \end{aligned} \tag{3.3}$$

where $\mathcal{H}_{\lambda,\delta} := E^H(\lambda;\delta)\mathcal{H}$. But we have

$$\left\| \left[(H')^2 E^H(\lambda;\delta) + \varepsilon \right]^{-1} \right\|_{\mathscr{B}(\mathcal{H}_{\lambda,\delta})} = (a+\varepsilon)^{-1},$$

where the number $a \geq 0$ is the infimum of the spectrum of $(H')^2 E^H(\lambda;\delta)$, considered as an operator in $\mathcal{H}_{\lambda,\delta}$. Therefore, Formula (3.3) entails the bound $a^{-1} \leq$ Const., which implies that $a > 0$. In consequence, the operator $(H')^2 E^H(\lambda;\delta)$ is strictly positive in $\mathcal{H}_{\lambda,\delta}$, namely,

$$(H')^2 E^H(\lambda;\delta) \geq a E^H(\lambda;\delta)$$

with $a > 0$. This implies that λ is a A-regular value of H, and $\kappa(H)$ is equal to $\kappa^A(H)$. □

We shall now state our main result on the nature of the spectrum of H, and exhibit a class of locally H-smooth operators. The space $\big(\mathcal{D}(A), \mathcal{H}\big)_{1/2,1}$, defined by real interpolation [1, Sec. 3.4.1], is denoted by $\mathscr{K}$. Since for each $j \in \{1, \ldots, d\}$ the operator Π_j belongs to $C^1(\Phi_j)$, we have $\mathcal{D}(\langle\Phi\rangle) \subset \mathcal{D}(A)$, and it follows from [1, Thm. 2.6.3] and [1, Thm. 3.4.3.(a)] that for $s > 1/2$ the continuous embeddings hold:

$$\mathcal{D}(\langle\Phi\rangle^s) \subset \mathscr{K} \subset \mathcal{H} \subset \mathscr{K}^* \subset \mathcal{D}(\langle\Phi\rangle^{-s}). \tag{3.4}$$

The symbol $\mathbb{C}_\pm$ stands for the half-plane $\mathbb{C}_\pm := \{\omega \in \mathbb{C} \mid \pm \mathsf{Im}(\omega) > 0\}$.

Theorem 3.6. *Let H satisfy Assumptions* 2.2 *and* 2.3. *Then,*

(a) *the spectrum of H in $\sigma(H) \setminus \kappa(H)$ is purely absolutely continuous,*
(b) *each operator $T \in \mathscr{B}\big(\mathcal{D}(\langle\Phi\rangle^{-s}), \mathcal{H}\big)$, with $s > 1/2$, is locally H-smooth on $\mathbb{R} \setminus \kappa(H)$.*

Proof. (a) This is a direct application of [31, Thm. 0.1] which takes Lemmas 3.3 and 3.5 into account.

(b) We know from [31, Thm. 0.1] that the map $\omega \mapsto R_\omega \in \mathscr{B}(\mathscr{K}, \mathscr{K}^*)$, which is holomorphic on the half-plane $\mathbb{C}_\pm$, extends to a weak*-continuous function on $\mathbb{C}_\pm \cup \{\mathbb{R} \setminus \kappa(H)\}$. Now, consider $T \in \mathscr{B}(\mathscr{K}^*, \mathcal{H})$. Then one has $T^* \in \mathscr{B}(\mathcal{H}, \mathscr{K})$, and it follows from the above continuity that for each compact subset $J \subset \mathbb{R} \setminus \kappa(H)$ there exists a constant $\mathrm{c} \geq 0$ such that for all $\omega \in \mathbb{C}$ with $\mathsf{Re}(\omega) \in J$ and $\mathsf{Im}(\omega) \in (0,1)$ one has

$$\|T R_\omega T^*\| + \|T R_{\bar{\omega}} T^*\| \leq \mathrm{c}.$$

A fortiori, one also has $\sup_\omega \|T(R_\omega - R_{\bar{\omega}})T^*\| \leq \mathrm{c}$, where the supremum is taken over the same set of complex numbers. This last property is equivalent to the local

H-smoothness of T on $\mathbb{R} \setminus \kappa(H)$. The claim is then obtained by using the last embedding of (3.4). □

4. Averaged localisation functions

In this section we recall some properties of a class of averaged localisation functions which appears naturally when dealing with quantum scattering theory. These functions, which are denoted R_f, are constructed in terms of functions $f \in \mathsf{L}^\infty(\mathbb{R}^d)$ of localisation around the origin 0 of $\mathbb{R}^d$. They were already used, in one form or another, in [14], [36], and [37].

Assumption 4.1. The function $f \in \mathsf{L}^\infty(\mathbb{R}^d)$ satisfies the following conditions:

(i) There exists $\rho > 0$ such that $|f(x)| \leq \text{Const.} \langle x \rangle^{-\rho}$ for a.e. $x \in \mathbb{R}^d$.
(ii) $f = 1$ on a neighbourhood of 0.

It is clear that s-$\lim_{r\to\infty} f(\Phi/r) = 1$ if f satisfies Assumption 4.1. Furthermore, one has for each $x \in \mathbb{R}^d \setminus \{0\}$

$$\left| \int_0^\infty \frac{\mathrm{d}\mu}{\mu} \left[f(\mu x) - \chi_{[0,1]}(\mu) \right] \right| \leq \int_0^1 \frac{\mathrm{d}\mu}{\mu} \, |f(\mu x) - 1| + \text{Const.} \int_1^{+\infty} \mathrm{d}\mu \, \mu^{-(1+\rho)} < \infty,$$

where $\chi_{[0,1]}$ denotes the characteristic function for the interval $[0, 1]$. Therefore the function $R_f : \mathbb{R}^d \setminus \{0\} \to \mathbb{C}$ given by

$$R_f(x) := \int_0^{+\infty} \frac{\mathrm{d}\mu}{\mu} \left[f(\mu x) - \chi_{[0,1]}(\mu) \right]$$

is well defined. If $\mathbb{R}_+^* := (0, \infty)$, endowed with the multiplication, is seen as a Lie group with Haar measure $\frac{\mathrm{d}\mu}{\mu}$, then R_f is the renormalised average of f with respect to the (dilation) action of $\mathbb{R}_+^*$ on $\mathbb{R}^d$.

In the next lemma we recall some differentiability and homogeneity properties of R_f. We also give the explicit form of R_f when f is a radial function. The reader is referred to [37, Sec. 2] for proofs and details. The symbol $\mathscr{S}(\mathbb{R}^d)$ stands for the Schwartz space on $\mathbb{R}^d$.

Lemma 4.2. *Let f satisfy Assumption* 4.1.

(a) *Assume that $(\partial_j f)(x)$ exists for all $j \in \{1, \ldots, d\}$ and $x \in \mathbb{R}^d$, and suppose that there exists some $\rho' > 0$ such that $|(\partial_j f)(x)| \leq \text{Const.} \langle x \rangle^{-(1+\rho')}$ for each $x \in \mathbb{R}^d$. Then R_f is differentiable on $\mathbb{R}^d \setminus \{0\}$, and its derivative is given by*

$$R_f'(x) = \int_0^\infty \mathrm{d}\mu \, f'(\mu x).$$

In particular, if $f \in \mathscr{S}(\mathbb{R}^d)$ then R_f belongs to $C^\infty(\mathbb{R}^d \setminus \{0\})$.

(b) *Assume that* R_f *belongs to* $C^m(\mathbb{R}^d \setminus \{0\})$ *for some* $m \geq 1$. *Then one has the homogeneity properties*

$$x \cdot R_f'(x) = -1, \tag{4.1}$$

$$t^{|\alpha|}(\partial^\alpha R_f)(tx) = (\partial^\alpha R_f)(x), \tag{4.2}$$

where $x \in \mathbb{R}^d \setminus \{0\}$, $t > 0$ *and* $\alpha \in \mathbb{N}^d$ *is a multi-index with* $1 \leq |\alpha| \leq m$.

(c) *Assume that* f *is radial,* i.e., *there exists* $f_0 \in \mathsf{L}^\infty(\mathbb{R})$ *such that* $f(x) = f_0(|x|)$ *for a.e.* $x \in \mathbb{R}^d$. *Then* R_f *belongs to* $C^\infty(\mathbb{R}^d \setminus \{0\})$, *and* $R_f'(x) = -x^{-2}x$.

Obviously, one can show as in Lemma 4.2.(a) that R_f is of class $C^m(\mathbb{R}^d \setminus \{0\})$ if one has for each $\alpha \in \mathbb{N}^d$ with $|\alpha| \leq m$ that $(\partial^\alpha f)(x)$ exists and that $|(\partial^\alpha f)(x)| \leq \text{Const.}\, \langle x \rangle^{-(|\alpha|+\rho')}$ for some $\rho' > 0$. However, this is not a necessary condition. In some cases (as in Lemma 4.2.(c)), the function R_f is very regular outside the point 0 even if f is not continuous.

5. Integral formula

In this section we prove our main result on the relation between the evolution of the localisation operators $f(\Phi/r)$ and the time operator T_f defined below. We begin with a technical lemma that will be used subsequently. Since this result could also be useful in other situations, we present here a general version of it. The symbol $\mathscr{F}$ stands for the Fourier transformation, and the measure $\underline{\mathrm{d}}x$ on $\mathbb{R}^n$ is chosen so that $\mathscr{F}$ extends to a unitary operator in $\mathsf{L}^2(\mathbb{R}^n)$.

Proposition 5.1. *Let* $C \equiv (C_1, \ldots, C_n)$ *and* $D \equiv (D_1, \ldots, D_d)$ *be two families of mutually commuting self-adjoint operators in a Hilbert space* $\mathscr{H}$. *Let* $k \geq 1$ *be an integer, and assume that each* C_j *is of class* $C^k(D)$. *Let* $f \in \mathsf{L}^\infty(\mathbb{R}^n)$, *set* $g(x) := f(x) \langle x_1 \rangle^{2k} \cdots \langle x_n \rangle^{2k}$, *and suppose that the functions* g *and*

$$x \mapsto (\mathscr{F}g)(x) \langle x_1 \rangle^{k+1} \cdots \langle x_n \rangle^{k+1}$$

are in $\mathsf{L}^1(\mathbb{R}^n)$. *Then the operator* $f(C)$ *belongs to* $C^k(D)$. *In particular, if* $f \in \mathscr{S}(\mathbb{R}^n)$ *then* $f(C)$ *belongs to* $C^k(D)$.

Proof. For each $y \in \mathbb{R}^d$, we set $D_y := \frac{1}{i|y|}(\mathrm{e}^{iy \cdot D} - 1)$. Then we know from [1, Lemma 6.2.3.(a)] that it is sufficient to prove that $\left\| \mathrm{ad}_{D_y}^k \big(f(C)\big) \right\|$ is bounded by a constant independent of y (the symbol $\mathrm{ad}_{D_y}^k \big(f(C)\big)$ refers to the kth iterated commutator of D_y with $f(C)$ in the sense of [1, Sec. 5.1.1]). By using the linearity

of $\mathrm{ad}^k_{D_y}(\cdot)$ and [1, Eq. 5.1.16], we get

$$\begin{aligned}\mathrm{ad}^k_{D_y}\big(f(C)\big) &= \mathrm{ad}^k_{D_y}\big(g(C)\,\langle C_1\rangle^{-2k}\cdots\langle C_n\rangle^{-2k}\big)\\ &= \int_{\mathbb{R}^n}\underline{\mathrm{d}}x\,(\mathscr{F}g)(x)\,\mathrm{ad}^k_{D_y}\big(\mathrm{e}^{ix_1C_1}\,\langle C_1\rangle^{-2k}\cdots\mathrm{e}^{ix_2C_n}\,\langle C_n\rangle^{-2k}\big)\\ &= \sum_{k_1+\cdots+k_n=k}\mathrm{c}_{k_1\cdots k_n}\int_{\mathbb{R}^n}\underline{\mathrm{d}}x\,(\mathscr{F}g)(x)\,\mathrm{ad}^{k_1}_{D_y}\\ &\qquad\times\big(\mathrm{e}^{ix_1C_1}\,\langle C_1\rangle^{-2k}\big)\cdots\mathrm{ad}^{k_n}_{D_y}\big(\mathrm{e}^{ix_2C_n}\,\langle C_n\rangle^{-2k}\big),\end{aligned}$$

where $\mathrm{c}_{k_1\cdots k_n}>0$ is some explicit constant. Furthermore, since C_j is of class $C^k(D)$, we know from [1, Eq. 6.2.13] that

$$\big\|\,\mathrm{ad}^{k_j}_{G_y}\big(\mathrm{e}^{ix_jC_j}\,\langle C_j\rangle^{-2k}\big)\big\|\le\mathrm{c}_{k_j}\,\langle x_j\rangle^{k+1},$$

where $\mathrm{c}_{k_j}\ge0$ is independent of y and x_j. This implies that

$$\big\|\,\mathrm{ad}^k_{D_y}\big(f(C)\big)\big\|\le\text{Const.}\int_{\mathbb{R}^n}\underline{\mathrm{d}}x\,|(\mathscr{F}g)(x)|\,\langle x_1\rangle^{k+1}\cdots\langle x_n\rangle^{k+1}\le\text{Const.},$$

and the claim is proved. □

In Lemma 2.6.(a) we have shown that the set $\kappa(H)$ is closed. So we can define for each $t\ge0$ the set

$$\mathscr{D}_t:=\big\{\varphi\in\mathcal{D}(\langle\Phi\rangle^t)\mid\varphi=\eta(H)\varphi\text{ for some }\eta\in C^\infty_{\mathrm{c}}\big(\mathbb{R}\setminus\kappa(H)\big)\big\}.$$

The set $\mathscr{D}_t$ is included in the subspace $\mathcal{H}_{\mathrm{ac}}(H)$ of absolute continuity of H, due to Theorem 3.6.(a), and $\mathscr{D}_{t_1}\subset\mathscr{D}_{t_2}$ if $t_1\ge t_2$. We refer the reader to Section 6 for an account on density properties of the sets $\mathscr{D}_t$.

In the sequel we consider the set of operators $\big\{H''_{jk}\big\}$ as the components of a d-dimensional (Hessian) matrix which we denote by H'' (H''^{T} stands for its matrix transpose). Furthermore we shall sometimes write C^{-1} for an operator C a priori not invertible. In such a case, the operator C^{-1} will always be restricted to a set where it is well defined. Namely, if $\mathcal{D}$ is a set on which C is invertible, then we shall simply write "C^{-1} acting on $\mathcal{D}$" instead of using the notation $C^{-1}|_{\mathcal{D}}$.

Proposition 5.2. *Let H and Φ satisfy Assumptions 2.2 and 2.3. Let f satisfy Assumption 4.1 and assume that R_f belongs to $C^1(\mathbb{R}^d\setminus\{0\})$. Then the map*

$$t_f:\mathscr{D}_1\to\mathbb{C},\quad\varphi\mapsto t_f(\varphi):=-\tfrac12\sum_j\big\{\big\langle\Phi_j\varphi,(\partial_jR_f)(H')\varphi\big\rangle+\big\langle\big(\partial_jR_{\overline{f}}\big)(H')\varphi,\Phi_j\varphi\big\rangle\big\},$$

is well defined. Moreover, if $(\partial_jR_f)(H')\varphi$ belongs to $\mathcal{D}(\Phi_j)$ for each j, then the linear operator $T_f:\mathscr{D}_1\to\mathcal{H}$ defined by

$$T_f\varphi:=-\tfrac12\Big(\Phi\cdot R'_f(H')+R'_f\big(\tfrac{H'}{|H'|}\big)\cdot\Phi\,|H'|^{-1}+iR'_f\big(\tfrac{H'}{|H'|}\big)\cdot\big(H''^{\mathsf{T}}H'\big)\,|H'|^{-3}\Big)\varphi\quad(5.1)$$

satisfies $t_f(\varphi)=\langle\varphi,T_f\varphi\rangle$ for each $\varphi\in\mathscr{D}_1$. In particular, T_f is a symmetric operator if f is real and if $\mathscr{D}_1$ is dense in $\mathcal{H}$.

Remark 5.3. Formula (5.1) is a priori rather complicated and one could be tempted to replace it by the simpler formula $-\frac{1}{2}\big(\Phi\cdot R_f'(H')+R_f'(H')\cdot\Phi\big)$. Unfortunately, a precise meaning of this expression is not available in general, and its full derivation can only be justified in concrete examples.

Remark 5.4. If $\varphi\in\mathscr{D}_1$ and if f either belongs to $\mathscr{S}(\mathbb{R}^d)$ or is radial, then the assumption $(\partial_j R_f)(H')\varphi\in\mathcal{D}(\Phi_j)$ holds for each j. Indeed, by Lemma 2.6.(d) there exists $\eta\in C_{\rm c}^\infty\big((0,\infty)\big)$ such that $(\partial_j R_f)(H')\varphi=(\partial_j R_f)(H')\eta\big((H')^2\big)\varphi$. By Lemma 4.2 and Proposition 5.1, it then follows that $(\partial_j R_f)(H')\eta\big((H')^2\big)\in C^1(\Phi_j)$, which implies the statement.

Proof of Proposition 5.2. Let $\varphi\in\mathscr{D}_1$. Then Lemma 2.6.(d) implies that there exists a function $\eta\in C_{\rm c}^\infty\big((0,\infty)\big)$ such that

$$(\partial_j R_f)(H')\varphi=(\partial_j R_f)(H')\eta\big((H')^2\big)\varphi.$$

Thus $\|(\partial_j R_f)(H')\varphi\|\le\text{Const.}\,\|\varphi\|$, and we have

$$|t_f(\varphi)|\le\text{Const.}\,\|\varphi\|\cdot\|\langle\Phi\rangle\varphi\|,$$

which implies the first part of the claim.

For the second part of the claim, it is sufficient to show that

$$\sum_j\big\langle\big(\partial_j R_{\overline{f}}\big)(H')\varphi,\Phi_j\varphi\big\rangle=\big\langle\varphi,\big\{R_f'\big(\tfrac{H'}{|H'|}\big)\cdot\Phi|H'|^{-1}+iR_f'\big(\tfrac{H'}{|H'|}\big)\cdot\big(H''^{\mathsf{T}}H'\big)|H'|^{-3}\big\}\varphi\big\rangle.$$

Using Formula (4.2), Lemma 2.6.(d), and [10, Eq. 4.3.2], one gets

$$\begin{aligned}
&\sum_j\big\langle\big(\partial_j R_{\overline{f}}\big)(H')\varphi,\Phi_j\varphi\big\rangle \qquad (5.2)\\
&\quad=\sum_j\big\langle(\partial_j R_{\overline{f}}\big)\big(\tfrac{H'}{|H'|}\big)|H'|^{-1}\varphi,\Phi_j\varphi\big\rangle\\
&\quad=\sum_j\lim_{\varepsilon\searrow0}\lim_{\delta\to0}\big\langle\big(\partial_j R_{\overline{f}}\big)\big(\frac{H'}{|H'|}\big)\varphi,[(H')^2+\varepsilon]^{-1/2}\Phi_j(1+i\delta\Phi_j)^{-1}\varphi\big\rangle\\
&\quad=\big\langle\varphi,R_f'\big(\frac{H'}{|H'|}\big)\cdot\Phi\,|H'|^{-1}\varphi\big\rangle+\pi^{-1}\sum_j\lim_{\varepsilon\searrow0}\lim_{\delta\to0}\int_0^\infty\mathrm{d}t\,t^{-1/2}\Big\langle\big(\partial_j R_{\overline{f}}\big)\big(\tfrac{H'}{|H'|}\big)\varphi,\\
&\qquad\qquad\big[[(H')^2+\varepsilon+t]^{-1},\Phi_j(1+i\delta\Phi_j)^{-1}\big]\varphi\Big\rangle.
\end{aligned}$$

Now, using Assumption 2.2, Lemma 2.4 and the usual mollifiers technics, one obtains that

$$\lim_{\delta\to0}\big[[(H')^2+\varepsilon+t]^{-1},\Phi_j(1+i\delta\Phi_j)^{-1}\big]\varphi=2i\big[(H')^2+\varepsilon+t\big]^{-2}\big(H''^{\mathsf{T}}H'\big)_j\varphi.$$

So, the term (5.2) is equal to

$$\begin{aligned}
&\pi^{-1}\sum_j \lim_{\varepsilon\searrow 0}\int_0^\infty \mathrm{d}t\, t^{-1/2}\big\langle \big(\partial_j R_{\overline{f}}\big)\big(\tfrac{H'}{|H'|}\big)\varphi, 2i[(H')^2+\varepsilon+t]^{-2}\big(H''^{\mathsf{T}}H'\big)_j\varphi\big\rangle \\
&= \sum_j \lim_{\varepsilon\searrow 0}\big\langle \big(\partial_j R_{\overline{f}}\big)\big(\tfrac{H'}{|H'|}\big)\varphi, i[(H')^2+\varepsilon]^{-3/2}\big(H''^{\mathsf{T}}H'\big)_j\varphi\big\rangle \\
&= \big\langle \varphi, iR_f'\big(\tfrac{H'}{|H'|}\big)\cdot\big(H''^{\mathsf{T}}H'\big)\,|H'|^{-3}\varphi\big\rangle,
\end{aligned}$$

and thus

$$\begin{aligned}
&\sum_j \big\langle \big(\partial_j R_{\overline{f}}\big)(H')\varphi, \Phi_j\varphi\big\rangle \\
&\quad = \big\langle \varphi, \big\{R_f'\big(\tfrac{H'}{|H'|}\big)\cdot\Phi\,|H'|^{-1} + iR_f'\big(\tfrac{H'}{|H'|}\big)\cdot\big(H''^{\mathsf{T}}H'\big)\,|H'|^{-3}\big\}\varphi\big\rangle. \qquad \square
\end{aligned}$$

Suppose for a while that f is radial. Then one has $(\partial_j R_f)(x) = -x^{-2}x_j$ due to Lemma 4.2.(c), and Formula (5.1) holds by Remark 5.4. This implies that T_f is equal to

$$T := \tfrac{1}{2}\Big(\Phi\cdot\tfrac{H'}{(H')^2} + \tfrac{H'}{|H'|}\cdot\Phi\,|H'|^{-1} + \tfrac{iH'}{(H')^4}\cdot\big(H''^{\mathsf{T}}H'\big)\Big) \tag{5.3}$$

on $\mathscr{D}_1$.

The next theorem is our main result; it relates the evolution of localisation operators $f(\Phi/r)$ to the operator T_f. In its proof, we freely use the notations of [1] for some regularity classes with respect to the unitary group generated by Φ. For us, a function $f:\mathbb{R}^d\to\mathbb{C}$ is even if $f(x)=f(-x)$ for *a.e.* $x\in\mathbb{R}^d$.

Theorem 5.5. *Let H and Φ satisfy Assumptions* 2.2 *and* 2.3. *Let $f\in\mathscr{S}(\mathbb{R}^d)$ be an even function such that $f=1$ on a neighbourhood of* 0. *Then we have for each $\varphi\in\mathscr{D}_2$*

$$\lim_{r\to\infty}\tfrac{1}{2}\int_0^\infty \mathrm{d}t\,\big\langle\varphi,\big[\,\mathrm{e}^{-itH}\,f(\Phi/r)\,\mathrm{e}^{itH} - \mathrm{e}^{itH}\,f(\Phi/r)\,\mathrm{e}^{-itH}\,\big]\varphi\big\rangle = t_f(\varphi). \tag{5.4}$$

Note that the integral on the l.h.s. of (5.4) is finite for each $r>0$ since $f(\Phi/r)$ can be factorized as

$$f(\Phi/r)\equiv |f(\Phi/r)|^{1/2}\cdot\mathrm{sgn}[f(\Phi/r)]\cdot|f(\Phi/r)|^{1/2},$$

with $|f(\Phi/r)|^{1/2}$ locally H-smooth on $\mathbb{R}\setminus\kappa(H)$ by Theorem 3.6. Furthermore, since Remark 5.4 applies, the r.h.s. can also be written as the expectation value $\langle\varphi,T_f\varphi\rangle$.

Proof. (i) Let $\varphi \in \mathscr{D}_2$, take a real $\eta \in C_{\mathrm{c}}^{\infty}\big(\mathbb{R} \setminus \kappa(H)\big)$ such that $\eta(H)\varphi = \varphi$, and set $\eta_t(H) := \mathrm{e}^{itH}\,\eta(H)$. Then we have

$$\begin{aligned}
&\big\langle \varphi, \big[\,\mathrm{e}^{itH}\,f(\Phi/r)\,\mathrm{e}^{-itH} - \mathrm{e}^{-itH}\,f(\Phi/r)\,\mathrm{e}^{itH}\,\big]\varphi\big\rangle \\
&= \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\big\langle \varphi, \big[\eta_t(H)\,\mathrm{e}^{i\frac{x}{r}\cdot\Phi}\,\eta_{-t}(H) - \eta_{-t}(H)\,\mathrm{e}^{i\frac{x}{r}\cdot\Phi}\,\eta_t(H)\big]\varphi\big\rangle \\
&= \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\big\langle \varphi, \big[\,\mathrm{e}^{i\frac{x}{r}\cdot\Phi}\,\eta_t\big(H(\tfrac{x}{r})\big)\eta_{-t}(H) - \eta_{-t}(H)\eta_t\big(H(-\tfrac{x}{r})\big)\,\mathrm{e}^{i\frac{x}{r}\cdot\Phi}\,\big]\varphi\big\rangle \\
&= \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\big\langle \varphi, \big\{\big(\,\mathrm{e}^{i\frac{x}{r}\cdot\Phi} - 1\big)\eta_t\big(H(\tfrac{x}{r})\big)\eta_{-t}(H) \qquad (5.5)\\
&\qquad + \eta_{-t}(H)\big[\eta_t\big(H(\tfrac{x}{r})\big) - \eta_t\big(H(-\tfrac{x}{r})\big)\big] - \eta_{-t}(H)\eta_t\big(H(-\tfrac{x}{r})\big)\big(\,\mathrm{e}^{i\frac{x}{r}\cdot\Phi} - 1\big)\big\}\varphi\big\rangle.
\end{aligned}$$

Since f is even, $\mathscr{F}f$ is also even, and

$$\int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\,\big\langle \varphi, \eta_{-t}(H)\big[\eta_t\big(H(\tfrac{x}{r})\big) - \eta_t\big(H(-\tfrac{x}{r})\big)\big]\varphi\big\rangle = 0.$$

Thus Formula (5.5), Lemma 2.4, and the change of variables $\mu := t/r$, $\nu := 1/r$, give

$$\begin{aligned}
&\lim_{r\to\infty} \tfrac{1}{2}\int_0^{\infty} \mathrm{d}t\,\big\langle \varphi, \big[\,\mathrm{e}^{-itH}\,f(\Phi/r)\,\mathrm{e}^{itH} - \mathrm{e}^{itH}\,f(\Phi/r)\,\mathrm{e}^{-itH}\,\big]\varphi\big\rangle \\
&\qquad = -\tfrac{1}{2}\lim_{\nu\searrow 0}\int_0^{\infty} \mathrm{d}\mu \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,K(\nu,\mu,x), \qquad (5.6)
\end{aligned}$$

where

$$\begin{aligned}
K(\nu,\mu,x) := (\mathscr{F}f)(x)\Big\langle \varphi, \Big\{ &\tfrac{1}{\nu}\big(\,\mathrm{e}^{i\nu x\cdot\Phi} - 1\big)\eta(H(\nu x))\,\mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x) - H]} \\
&- \eta(H(-\nu x))\,\mathrm{e}^{i\frac{\mu}{\nu}[H(-\nu x) - H]}\,\tfrac{1}{\nu}\big(\,\mathrm{e}^{i\nu x\cdot\Phi} - 1\big)\Big\}\varphi\Big\rangle.
\end{aligned}$$

(ii) To prove the statement, we shall show that one may interchange the limit and the integrals in (5.6), by invoking Lebesgue's dominated convergence theorem. This will be done in (iii) below. Here we pursue the calculations assuming that these interchanges are justified.

There exists a bounded interval $J \subset \mathbb{R}$ such that $\varphi = E^H(J)\varphi$. Thus

$$\mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x) - H]}\,\varphi = \mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x) - H]E^H(J)}\,\varphi.$$

Furthermore, it follows from Assumption 2.2 and [1, Lemma 5.1.2.(b)] that $H \in C^2(\Phi, \mathcal{G}, \mathcal{H})$, where $\mathcal{G}$ denotes the space $\mathcal{D}(H)$ endowed with the graph topology. In particular, we have $H \in C_{\mathrm{u}}^1(\Phi, \mathcal{G}, \mathcal{H})$ (see [1, Sec. 5.2.2]), and therefore the map

$$\mathbb{R} \setminus \{0\} \ni \nu \mapsto i\tfrac{\mu}{\nu}[H(\nu x) - H]E^H(J) \in \mathscr{B}(\mathcal{H})$$

extends to a continuous map defined on $\mathbb{R}$ and taking value $i\mu x \cdot H'E^H(J)$ at $\nu = 0$. Since the exponential $B \mapsto \mathrm{e}^{iB}$ is continuous from $\mathscr{B}(\mathcal{H})$ to $\mathscr{B}(\mathcal{H})$, the composed map

$$\mathbb{R} \ni \nu \mapsto \mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x) - H]E^H(J)} \in \mathscr{B}(\mathcal{H})$$

is also continuous, and takes value $\mathrm{e}^{i\mu x\cdot H' E^H(J)}$ at $\nu = 0$. Summing up, we obtain that

$$\lim_{\nu \searrow 0} \mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x)-H]}\,\varphi = \mathrm{e}^{i\mu x\cdot H'}\,\varphi.$$

This identity, together with the symmetry of f, Lemma 4.2.(a), and Proposition 5.2, implies that for $\varphi \in \mathscr{D}_2$

$$\begin{aligned}
&\lim_{r\to\infty} \tfrac{1}{2}\int_0^\infty \mathrm{d}t\,\big\langle \varphi, \big[\,\mathrm{e}^{-itH}\,f(\Phi/r)\,\mathrm{e}^{itH} - \mathrm{e}^{itH}\,f(\Phi/r)\,\mathrm{e}^{-itH}\,\big]\varphi\big\rangle \\
&\quad = -\tfrac{i}{2}\int_0^\infty \mathrm{d}\mu \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\big\{\big\langle\,(x\cdot\Phi)\,\varphi, \mathrm{e}^{i\mu x\cdot H'}\,\varphi\big\rangle - \big\langle\varphi, \mathrm{e}^{-i\mu x\cdot H'}\,(x\cdot\Phi)\,\varphi\big\rangle\big\} \\
&\quad = -\tfrac{1}{2}\sum_j \int_0^\infty \mathrm{d}\mu \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,[\mathscr{F}(\partial_j f)](x)\big[\big\langle\Phi_j\varphi, \mathrm{e}^{i\mu x\cdot H'}\,\varphi\big\rangle + \big\langle\varphi, \mathrm{e}^{i\mu x\cdot H'}\,\Phi_j\varphi\big\rangle\big] \\
&\quad = -\tfrac{1}{2}\sum_j \int_0^\infty \mathrm{d}\mu\,\big[\big\langle\Phi_j\varphi, (\partial_j f)\big(\mu H'\big)\varphi\big\rangle + \big\langle\big(\partial_j\overline{f}\big)\big(\mu H'\big)\varphi, \Phi_j\varphi\big\rangle\big] \\
&\quad = t_f(\varphi).
\end{aligned}$$

(iii) To interchange the limit $\nu \searrow 0$ and the integration over μ in (5.6), one has to bound $\int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,K(\nu,\mu,x)$ uniformly in ν by a function in $\mathsf{L}^1\big((0,\infty),\mathrm{d}\mu\big)$. We begin with the first term of $\int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,K(\nu,\mu,x)$:

$$K_1(\nu,\mu) := \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\,\big\langle\langle\Phi\rangle^2\varphi, \tfrac{1}{\nu}\big(\,\mathrm{e}^{i\nu x\cdot\Phi} - 1\big)\langle\Phi\rangle^{-2}\eta(H(\nu x))\,\mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x)-H]}\,\varphi\big\rangle\,.$$

Observe that for each multi-index $\alpha \in \mathbb{N}^d$ with $|\alpha| \leq 2$ one has

$$\big\|\partial_x^\alpha \tfrac{1}{\nu}\big(\,\mathrm{e}^{i\nu x\cdot\Phi} - 1\big)\langle\Phi\rangle^{-2}\big\| \leq \mathrm{Const.}\,\langle x\rangle, \tag{5.7}$$

where the derivatives are taken in the strong topology and where the constant is independent of $\nu \in (-1,1)$. Since $\mathscr{F}f \in \mathscr{S}(\mathbb{R}^d)$ it follows that

$$\big|K_1(\nu,\mu)\big| \leq \mathrm{Const.}, \tag{5.8}$$

and thus $K_1(\nu,\mu)$ is bounded uniformly in ν by a function in $\mathsf{L}^1\big((0,1],\mathrm{d}\mu\big)$.

For the case $\mu > 1$ we first remark that there exists a compact set $J \subset \mathbb{R}\setminus\kappa(H)$ such that $\varphi = E^H(J)\varphi$. There also exists $\zeta \in C_{\mathrm{c}}^\infty\big((0,\infty)\big)$ such that $\zeta\big((H')^2\big)\eta(H) = \eta(H)$ due to Lemma 2.6.(d). It then follows that

$$\eta(H(\nu x))\,\mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x)-H]}\,\varphi = \zeta\big(H'(\nu x)^2\big)\eta(H(\nu x))\,\mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x)-H]}\,\varphi.$$

Moreover, from Assumption 2.3, we also get that

$$B^J_{\nu,\mu}(x)\varphi := E^H(J)\,\mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x)-H]}\,E^H(J)\varphi = \mathrm{e}^{i\frac{\mu}{\nu}[H(\nu x)-H]}\,\varphi.$$

So, $K_1(\nu,\mu)$ can be rewritten as

$$\int_{\mathbb{R}^d} \underline{\mathrm{d}}x\,(\mathscr{F}f)(x)\,\big\langle\langle\Phi\rangle^2\varphi, \tfrac{1}{\nu}\big(\,\mathrm{e}^{i\nu x\cdot\Phi} - 1\big)\langle\Phi\rangle^{-2}\zeta\big(H'(\nu x)^2\big)\eta(H(\nu x))B^J_{\nu,\mu}(x)\varphi\big\rangle\,.$$

Now, it is easily shown by using Assumption 2.2 and Lemma 2.4 that the function $B^J_{\nu,\mu} : \mathbb{R}^d \to \mathscr{B}(\mathcal{H})$ is differentiable with derivative equal to

$$\big(\partial_j B^J_{\nu,\mu}\big)(x) = i\mu H'_j(\nu x) B^J_{\nu,\mu}(x).$$

Furthermore, the bounded operator

$$A_{j,\nu}(x) := (\mathscr{F}f)(x)\tfrac{1}{\nu}\big(\mathrm{e}^{i\nu x\cdot\Phi} - 1\big)\langle\Phi\rangle^{-2} H'_j(\nu x)|H'(\nu x)|^{-2}\zeta\big(H'(\nu x)^2\big)\eta(H(\nu x))$$

satisfies for each integer $k \geq 1$ the bound

$$\big\|A_{j,\nu}(x)\big\| \leq \text{Const.}\,\langle x\rangle^{-k},$$

due to Assumption 2.2, Lemma 2.4, Equation (5.7) and the rapid decay of $\mathscr{F}f$. Thus $K_1(\nu,\mu)$ can be written as

$$K_1(\nu,\mu) = -i\mu^{-1}\sum_j \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\, \big\langle \langle\Phi\rangle^2\varphi, A_{j,\nu}(x)\big(\partial_j B^J_{\nu,\mu}\big)(x)\varphi\big\rangle\,.$$

Now, calculations as in the proof of Lemma 3.1.(d) show that each operator H'_j is of class $C^2(\Phi)$. So, the factor $H'_j(\nu x)|H'(\nu x)|^{-2}\zeta\big(H'(\nu x)^2\big)\eta(H(\nu x))$ in $A_{j,\nu}(x)$ can be rewritten as $\mathrm{e}^{-i\nu x\cdot\Phi}\, g(H, H'_1, \ldots, H'_d)\,\mathrm{e}^{i\nu x\cdot\Phi}$, with $g \in \mathscr{S}(\mathbb{R}^{d+1})$ and $H, H'_1, \ldots, H'_d$ mutually commuting and of class $C^2(\Phi)$. It follows by Equation (5.7) and Proposition 5.1 that the map $\mathbb{R}^d \ni x \mapsto A_{j,\nu}(x) \in \mathscr{B}(\mathcal{H})$ is twice strongly differentiable and satisfies

$$\big\|(\partial_j A_{j,\nu})(x)\big\| \leq \text{Const.}\,\langle x\rangle^{-k}$$

and

$$\big\|\partial_\ell\big\{(\partial_j A_{j,\nu})H'_\ell(\nu\cdot)(H'(\nu\cdot))^{-2}\big\}(x)\big\| \leq \text{Const.}\,(1+|\nu|)\,\langle x\rangle^{-k} \tag{5.9}$$

for any integer $k \geq 1$. Therefore one can perform two successive integrations by parts (with vanishing boundary contributions) and obtain

$$\begin{aligned} K_1(\nu,\mu) &= i\mu^{-1}\sum_j \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\, \big\langle \langle\Phi\rangle^2\varphi, (\partial_j A_{j,\nu})(x) B^J_{\nu,\mu}(x)\varphi\big\rangle \\ &= -\mu^{-2}\sum_{j,\ell} \int_{\mathbb{R}^d} \underline{\mathrm{d}}x\, \big\langle \langle\Phi\rangle^2\varphi, \partial_\ell\big\{(\partial_j A_{j,\nu})H'_\ell(\nu\cdot)(H'(\nu\cdot))^{-2}\big\}(x) B^J_{\nu,\mu}(x)\varphi\big\rangle. \end{aligned}$$

This together with Formula (5.9) implies for each $\nu < 1$ and each $\mu > 1$ that

$$\big|K_1(\nu,\mu)\big| \leq \text{Const.}\,\mu^{-2}. \tag{5.10}$$

The combination of the bounds (5.8) and (5.10) shows that $K_1(\nu,\mu)$ is bounded uniformly for $\nu < 1$ by a function in $\mathsf{L}^1\big((0,\infty), \mathrm{d}\mu\big)$. Since similar arguments show that the same holds for the second term of $\int_{\mathbb{R}^d} \underline{\mathrm{d}}x\, K(\nu,\mu,x)$, one can interchange the limit $\nu \searrow 0$ and the integration over μ in (5.6).

The interchange of the limit $\nu \searrow 0$ and the integration over x in (5.6) is justified by the bound

$$\big|K(\nu,\mu,x)\big| \leq \text{Const.}\,\big|x(\mathscr{F}f)(x)\big|,$$

which follows from Formula (5.7). □

When the localisation function f is radial, the operator T_f is equal to the operator T, which is independent of f. The next result, which depicts this situation of particular interest, is a direct consequence of Lemma 4.2.(c) and Theorem 5.5.

Corollary 5.6. *Let H and Φ satisfy Assumptions* 2.2 *and* 2.3. *Let $f \in \mathscr{S}(\mathbb{R}^d)$ be a radial function such that $f = 1$ on a neighbourhood of* 0. *Then we have for each $\varphi \in \mathscr{D}_2$*

$$\lim_{r\to\infty} \tfrac{1}{2} \int_0^\infty \mathrm{d}t \, \big\langle \varphi, \big[\mathrm{e}^{-itH} \, f(\Phi/r) \, \mathrm{e}^{itH} - \mathrm{e}^{itH} \, f(\Phi/r) \, \mathrm{e}^{-itH} \big] \varphi \big\rangle = \langle \varphi, T\varphi \rangle, \quad (5.11)$$

with T defined by (5.3).

6. Interpretation of the integral formula

This section is devoted to the interpretation of Formula (5.4) and to the description of the sets $\mathscr{D}_t$. We begin by stressing some properties of the subspace $\mathcal{K} := \ker\big((H')^2\big)$ of $\mathcal{H}$, which plays an important role in the sequel.

Lemma 6.1.

(a) *The eigenvectors of H belong to $\mathcal{K}$,*
(b) *If $\varphi \in \mathcal{K}$, then the spectral support of φ with respect to H is contained in $\kappa(H)$,*
(c) *For each $t \geq 0$, the set $\mathcal{K}$ is orthogonal to $\mathscr{D}_t$,*
(d) *For each $t \geq 0$, the set $\mathscr{D}_t$ is dense in $\mathcal{H}$ only if $\mathcal{K}$ is trivial.*

Proof. As observed in the proof of Lemma 2.6.(b), if λ is an eigenvalue of H then one has $E^H(\{\lambda\})H'_jE^H(\{\lambda\}) = 0$ for each j. If φ_λ is some corresponding eigenvector, it follows that $H'_j\varphi_\lambda = E^H(\{\lambda\})H'_jE^H(\{\lambda\})\varphi_\lambda = 0$. Thus, all eigenvectors of H belong to the kernel of H'_j, and a fortiori to the kernels of $(H'_j)^2$ and $(H')^2$.

Now, let $\varphi \in \mathcal{K}$ and let J be the minimal closed subset of $\mathbb{R}$ such that $E^H(J)\varphi = \varphi$. It follows then from Definition 2.5 that $J \subset \kappa(H)$. This implies that $\varphi \perp \mathscr{D}_t$, and thus $\mathcal{K} \perp \mathscr{D}_t$. The last statement is a straightforward consequence of point (c). □

Let us now proceed to the interpretation of Formula (5.4). We consider first the term $t_f(\varphi)$ on the r.h.s., and recall that f is an even element of $\mathscr{S}(\mathbb{R}^d)$ with $f = 1$ in a neighbourhood of 0. We also assume that f is real.

Due to Remark 5.4 with $\varphi \in \mathscr{D}_1$, the term $t_f(\varphi)$ reduces to the expectation value $\langle \varphi, T_f\varphi \rangle$, with T_f given by (5.1). Now, a direct calculation using Formulas (4.1), (4.2), and (5.1) shows that the operators T_f and H satisfy in the form sense on $\mathscr{D}_1$ the canonical commutation relation

$$\big[T_f, H\big] = i. \quad (6.1)$$

Therefore, since the group $\{\mathrm{e}^{-itH}\}_{t\in\mathbb{R}}$ leaves $\mathscr{D}_1$ invariant, the following equalities hold in the form sense on $\mathscr{D}_1$:

$$T_f\,\mathrm{e}^{-itH} = \mathrm{e}^{-itH}\,T_f + \big[T_f, \mathrm{e}^{-itH}\,\big] = \mathrm{e}^{-itH}\,T_f - i\int_0^t \mathrm{d}s\;\mathrm{e}^{-i(t-s)H}\,\big[T_f, H\big]\,\mathrm{e}^{-isH}$$
$$= \mathrm{e}^{-itH}\,\big(T_f + t\big).$$

In other terms, one has

$$\big\langle \psi, T_f\,\mathrm{e}^{-itH}\,\varphi\big\rangle = \big\langle \psi, \mathrm{e}^{-itH}\,\big(T_f + t\big)\varphi\big\rangle \tag{6.2}$$

for each $\psi, \varphi \in \mathscr{D}_1$, and the operator T_f satisfies on $\mathscr{D}_1$ the so-called infinitesimal Weyl relation in the weak sense [18, Sec. 3]. Note that we have not supposed that $\mathscr{D}_1$ is dense. However, if $\mathscr{D}_1$ is dense in $\mathcal{H}$, then the infinitesimal Weyl relation in the strong sense holds:

$$T_f\,\mathrm{e}^{-itH}\,\varphi = \mathrm{e}^{-itH}\,\big(T_f + t\big)\varphi, \qquad \varphi \in \mathscr{D}_1. \tag{6.3}$$

This relation, also known as T_f-weak Weyl relation [21, Def. 1.1], has deep implications on the spectral nature of H and on the form of T_f in the spectral representation of H. Formally, it suggests that $T_f = i\frac{\mathrm{d}}{\mathrm{d}H}$, and thus $-iT_f$ can be seen as the operator of differentiation with respect to the Hamiltonian H. Moreover, being a weak version of the usual Weyl relation, Relation (6.3) also suggests that the spectrum of H may not differ too much from a purely absolutely continuous spectrum. These properties are now discussed more rigorously in particular situations. In the first two cases, the density of $\mathscr{D}_1$ in $\mathcal{H}$ is assumed, and so the point spectrum of H is empty by Lemma 6.1.

Case 1 (T_f essentially self-adjoint): If the set $\mathscr{D}_1$ is dense in $\mathcal{H}$, and T_f is essentially self-adjoint on $\mathscr{D}_1$, then it has been shown in [18, Lemma 4] that (6.3) implies that the pair $\{\overline{T_f}, H\}$ satisfies the usual Weyl relation, *i.e.*,

$$\mathrm{e}^{isH}\,\mathrm{e}^{it\overline{T_f}} = \mathrm{e}^{ist}\,\mathrm{e}^{it\overline{T_f}}\,\mathrm{e}^{isH}, \qquad s,t \in \mathbb{R}.$$

It follows by the Stone-von Neumann theorem [26, VIII.14] that there exists a unitary operator $\mathscr{U} : \mathcal{H} \to \mathsf{L}^2(\mathbb{R};\mathbb{C}^N,\mathrm{d}\lambda)$, with N finite or infinite, such that $\mathscr{U}\,\mathrm{e}^{it\overline{T_f}}\,\mathscr{U}^*$ is the operator of translation by t, and $\mathscr{U}\,\mathrm{e}^{isH}\,\mathscr{U}^*$ is the operator of multiplication by $\mathrm{e}^{is\lambda}$. In terms of the generator H, this means that $\mathscr{U}H\mathscr{U}^* = \lambda$, where "$\lambda$" stands for the multiplication operator by λ in $\mathsf{L}^2(\mathbb{R};\mathbb{C}^N,\mathrm{d}\lambda)$. Therefore the spectrum of H is purely absolutely continuous and covers the whole real line. Moreover, we have for each $\psi \in \mathcal{H}$ and $\varphi \in \mathscr{D}_1$

$$\langle \psi, T_f\varphi\rangle = \langle \psi, \overline{T_f}\varphi\rangle = \int_{\mathbb{R}} \mathrm{d}\lambda\,\big\langle (\mathscr{U}\psi)(\lambda), i\,\tfrac{\mathrm{d}(\mathscr{U}\varphi)}{\mathrm{d}\lambda}(\lambda)\big\rangle_{\mathbb{C}^N},$$

where $\frac{\mathrm{d}}{\mathrm{d}\lambda}$ denotes the distributional derivative (see for instance [2, Rem. 1] for an interpretation of the derivative $\frac{\mathrm{d}}{\mathrm{d}\lambda}$).

Case 2 (T_f symmetric): If the set $\mathscr{D}_1$ is dense in $\mathcal{H}$, then we know from Proposition 5.2 and Remark 5.4 that T_f is symmetric. In such a situation, (6.3) once more implies that the spectrum of H is purely absolutely continuous [21, Thm. 4.4], but

it may not cover the whole real line. We expect that the operator T_f is still equal to $i\frac{\mathrm{d}}{\mathrm{d}\lambda}$ (on a suitable subspace) in the spectral representation of H, but we have not been able to prove it in this generality. However, this property holds in most of the examples presented below. If T_f and H satisfy more assumptions, then more can be said (see for instance [33]).

Case 3 (T_f not densely defined): If $\mathscr{D}_1$ is not dense in $\mathcal{H}$, then we are not aware of general works using a relation like (6.2) to deduce results on the spectral nature of H or on the form of T_f in the spectral representation of H. In such a case, we only know from Theorem 3.6 that the spectrum of H is purely absolutely continuous in $\sigma(H)\setminus\kappa(H)$, but we have no general information on the form of T_f in the spectral representation of H. However, with a suitable additional assumption the analysis can be continued. Indeed, consider the orthogonal decomposition $\mathcal{H} := \mathcal{K}\oplus\mathcal{G}$, with $\mathcal{K}\equiv\ker\big((H')^2\big)$. Then the operators H, H'_j, and $H''_{k\ell}$ are all reduced by this decomposition, due to Lemma 2.4. If we assume additionally that $T_f\mathscr{D}_1\subset\mathcal{G}$, then the analysis can be performed in the subspace $\mathcal{G}$.

Since $\mathscr{D}_1\subset\mathcal{G}$ by Lemma 6.1, the additional hypothesis allows us to consider the restriction of T_f to $\mathcal{G}$, which we denote by T_f. Let also H, H'_j, and $\mathsf{H}''_{k\ell}$ denote the restrictions of the corresponding operators in $\mathcal{G}$. We then set

$$\mathsf{D}_t := \big\{\varphi\in\mathcal{D}(\langle\Phi\rangle^t)\cap\mathcal{G}\mid\varphi=\eta(\mathsf{H})\varphi\text{ for some }\eta\in C_{\mathrm{c}}^\infty\big(\mathbb{R}\setminus\kappa(H)\big)\big\}\subset\mathcal{G},$$

and observe that the equality (6.1) holds in the form sense on D_1. In other words, (6.1) can be considered in the reduced Hilbert space $\mathcal{G}$ instead of $\mathcal{H}$. The interest of the above decomposition comes from the following fact: If D_1 is dense in $\mathcal{G}$, then T_f is symmetric and the situation reduces to Case 2 with the operators H and T_f. If in addition T_f is essentially self-adjoint on D_1, the situation even reduces to the case 1 with the operators H and T_f. In both situations, the spectrum of H is purely absolutely continuous. In Section 7, we shall present 2 examples corresponding to these situations.

Remark 6.2. The implicit condition $T_f\mathscr{D}_1\subset\mathcal{G}$ can be made more explicit. For example, if the collection Φ is reduced by the decomposition $\mathcal{H}=\mathcal{K}\oplus\mathcal{G}$, then the condition holds (and (5.4) also holds on D_2). More generally, if $\Phi_j\mathscr{D}_1\subset\mathcal{G}$ for each j, then the condition holds. Indeed, if $\varphi\in\mathscr{D}_1$ one knows from Remark 5.4 that $(\partial_jR_f)(H')\varphi\in\mathcal{D}(\langle\Phi\rangle)$, and one can prove similarly that $|H'|^{-1}\varphi\in\mathcal{D}(\langle\Phi\rangle)$. Furthermore, there exists $\eta\in C_{\mathrm{c}}^\infty\big(\mathbb{R}\setminus\kappa(H)\big)$ such that $(\partial_jR_f)(H')\varphi=\eta(H)(\partial_jR_f)(H')\varphi$ and $|H'|^{-1}\varphi=\eta(H)|H'|^{-1}\varphi$, which means that both vectors $\partial_jR_f(H')\varphi$ and $|H'|^{-1}\varphi$ belong to $\mathscr{D}_1$. It follows that $T_f\varphi\in\mathcal{G}$ by taking the explicit form (5.1) of T_f into account.

Let us now concentrate on the other term in Formula (5.4). If we consider the operators Φ_j as the components of an abstract position operator Φ, then the l.h.s. of Formula (5.4) has the following meaning: For r fixed, it can be interpreted as the difference of times spent by the evolving state $\mathrm{e}^{-itH}\,\varphi$ in the past (first term) and in the future (second term) within the region defined by the localisation operator

$f(\Phi/r)$. Thus, Formula (5.4) shows that this difference of times tends as $r \to \infty$ to the expectation value in φ of the operator T_f.

On the other hand, let us consider a quantum scattering pair $\{H, H+V\}$, with V an appropriate perturbation of H. Let us also assume that the corresponding scattering operator S is unitary, and recall that S commute with H. In this framework, the global time delay $\tau(\varphi)$ for the state φ defined in terms of the localisation operators $f(\Phi/r)$ can usually be reexpressed as follows: it is equal to the l.h.s. of (5.4) minus the same quantity with φ replaced by $S\varphi$. Therefore, if φ and $S\varphi$ are elements of $\mathscr{D}_2$, then the time delay for the scattering pair $\{H, H+V\}$ should satisfy the equation

$$\tau(\varphi) = -\langle \varphi, S^*[T_f, S]\varphi \rangle. \tag{6.4}$$

In addition, if T_f acts in the spectral representation of H as a differential operator $i\frac{\mathrm{d}}{\mathrm{d}H}$, then $\tau(\varphi)$ would verify, in our complete abstract setting, the Eisenbud-Wigner formula

$$\tau(\varphi) = \big\langle \varphi, -iS^* \tfrac{\mathrm{d}S}{\mathrm{d}H} \varphi \big\rangle.$$

Summing up, as soon as the position operator Φ and the operator H satisfy Assumptions 2.2 and 2.3, then our study establishes a preliminary relation between time operators T_f given by (5.1) and the theory of quantum time delay. Many concrete examples discussed in the literature [2, 3, 4, 14, 22, 35, 37] turn out to fit in the present framework, and several old or new examples are presented in the following section. Further investigations in relation with the abstract Formula (6.4) will be considered elsewhere.

Now, most of the above discussion depends on the size of $\mathscr{D}_1$ in $\mathcal{H}$, and implicitly on the size of $\kappa(H)$ in $\sigma(H)$. We collect some information about these sets. It has been proved in Lemma 2.6.(d) that $\kappa(H)$ is closed and corresponds to the complement in $\sigma(H)$ of the Mourre set (see the comment after Definition 3.4). It always contains the eigenvalues of H. Furthermore, since the spectrum of H is absolutely continuous on $\sigma(H) \setminus \kappa(H)$, the support of the singularly continuous spectrum, if any, is contained in $\kappa(H)$. In particular, if $\kappa(H)$ is discrete, then H has no singularly continuous spectrum. Thus, the determination of the size of $\kappa(H)$ is an important issue for the spectral analysis of H. More will be said in the concrete examples of the next section.

Let us now turn to the density properties of the sets $\mathscr{D}_t$. For this, we recall that a subset $K \subset \mathbb{R}$ is said to be uniformly discrete if

$$\inf\{|x-y| \mid x, y \in K \text{ and } x \neq y\} > 0.$$

Lemma 6.3. *Assume that $\kappa(H)$ is uniformly discrete. Then*

(a) *$\mathscr{D}_0$ is dense in $\mathcal{H}_{\mathrm{ac}}(H)$.*
(b) *If $\sigma_{\mathrm{p}}(H) = \varnothing$ and if H is of class $C^k(\Phi)$ for some integer k, then $\mathscr{D}_t$ is dense in $\mathcal{H}$ for any $t \in [0, k)$.*

Proof. (a) Let $\varphi \in \mathcal{H}_{\mathrm{ac}}(H)$ and $\varepsilon > 0$. Then there exists a finite interval $[a, b]$ such that $\big\| \big[1 - E^H([a,b])\big]\varphi \big\| \leq \varepsilon/2$. Since $\kappa(H)$ is uniformly discrete, the set

$\kappa(H) \cap (a,b)$ contains only a finite number N of points $x_1 < x_2 < \cdots < x_N$. Let us set $x_0 := a$ and $x_{N+1} := b$. Since $\varphi \in \mathcal{H}_{\rm ac}$, there exists $\delta > 0$ such that $x_j + \delta < x_{j+1} - \delta$ for each $j \in \{0, \ldots, N\}$, and $\|E^H(L_\delta)\varphi\| \leq \varepsilon/2$, where

$$L_\delta := \{x \in [a,b] \mid |x - x_j| \leq \delta \text{ for each } j = 0, 1, \ldots, N+1\}.$$

Now, for any $j \in \{0, \ldots, N\}$ there exist $\eta_j, \widetilde{\eta}_j \in C_{\rm c}^\infty\big((x_j, x_{j+1}); [0,1]\big)$ such that $\widetilde{\eta}_j(x) = 1$ for $x \in [x_j + \delta, x_{j+1} - \delta]$ and $\eta_j \widetilde{\eta}_j = \widetilde{\eta}_j$. Therefore, if $\eta := \sum_{j=0}^N \eta_j$, $\widetilde{\eta} := \sum_{j=0}^N \widetilde{\eta}_j$ and $\psi := \widetilde{\eta}(H)\varphi$, one verifies that $\eta \in C_{\rm c}^\infty\big((a,b); [0,1]\big) \subset C_{\rm c}^\infty\big(\mathbb{R} \setminus \kappa(H)\big)$ and that $\psi = \eta(H)\psi$, which imply that $\psi \in \mathscr{D}_0$. Moreover, one has

$$\begin{aligned} \|\varphi - \psi\| &\leq \big\|[1 - \widetilde{\eta}(H)]E^H([a,b])\varphi\big\| + \big\|[1 - \widetilde{\eta}(H)]\big[1 - E^H([a,b])\big]\varphi\big\| \\ &\leq \big\|[1 - \widetilde{\eta}(H)]E^H(L_\delta)\varphi\big\| + \big\|\big[1 - E^H([a,b])\big]\varphi\big\| \\ &\leq \tfrac{\varepsilon}{2} + \tfrac{\varepsilon}{2}\,. \end{aligned}$$

Thus $\|\varphi - \psi\| \leq \varepsilon$ for $\psi \in \mathscr{D}_0$, and the claim is proved.

(b) If $\sigma_{\rm p}(H) = \varnothing$, then it follows from the above discussion that $\mathcal{H}_{\rm ac}(H) = \mathcal{H}$. In view of what precedes, it is enough to show that the vector $\psi \equiv \widetilde{\eta}(H)\varphi$ of point (a) belongs to $\mathcal{D}(\langle\Phi\rangle^t)$: The operator $\widetilde{\eta}(H)$ belongs to $C^k(\Phi)$, since H is of class $C^k(\Phi)$ and $\widetilde{\eta} \in C_{\rm c}^\infty(\mathbb{R})$ (see [1, Thm. 6.2.5]). So, we obtain from [1, Prop. 5.3.1] that $\langle\Phi\rangle^t\, \widetilde{\eta}(H)\, \langle\Phi\rangle^{-t}$ is bounded on $\mathcal{H}$, which implies the claim. □

7. Examples

In this section we show that Assumptions 2.2 and 2.3 are satisfied in various general situations. In these situations all the results of the preceding sections such as Theorem 3.6 or Formula (5.4) hold. However, it is usually impossible to determine explicitly the set $\kappa(H)$ when the framework is too general. Therefore, we also illustrate our approach with some concrete examples for which everything can be computed explicitly. When possible, we also relate these examples with the different cases presented in Section 6. For that purpose, we shall always assume that f is a real and even function in $\mathscr{S}(\mathbb{R}^d)$ with $f = 1$ on a neighbourhood of 0.

The configuration space of the system under consideration will sometimes be $\mathbb{R}^n$, and the corresponding Hilbert space $\mathsf{L}^2(\mathbb{R}^n)$. In that case, the notations $Q \equiv (Q_1, \ldots, Q_n)$ and $P \equiv (P_1, \ldots, P_n)$ refer to the families of position operators and momentum operators. More precisely, for suitable $\varphi \in \mathsf{L}^2(\mathbb{R}^n)$ and each $j \in \{1, \ldots, n\}$, we have $(Q_j\varphi)(x) = x_j\varphi(x)$ and $(P_j\varphi)(x) = -i(\partial_j\varphi)(x)$ for each $x \in \mathbb{R}^n$.

7.1. H' constant

Suppose that H is of class $C^1(\Phi)$, and assume that there exists $v \in \mathbb{R}^d \setminus \{0\}$ such that $H' = v$. Then H is of class $C^\infty(\Phi)$, Assumption 2.2 is directly verified, and

one has on $\mathcal{D}(H)$

$$H(x) = H(0) + \int_0^1 \mathrm{d}t \, \big(x \cdot H'(tx)\big) = H + \int_0^1 \mathrm{d}t \, \mathrm{e}^{-itx\cdot\Phi} \, \big(x \cdot H'\big) \, \mathrm{e}^{itx\cdot\Phi} = H + x \cdot v.$$

This implies Assumption 2.3. Furthermore $\kappa(H) = \varnothing$, and $\sigma(H) = \sigma_{\mathrm{ac}}(H)$ due to Theorem 3.6. So, the set $\mathscr{D}_t$ is dense in $\mathcal{H}$ for each $t \geq 0$, due to Lemma 6.3.(b). The operator $R'_f(H')$ reduces to the constant vector $R'_f(v)$. Therefore, we have the equality $T_f = -R'_f(v) \cdot \Phi$ on $\mathscr{D}_1$, and it is easily shown that T_f is essentially self-adjoint on $\mathscr{D}_1$. It follows from Case 1 of Section 6 that the spectrum of H covers the whole real line, and there exists a unitary operator $\mathscr{U} : \mathcal{H} \to \mathsf{L}^2(\mathbb{R}; \mathbb{C}^N, \mathrm{d}\lambda)$ such that

$$\langle \psi, T_f \varphi \rangle = \int_{\mathbb{R}} \mathrm{d}\lambda \, \big\langle (\mathscr{U}\psi)(\lambda), i \, \tfrac{\mathrm{d}(\mathscr{U}\varphi)}{\mathrm{d}\lambda}(\lambda) \big\rangle_{\mathbb{C}^N}$$

for each $\psi \in \mathcal{H}$ and $\varphi \in \mathscr{D}_1$.

Typical examples of operators H and Φ fitting into this construction are Friedrichs-type Hamiltonians and position operators. For illustration, we mention the case $H := v \cdot P + V(Q)$ and $\Phi := Q$ in $\mathsf{L}^2(\mathbb{R}^d)$, with $v \in \mathbb{R}^d \setminus \{0\}$ and $V \in \mathsf{L}^\infty(\mathbb{R}^d; \mathbb{R})$ (see also [37, Sec. 5] for information on quantum time delay in a similar case).

Stark Hamiltonians and momentum operators also fit into the construction, *i.e.*, $H := P^2 + v \cdot Q$ in $\mathsf{L}^2(\mathbb{R}^d)$ with $v \in \mathbb{R}^d \setminus \{0\}$, and $\Phi := P$. We refer to [25, 29, 30] for previous accounts on the theory of time operators and quantum time delay in similar situations.

Note that these first two examples are interesting since the operators H contain not only a kinetic part, but also a potential perturbation.

Another example is provided by the Jacobi operator related to the family of Hermite polynomials (see [32, Appendix A] for details). In the Hilbert space $\mathcal{H} := \ell^2(\mathbb{N})$, consider the Jacobi operator given for $\varphi \in \mathcal{H}$ by

$$(H\varphi)(n) := \tfrac{\sqrt{n-1}}{2} \, \varphi(n-1) + \tfrac{\sqrt{n}}{2} \, \varphi(n+1),$$

with the convention that $\varphi(0) = 0$. The operator H is essentially self-adjoint on ℓ^2_0, the subspace of sequences in $\mathcal{H}$ with only finitely many non-zero components. As operator Φ (with one component), take

$$(\Phi\varphi)(n) := -i\big\{\sqrt{n-1} \, \varphi(n-1) - \sqrt{n} \, \varphi(n+1)\big\},$$

which is also essentially self-adjoint on ℓ^2_0. Then H is of class $C^1(\Phi)$ and $H' \equiv i[H, \Phi] = 1$, and so the preceding results hold.

7.2. $H' = H$

Suppose that Φ has only one component, and assume that H is Φ-homogeneous of degree 1, *i.e.*, $H(x) \equiv \mathrm{e}^{-ix\Phi} \, H \, \mathrm{e}^{ix\Phi} = \mathrm{e}^x \, H$ for all $x \in \mathbb{R}$. This implies that H is of class $C^\infty(\Phi)$ and that $H' = H$. So, Assumptions 2.2 and 2.3 are readily verified. Moreover, since $\kappa(H) = \{0\}$, Theorem 3.6 implies that H is purely absolutely continuous except at the origin, where it may have the eigenvalue 0.

Now, let us show that the formal formula of Remark 5.3 holds in this case. For any $\varphi \in \mathscr{D}_1$ one has by Remark 5.4 that $R'_f(H')\varphi \equiv R'_f(H)\varphi$ belongs to $\mathcal{D}(\Phi)$. On another hand, we have

$$\Phi\varphi = \big\{H\Phi + [\Phi, H]\big\}H^{-1}\varphi = H(\Phi + i)H^{-1}\varphi,$$

which implies that $R'_f(H)\Phi\varphi = R'_f\big(\frac{H}{|H|}\big)\frac{H}{|H|}(\Phi+i)H^{-1}\varphi \in \mathcal{H}$. In consequence, the operator

$$T_f = -\tfrac{1}{2}\big(\Phi R'_f(H) + R'_f(H)\Phi\big)$$

is well defined on $\mathscr{D}_1$. In particular, if 0 is not an eigenvalue of H, then T_f is a symmetric operator and the discussion of Case 2 of Section 6 is relevant (if T_f is essentially self-adjoint, Case 1 is relevant).

We now give two examples of pairs $\{H, \Phi\}$ satisfying the preceding assumptions. Other examples are presented in [8, Sec. 10]. Suppose that $H := P^2$ is the free Schrödinger operator in $\mathcal{H} := \mathsf{L}^2(\mathbb{R}^n)$ and $\Phi := \frac{1}{4}(Q \cdot P + P \cdot Q)$ is the generator of dilations in $\mathcal{H}$. Then the relation $\mathrm{e}^{-ix\Phi}\, H\, \mathrm{e}^{ix\Phi} = \mathrm{e}^{x}\, H$ is satisfied, and $\sigma(H) = \sigma_{\mathrm{ac}}(H) = [0, \infty)$. Furthermore, for $\psi \in \mathcal{H}$ and $\varphi \in \mathscr{F}C_{\mathrm{c}}^{\infty}\big(\mathbb{R}^n \setminus \{0\}\big) \subset \mathscr{D}_1$ a direct calculation using Formula (4.1) shows that

$$\langle \psi, T_f\varphi\rangle = \big\langle \psi, \tfrac{1}{4}\big(Q\cdot PP^{-2} + PP^{-2}\cdot Q\big)\varphi\big\rangle = \int_0^{\infty} \mathrm{d}\lambda\, \big\langle (\mathscr{U}\psi)(\lambda), i\,\tfrac{\mathrm{d}(\mathscr{U}\varphi)}{\mathrm{d}\lambda}(\lambda)\big\rangle_{\mathsf{L}^2(\mathbb{S}^{n-1})},$$

where $\mathscr{U} : \mathcal{H} \to \int_{[0,\infty)}^{\oplus} \mathrm{d}\lambda\, \mathsf{L}^2(\mathbb{S}^{n-1})$ is the spectral transformation for P^2. This example corresponds to Case 2 of Section 6.

Another example of Φ-homogeneous operator is provided by the Jacobi operator related to the family of Laguerre polynomials (see [32, Appendix A] for details). In the Hilbert space $\mathcal{H} := \ell^2(\mathbb{N})$, consider the Jacobi operator given for $\varphi \in \mathcal{H}$ by

$$(H\varphi)(n) := (n-1)\varphi(n-1) + (2n-1)\varphi(n) + n\varphi(n+1),$$

with the convention that $\varphi(0) = 0$. The operator H is essentially self-adjoint on ℓ_0^2. As operator Φ (with one component), take

$$(\Phi\varphi)(n) := -\tfrac{i}{2}\big\{(n-1)\varphi(n-1) - n\varphi(n+1)\big\}.$$

Then one has $H' \equiv i[H, \Phi] = H$, which implies that H is Φ-homogeneous of degree 1 and so the preceding results hold.

7.3. Dirac operator

In the Hilbert space $\mathcal{H} := \mathsf{L}^2(\mathbb{R}^3; \mathbb{C}^4)$ we consider the Dirac operator for a spin-$\frac{1}{2}$ particle of mass $m > 0$

$$H := \alpha \cdot P + \beta m,$$

where $\alpha \equiv (\alpha_1, \alpha_2, \alpha_3)$ and β denote the usual 4×4 Dirac matrices. It is known that H has domain $\mathcal{H}^1(\mathbb{R}^3; \mathbb{C}^4)$, that $|H| = (P^2 + m^2)^{1/2}$ and that $\sigma(H) = \sigma_{\mathrm{ac}}(H) = (-\infty, -m] \cup [m, \infty)$.

We also let $\Phi := \mathscr{U}_{\mathrm{FW}}^{-1} Q \mathscr{U}_{\mathrm{FW}} \equiv Q_{\mathrm{NW}}$ be the Wigner-Newton position operator, with $\mathscr{U}_{\mathrm{FW}}$ the usual Foldy-Wouthuysen transformation [34, Sec. 1.4.3]. Then a direct calculation shows that

$$H(x) = \sqrt{\tfrac{(P+x)^2+m^2}{P^2+m^2}}\, H$$

for each $x \in \mathbb{R}^3$, and thus Assumptions 2.2 and 2.3 are easily verified. Furthermore, since $H'_j = P_j H^{-1}$ for each $j = 1, 2, 3$, it follows that

$$(H')^2 = P^2 H^{-2} = (H^2 - m^2) H^{-2}.$$

Clearly, $\ker\big((H')^2\big) = \{0\}$ and one infers from Definition 2.5 that $\kappa(H) = \{\pm m\}$, and from Lemma 6.3.(b) that the sets

$$\mathscr{D}_t = \big\{\varphi \in \mathscr{U}_{\mathrm{FW}}^{-1} \mathcal{D}\big(\langle Q\rangle^t\big) \mid \eta(H)\varphi = \varphi \text{ for some } \eta \in C_{\mathrm{c}}^{\infty}\big(\mathbb{R} \setminus \{\pm m\}\big)\big\},$$

are dense in $\mathcal{H}$. So the discussion of Case 2 of Section 6 is relevant.

We now show that the formal formula of Remark 5.3 holds if f is radial. Indeed, each $\varphi \in \mathscr{D}_1$ satisfies $\varphi = \eta(H)\mathscr{U}_{\mathrm{FW}}^{-1}\psi$ for some $\eta \in C_{\mathrm{c}}^{\infty}\big(\mathbb{R} \setminus \{\pm m\}\big)$ and some $\psi \in \mathcal{D}(\langle Q\rangle)$. So, we have

$$\begin{aligned} H'(H')^{-2} \cdot Q_{\mathrm{NW}}\varphi &= PP^{-2}H \cdot \mathscr{U}_{\mathrm{FW}}^{-1} Q \mathscr{U}_{\mathrm{FW}} \eta(H) \mathscr{U}_{\mathrm{FW}}^{-1}\psi \\ &= \mathscr{U}_{\mathrm{FW}}^{-1} PP^{-2}\beta|H| \cdot Q\eta(\beta|H|)\psi \in \mathcal{H}, \end{aligned}$$

and the operator T of (5.3) is symmetric and can be written on $\mathscr{D}_1$ in the simpler form

$$T = \tfrac{1}{2}\big\{Q_{\mathrm{NW}} \cdot H'(H')^{-2} + H'(H')^{-2} \cdot Q_{\mathrm{NW}}\big\} \equiv \tfrac{1}{2}\big\{Q_{\mathrm{NW}} \cdot PP^{-2}H + PP^{-2}H \cdot Q_{\mathrm{NW}}\big\}.$$

Now let $h : \mathbb{R}^3 \to \mathbb{R}$ be defined by $h(\xi) := (\xi^2 + m^2)^{1/2}$. Then it is known that $\mathscr{U}_{\mathrm{FW}} H \mathscr{U}_{\mathrm{FW}}^{-1} = \beta h(P)$, and a direct calculation shows that

$$\begin{aligned} \mathscr{U}_{\mathrm{FW}} T \mathscr{U}_{\mathrm{FW}}^{-1} &= \tfrac{1}{2}\beta\big\{Q \cdot PP^{-2}(P^2+m^2)^{1/2} + PP^{-2}(P^2+m^2)^{1/2} \cdot Q\big\} \\ &= \tfrac{1}{2}\beta\big\{Q \cdot \tfrac{h'(P)}{h'(P)^2} + \tfrac{h'(P)}{h'(P)^2} \cdot Q\big\} \end{aligned}$$

on $\mathscr{U}_{\mathrm{FW}}\mathscr{D}_1$. Furthermore there exists a spectral transformation $\mathscr{U}_0 : \mathsf{L}^2(\mathbb{R}^3) \to \int_{[m,\infty)}^{\oplus} \mathrm{d}\lambda\, \mathsf{L}^2(\mathbb{S}^2)$ for $h(P)$ such that

$$\mathscr{U}_0\big\{Q \cdot \tfrac{h'(P)}{h'(P)^2} + \tfrac{h'(P)}{h'(P)^2} \cdot Q\big\}\mathscr{U}_0^{-1}$$

is equal to the operator $2i\frac{\mathrm{d}}{\mathrm{d}\lambda}$ of differentiation with respect to the spectral parameter λ of $h(P)$ (see [37, Lemma 3.6] for a precise statement). Combining the preceding transformations we obtain for each $\psi \in \mathcal{H}$ and $\varphi \in \mathscr{D}_1$ that

$$\langle \psi, T\varphi\rangle = \int_{\sigma(H)} \mathrm{d}\lambda\, \big\langle (\mathscr{U}\psi)(\lambda), i\tfrac{\mathrm{d}(\mathscr{U}\varphi)}{\mathrm{d}\lambda}(\lambda)\big\rangle_{\mathsf{L}^2(\mathbb{S}^2;\mathbb{C}^2)},$$

where $\mathscr{U} : \mathcal{H} \to \int_{\sigma(H)}^{\oplus} \mathrm{d}\lambda\, \mathsf{L}^2(\mathbb{S}^2;\mathbb{C}^2)$ is the spectral transformation for the free Dirac operator H.

7.4. Convolution operators on locally compact groups

This example is partially inspired from [20], where the spectral nature of convolution operators on locally compact groups is studied.

Let G be a locally compact group with identity e and a left Haar measure ρ. In the Hilbert space $\mathcal{H} := \mathsf{L}^2(G, \mathrm{d}\rho)$ we consider the operator H of convolution by $\mu \in \mathsf{M}(G)$, where $\mathsf{M}(G)$ is the set of complex bounded Radon measures on G. Namely, for $\varphi \in \mathcal{H}$ one sets

$$(H\varphi)(g) := (\mu * \varphi)(g) \equiv \int_G \mathrm{d}\mu(h)\, \varphi(h^{-1}g) \quad \text{for } a.e.\ g \in G,$$

where the notation *a.e.* stands for "almost everywhere" and refers to the Haar measure ρ. The operator H is bounded with norm $\|H\| \leq |\mu|(G)$, and it is self-adjoint if μ is symmetric, *i.e.*, $\mu(E) = \overline{\mu(E^{-1})}$ for each Borel subset E of G. For simplicity, we also assume that μ is central and with compact support, where central means that $\mu(h^{-1}Eh) = \mu(E)$ for each $h \in G$ and each Borel subset E of G.

We recall that given two measures $\mu, \nu \in \mathsf{M}(G)$, their convolution $\mu * \nu \in \mathsf{M}(G)$ is defined by the relation [11, Eq. 2.34]

$$\int_G \mathrm{d}(\mu * \nu)(g)\, \psi(g) := \int_G \int_G \mathrm{d}\mu(g)\mathrm{d}\nu(h)\, \psi(gh) \qquad \forall \psi \in C_0(G),$$

where $C_0(G)$ denotes the C^*-algebra of continuous complex functions on G vanishing at infinity. If $\mu \in \mathsf{M}(G)$ has compact support and $\zeta : G \to \mathbb{C}$ is continuous, then the linear functional

$$C_0(G) \ni \psi \mapsto \int_G \mathrm{d}\mu(g)\, \zeta(g)\psi(g) \in \mathbb{C}$$

is bounded, and there exists a unique measure with compact support associated with it, due to the Riesz-Markov representation theorem. We write $\zeta\mu$ for this measure.

A natural choice for the family of operators $\Phi \equiv (\Phi_1, \dots, \Phi_d)$ are, if they exist, real characters $\Phi_j \in \mathrm{Hom}(G; \mathbb{R})$, *i.e.*, continuous group morphisms from G to $\mathbb{R}$. With this choice, one obtains that

$$[H(x)\varphi](g) \equiv \big(\mathrm{e}^{-ix\cdot\Phi}\, H\, \mathrm{e}^{ix\cdot\Phi}\, \varphi\big)(g) = \int_G \mathrm{d}\mu(h)\ \mathrm{e}^{-ix\cdot\Phi(h)}\, \varphi(h^{-1}g)$$

for each $x \in \mathbb{R}^d$, $\varphi \in \mathcal{H}$, and *a.e.* $g \in G$. Namely, $H(x)$ is equal to the operator of convolution by the measure $\mathrm{e}^{-ix\cdot\Phi}\, \mu$. Since μ has compact support and each Φ_j is continuous, this implies that H is of class $C^\infty(\Phi)$, with all the operators $H'_j, H''_{jk}, H'''_{jk\ell}$ belonging to $\mathscr{B}(\mathcal{H})$. So Assumption 2.2 is satisfied. Furthermore, the commutativity of central measures with respect to the convolution product implies that $\mu * \mathrm{e}^{-ix\cdot\Phi}\, \mu = \mathrm{e}^{-ix\cdot\Phi}\, \mu * \mu$ or equivalently that $HH(x) = H(x)H$. So Assumption 2.3 is satisfied. Finally, since $H(x)$ is the operator of convolution by the measure $\mathrm{e}^{-ix\cdot\Phi}\, \mu$, one readily obtains that H'_j is the operator of convolution with the measure $-i\Phi_j\mu$.

Since both Assumptions 2.2 and 2.3 are satisfied, the general results of the previous sections apply. However, it is very complicated to describe the set $\kappa(H)$ in the present generality. Therefore, we shall now assume that the group G is abelian in order to use the Fourier transformation to determine some properties of $\kappa(H)$. So let us assume that G is a locally compact abelian group. Then any measure on G is automatically central, and thus we only need to suppose that μ is symmetric and with compact support. For a suitably normalised Haar measure $\rho_\wedge$ on the dual group $\widehat{G}$, the Fourier transformation $\mathscr{F}$ defines a unitary isomorphism from $\mathcal{H}$ onto $\mathsf{L}^2(\widehat{G}, \mathrm{d}\rho_\wedge)$. It maps unitarily H on the operator M_m of multiplication with the bounded continuous real function $m := \mathscr{F}(\mu)$ on $\widehat{G}$. Furthermore, one has

$$\begin{aligned} \sigma(H) &= \sigma(M_m) = \overline{m(\widehat{G})}, \\ \sigma_{\mathrm{p}}(H) &= \sigma_{\mathrm{p}}(M_m) = \overline{\big\{s \in \mathbb{R} \mid \rho_\wedge\big(m^{-1}(s)\big) > 0\big\}}, \end{aligned} \tag{7.1}$$

where the overlines denote the closure in $\mathbb{R}$.

Let us recall that there is an almost canonical identification of $\mathrm{Hom}(G, \mathbb{R})$ with the vector space $\mathrm{Hom}(\mathbb{R}, \widehat{G})$ of all continuous one-parameter subgroups of $\widehat{G}$. Given the real character Φ_j, we denote by $\Upsilon_j \in \mathrm{Hom}(\mathbb{R}, \widehat{G})$ the unique element satisfying

$$\big\langle g, \Upsilon_j(t)\big\rangle = \mathrm{e}^{it\Phi_j(g)} \quad \text{for all } t \in \mathbb{R} \text{ and } g \in G,$$

where $\langle \cdot, \cdot \rangle : G \times \widehat{G} \to \mathbb{C}$ is the duality between G and $\widehat{G}$.

Definition 7.1. A function $m : \widehat{G} \to \mathbb{C}$ is *differentiable at* $\xi \in \widehat{G}$ *along the one-parameter subgroup* $\Upsilon_j \in \mathrm{Hom}(\mathbb{R}, \widehat{G})$ if the function $\mathbb{R} \ni t \mapsto m\big(\xi + \Upsilon_j(t)\big) \in \mathbb{C}$ is differentiable at $t = 0$. In such a case we write $(d_j m)(\xi)$ for $\frac{\mathrm{d}}{\mathrm{d}t}\, m\big(\xi + \Upsilon_j(t)\big)\big|_{t=0}$. Higher-order derivatives, when existing, are denoted by $d_j^k m$, $k \in \mathbb{N}$.

We refer to [28] for more details on differential calculus on locally compact groups. Here we only note that (since μ has compact support) the function $m = \mathscr{F}(\mu)$ is differentiable at any point ξ along the one-parameter subgroup Υ_j, and $-i\mathscr{F}(\Phi_j \mu) = d_j m$ [28, p. 68]. This implies that the operator H'_j is mapped unitarily by $\mathscr{F}$ on the multiplication operator $M_{d_j m}$, and thus $(H')^2$ is unitarily equivalent to the operator of multiplication by the function $\sum_j (d_j m)^2$. It follows that

$$\kappa(H) \supset \big\{\lambda \in \mathbb{R} \mid \exists \xi \in \widehat{G} \text{ such that } m(\xi) = \lambda \text{ and } \textstyle\sum_j (d_j m)(\xi)^2 = 0\big\}.$$

This property of $\kappa(H)$ suggests a way to justify the formal formula of Remark 5.3 and to write nice formulas for the operator T given by (5.3). Indeed, since $\mathscr{F}\Phi_j\mathscr{F}^{-1}$ acts as the differential operator id_j in $\mathsf{L}^2(\widehat{G}, \mathrm{d}\rho_\wedge)$, it follows that Φ_j leaves invariant the complement of the support of the functions on which it acts. Therefore, the set $\Phi_j \mathscr{D}_1 \equiv \mathscr{F}^{-1}(id_j)\mathscr{F}\mathscr{D}_1$ is included in the domain of the operator

$$\tfrac{H'_j}{(H')^2} \equiv \mathscr{F}^{-1} \tfrac{M_{d_j m}}{M_{\sum_k (d_k m)^2}}\, \mathscr{F}.$$

Thus the formula (5.3) takes the form

$$\mathscr{F}T\mathscr{F}^{-1} = \tfrac{i}{2}\sum_j \left\{ d_j \tfrac{M_{d_j m}}{M_{\sum_k (d_k m)^2}} + \tfrac{M_{d_j m}}{M_{\sum_k (d_k m)^2}}\, d_j \right\} \tag{7.2}$$

on $\mathscr{F}\mathscr{D}_1$ (note that the last expression is well defined on $\mathscr{F}\mathscr{D}_1$, since $m = \mathscr{F}(\mu)$ is of class C^2 in the sense of Definition 7.1).

In simple situations, everything can be calculated explicitly. For instance, when $G = \mathbb{Z}^d$, the Haar measure ρ is the counting measure, and the most natural real characters Φ_j are the position operators given by

$$(\Phi_j \varphi)(g) := g_j \varphi(g), \qquad \varphi \in \mathsf{L}^2(\mathbb{Z}^d),$$

where g_j is the jth component of $g \in \mathbb{Z}^d$. The operators H and $(H')^2$ are unitarily equivalent to multiplication operators on $\widehat{G} = (-\pi, \pi]^d$. Since the measures μ and $\Phi_j \mu$ have compact (and thus finite) support, these operators are just multiplication operators by polynomials of finite degree in the variables $\mathrm{e}^{-i\xi_1}, \ldots, \mathrm{e}^{-i\xi_d}$, with $\xi_j \in (-\pi, \pi]$. So, the set $\kappa(H)$ is finite, and the characterisation (7.1) of the point spectrum of H implies that $\sigma_{\mathrm{p}}(H) = \varnothing$ if $\mathrm{supp}(\mu) \neq \{e\}$. By taking into account Lemma 6.3.(b) and Theorem 3.6, we infer that the sets $\mathscr{D}_t$ are dense in $\mathcal{H}$ for each $t \geq 0$, and thus Case 2 of Section 6 applies. Finally, we mention as a corollary the following spectral result:

Corollary 7.2. *Let μ be a symmetric measure on $\mathbb{Z}^d$ with finite support. If $\mathrm{supp}(\mu) \neq \{e\}$, then the convolution operator H in $\mathcal{H} := \mathsf{L}^2(\mathbb{Z}^d)$ is purely absolutely continuous.*

7.5. $H = h(P)$

Consider in $\mathcal{H} := \mathsf{L}^2(\mathbb{R}^d)$ the dispersive operator $H := h(P)$, where $h \in C^3(\mathbb{R}^d; \mathbb{R})$ satisfies the following condition: For each multi-indices $\alpha, \beta \in \mathbb{N}^d$ with $\alpha > \beta$, $|\alpha| = |\beta| + 1$, and $|\alpha| \leq 3$, we have

$$|\partial^\alpha h| \leq \mathrm{Const.}\big(1 + |\partial^\beta h|\big). \tag{7.3}$$

Note that this class of operators $h(P)$ contains all the usual elliptic free Hamiltonians appearing in physics.

Take for the family $\Phi \equiv (\Phi_1, \ldots, \Phi_d)$ the position operators $Q \equiv (Q_1, \ldots, Q_d)$. Then we have for each $x \in \mathbb{R}^d$

$$H(x) = \mathrm{e}^{-ix\cdot Q}\, H\, \mathrm{e}^{ix\cdot Q} = h(P + x),$$

and $H' = h'(P)$. So Assumption 2.3 is directly verified and Assumption 2.2 follows from (7.3). Therefore all the results of the previous sections are valid. We do not give more details since many aspects of this example, including the existence of time delay, have already been extensively discussed in [37]. We only add some comments in relation with Case 3 of Section 6.

Assume that there exist $\lambda \in \mathbb{R}$ and a maximal subset $\Omega \subset \mathbb{R}^d$ of strictly positive Lebesgue measure such that $h(x) = \lambda$ for all $x \in \Omega$. Then any φ in $\mathcal{H}_\Omega := \{\psi \in \mathcal{H} \mid \mathrm{supp}(\mathscr{F}\psi) \subset \Omega\}$ is an eigenvector of $h(P)$ with eigenvalue λ. Furthermore, one has $\mathscr{F}^{-1}\mathcal{H}_\Omega \subset \mathcal{K} \equiv \ker\big(h'(P)^2\big)$, and for simplicity we assume

that the first inclusion is an equality. Then, an application of the Fourier transformation shows that $Q_j\mathscr{D}_1 \subset \mathcal{G}$ for each j, where $\mathcal{G}$ is the orthocomplement of $\mathcal{K}$ in $\mathcal{H}$. Thus Remark 6.2 applies, and one can consider the restrictions of H and T_f to the subspace $\mathcal{G}$, as described in Case 3 of Section 6. In favorable situations, we expect that the restriction of T_f to $\mathcal{G}$ acts as $i\frac{\mathrm{d}}{\mathrm{d}\lambda}$ in the spectral representation of the restriction of H to $\mathcal{G}$.

7.6. Adjacency operators on admissible graphs

Let $(X, \sim)$ be a graph X with no multiple edges or loops. We write $g \sim h$ whenever the vertices g and h of X are connected. In the Hilbert space $\mathcal{H} := \ell^2(X)$ we consider the adjacency operator

$$(H\varphi)(g) := \sum_{h\sim g} \varphi(h), \quad \varphi \in \mathcal{H},\ g \in X.$$

We denote by $\deg(g) := \#\{h \in X \mid h \sim g\}$ the degree of the vertex g. Under the assumption that $\deg(X) := \sup_{g\in X} \deg(g)$ is finite, H is a bounded self-adjoint operator in $\mathcal{H}$. The spectral analysis of the adjacency operator on some general graphs has been performed in [19]. Here we consider only a subclass of such graphs called admissible graphs.

A directed graph $(X, \sim, <)$ is a graph $(X, \sim)$ and a relation $<$ on the graph such that, for any $g, h \in X$, $g \sim h$ is equivalent to $g < h$ or $h < g$, and one cannot have both $h < g$ and $g < h$. We also write $h > g$ for $g < h$. For a fixed g, we denote by $N^-(g) \equiv \{h \in X \mid g < h\}$ the set of fathers of g and by $N^+(g) \equiv \{h \in X \mid h < g\}$ the set of sons of g. The set $\{h \in X \mid g \sim h\}$ of neighbours of g is denoted by $N(g) \equiv N^-(g) \cup N^+(g)$. When using drawings, one has to choose a direction (an arrow) for any edge. By convention, we set $g \leftarrow h$ if $g < h$, *i.e.*, any arrow goes from a son to a father. When directions have been fixed, we use the simpler notation $(X, <)$ for the directed graph $(X, \sim, <)$.

Definition 7.3. A directed graph $(X, <)$ is called admissible if

(a) any closed path in X has index zero (the index of a path is the difference between the number of positively oriented edges in the path and that of the negatively oriented ones),

(b) for any $g, h \in X$, one has $\#\{N^-(g) \cap N^-(h)\} = \#\{N^+(g) \cap N^+(h)\}$.

It is proved in [19, Lemma 5.3] that for admissible graphs there exists a unique (up to constant) map $\Phi : X \to \mathbb{Z}$ satisfying $\Phi(h) + 1 = \Phi(g)$ whenever $h < g$. With this choice of operator Φ, one obtains that

$$[H(x)\varphi](g) = \sum_{h\sim g} \mathrm{e}^{ix[\Phi(h)-\Phi(g)]}\, \varphi(h) \tag{7.4}$$

for each $x \in \mathbb{R}$, $\varphi \in \mathcal{H}$, and $g \in X$. Therefore, the commutativity of H and $H(x)$ is equivalent to the condition

$$\sum_{h\in N(g)\cap N(\ell)} \left(\mathrm{e}^{ix[\Phi(\ell)-\Phi(h)]} - \mathrm{e}^{ix[\Phi(h)-\Phi(g)]} \right) = 0$$

for each $g, \ell \in X$. By taking into account the growth property of Φ and Hypothesis (b) of Definition 7.3, one obtains that the parts $h \in N^-(g) \cap N^-(\ell)$ and $h \in N^+(g) \cap N^+(\ell)$ of the sum are of opposite sign, and that the parts $h \in N^-(g) \cap N^+(\ell)$ and $h \in N^+(g) \cap N^-(\ell)$ are null. So Assumption 2.3 is satisfied. One also verifies by using Formula (7.4) that H belongs to $C^\infty(\Phi)$, and that Assumption 2.2 holds. It follows that the general results presented before apply.

Now, the operator H' acts as $(H'\varphi)(g) = i\big(\sum_{h>g} \varphi(h) - \sum_{h<g} \varphi(h)\big)$, and it is proved in [19, Sec. 5] that

$$\begin{aligned} \mathcal{H}_{\rm p}(H) &= \ker(H) = \ker(H') \\ &= \big\{\varphi \in \mathcal{H} \mid \textstyle\sum_{h>g} \varphi(h) = 0 = \sum_{h<g} \varphi(h) \text{ for each } g \in X\big\}. \end{aligned} \tag{7.5}$$

It is also proved that H is purely absolutely continuous, except at the origin where it may have an eigenvalue with eigenspace given by (7.5). The proof of these statements is based on the method of the weakly conjugate operator [9].

However, in the present generality, it is hardly possible to obtain a simple description of the set $\kappa(H)$ or the operator T_f. We refer then to [19, Sec. 6] for explicit examples of admissible graphs with adjacency operators whose kernels are either trivial or non trivial, and develop one example for which more explicit computations can be performed. This example furnishes an illustration of the discussion in Case 3 of Section 6.

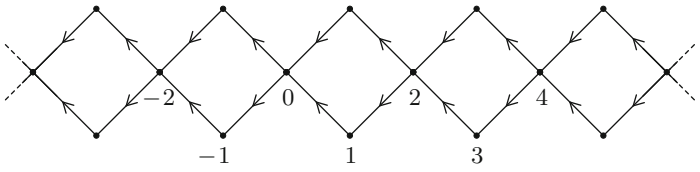

FIGURE 1. Example of an admissible directed graph X

We consider the admissible graph of Figure 1, and endow it with the function $\Phi : X \to \mathbb{Z}$ as shown on the picture. The vertices of the graph are denoted by z_- and z_+ when Φ takes an odd value, and by z when Φ takes an even value. More precisely, $\Phi(z) = z$ for z even, and $\Phi(z_-) = \Phi(z_+) = z$ for z odd. By using (7.5), it is easily observed that $\mathcal{K} \equiv \ker\big((H')^2\big)$ is equal to

$$\big\{\varphi \in \mathsf{l}^2(X) \mid \varphi(z) = 0 \text{ for } z \text{ even, and } \varphi(z_-) = -\varphi(z_+) \text{ for } z \text{ odd}\big\}.$$

On the other hand, the orthocomplement $\mathcal{G}$ of $\mathcal{K}$ in $\mathsf{l}^2(X)$ is unitarily equivalent to $\ell^2(\mathbb{Z})$, and the restriction H of H to $\mathcal{G}$ is unitarily equivalent to the operator in $\ell^2(\mathbb{Z})$ defined by

$$\big(\widetilde{\mathsf{H}}\varphi\big)(z) := \sqrt{2}\big\{\varphi(z-1) + \varphi(z+1)\big\}, \qquad \varphi \in \ell^2(\mathbb{Z}).$$

Using the Fourier transformation, one shows that this operator is unitarily equivalent to the multiplication operator M in $\mathsf{l}^2\big((-\pi, \pi]\big)$ given by the function $(-\pi, \pi] \ni \xi \mapsto 2\sqrt{2}\cos(\xi)$.

Now, the operator Φ in $\mathsf{L}^2(X)$ is clearly reduced by the decomposition $\mathcal{K} \oplus \mathcal{G}$. As mentioned in Remark 6.2, this implies that the operator T_f is also reduced by this decomposition. By taking Formula (7.2) into account, one obtains that the restriction T_f of T_f to $\mathcal{G}$ is unitarily equivalent to the operator

$$\tfrac{i}{2}\Big\{\tfrac{\mathrm{d}}{\mathrm{d}\xi}\big[-2\sqrt{2}\sin(\xi)\big]^{-1} + \big[-2\sqrt{2}\sin(\xi)\big]^{-1}\tfrac{\mathrm{d}}{\mathrm{d}\xi}\Big\}$$

on $\mathscr{F}\mathscr{D}_1 \subset \mathsf{L}^2\big((-\pi,\pi]\big)$. This implies, as expected, that T_f acts as $i\frac{\mathrm{d}}{\mathrm{d}\lambda}$ in the spectral representation of H.

7.7. Direct integral operators

Let Ω be a measurable subset of $\mathbb{R}^n$ and let us consider a direct integral

$$\mathcal{H} := \int_\Omega^\oplus \mathrm{d}\xi\, \mathcal{H}_\xi,$$

where $\mathrm{d}\xi$ is the usual Lebesgue measure on $\mathbb{R}^n$ and $\mathcal{H}_\xi$ are Hilbert spaces. Take a decomposable self-adjoint operator $H \equiv \int_\Omega^\oplus \mathrm{d}\xi\, H(\xi)$ in $\mathcal{H}$. Assume that there exists a family $\Phi \equiv (\Phi_1, \ldots, \Phi_d)$ of operators in $\mathcal{H}$ such that Assumption 2.2 is satisfied. Assume also for each $x \in \mathbb{R}^d$ that the operator $H(x)$ defined by (2.4) is decomposable, *i.e.*, there exists a family of self-adjoint operators $H(\xi, x)$ in $\mathcal{H}_\xi$ such that $H(x) = \int_\Omega^\oplus \mathrm{d}\xi\, H(\xi, x)$. Finally, assume that the operators $H(\xi)$ and $H(\xi, x)$ commute for each $x \in \mathbb{R}^d$ and *a.e.* $\xi \in \Omega$, so that H and $H(x)$ commute. Then Assumption 2.3 holds, and the general theory developed in the preceding sections applies. Moreover, it is easily observed that the fibered structure of the map $x \mapsto H(x)$ implies that the operators H'_j are also decomposable. Therefore, there exists for each $j \in \{1, \ldots, d\}$ a family of self-adjoint operators $H'_j(\xi)$ such that $H'_j = \int_\Omega^\oplus \mathrm{d}\xi\, H'_j(\xi)$. In consequence $\lambda \in \mathbb{R}$ is a regular value of H if there exists $\delta > 0$ and $\mathrm{c} < \infty$ such that

$$\lim_{\varepsilon \searrow 0} \Big\| \big[\big(H'(\xi)\big)^2 + \varepsilon\big]^{-1} E^{H(\xi)}(\lambda; \delta) \Big\|_{\mathcal{H}_\xi} < \mathrm{c} \tag{7.6}$$

for *a.e.* $\xi \in \Omega$. We also recall that $\ker\big((H')^2\big) \neq \{0\}$ if and only if there exists a measurable subset $\Omega_0 \subset \Omega$ with positive measure such that $\ker\big(H'(\xi)^2\big) \neq \{0\}$ for each $\xi \in \Omega_0$.

We now give an example of quantum waveguide fitting into this setting (see [35] for more details). Let Σ be a bounded open connected set in $\mathbb{R}^m$, and consider in the Hilbert space $\mathsf{L}^2(\Sigma \times \mathbb{R})$ the Dirichlet Laplacian $-\Delta_{\mathrm{D}}$. The partial Fourier transformation along the longitudinal axis sends the initial Hilbert space onto the direct integral $\mathcal{H} := \int_{\mathbb{R}}^\oplus \mathrm{d}\xi\, \mathcal{H}_0$, with $\mathcal{H}_0 := \mathsf{L}^2(\Sigma)$, and it sends $-\Delta_{\mathrm{D}}$ onto the fibered operator $H := \int_{\mathbb{R}}^\oplus \mathrm{d}\xi\, H(\xi)$, with $H(\xi) := \xi^2 - \Delta_{\mathrm{D}}^\Sigma$. Here, $-\Delta_{\mathrm{D}}^\Sigma$ denotes the Dirichlet Laplacian in Σ. By choosing for Φ the position operator Q along the longitudinal axis one obtains that $H(x) = \int_{\mathbb{R}}^\oplus \mathrm{d}\xi\, H(\xi, x)$ with $H(\xi, x) = (\xi + x)^2 - \Delta_{\mathrm{D}}^\Sigma$. Clearly, $H(\xi)$ and $H(\xi, x)$ commute, and so do H and $H(x)$. Furthermore, the operator H is of class $C^\infty(\Phi)$, and H' is the fibered operator given by $H'(\xi) = 2\xi$.

It follows that both Assumptions 2.2 and 2.3 hold, and thus the general theory applies. Now a simple calculation using (7.6) shows that $\kappa(H) = \sigma(-\Delta_{\mathrm{D}}^{\Sigma})$. Furthermore, in the tensorial representation $\mathsf{L}^2(\Sigma) \otimes \mathsf{L}^2(\mathbb{R})$ of $\mathsf{L}^2(\Sigma \times \mathbb{R})$, one obtains that $T_f = T = \frac{1}{4} \otimes (QP^{-1} + P^{-1}Q)$ on the dense set

$$\mathscr{D}_1 = \big\{\varphi \in \mathsf{L}^2(\Sigma) \otimes \mathcal{D}(\langle Q \rangle) \mid \varphi = \eta(-\Delta_{\mathrm{D}})\varphi \text{ for some } \eta \in C_{\mathrm{c}}^{\infty}\big(\mathbb{R} \setminus \kappa(H)\big)\big\},$$

and T_f is equal to $i\frac{\mathrm{d}}{\mathrm{d}\lambda}$ in the spectral representation of $-\Delta_{\mathrm{D}}$. In [35] it is even shown that the quantum time delay exists and is given by Formula (6.4) for appropriate scattering pairs $\{-\Delta_{\mathrm{D}}, -\Delta_{\mathrm{D}} + V\}$.

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