Mathematical Results in QUANTUM PHYSICS

edited by *Pavel Exner*

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Mathematical Results in QUANTUM PHYSICS

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edited by

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PREFACE

Conference series are more than just collections of scientific meetings; they make it possible to follow the life of a community of people with shared interest over a certain period of time. True, very few series reach the state of effective immortality spanning several generations; most of them die at a young age due to the lack of people willing to take the burden of organizing such a meeting, a task which usually distracts you from your normal activity for months if not more.

The *QMath* series has managed to pass its teens and enter the third decade of its existence. It was begotten in 1987 in Dubna as an attempt to foster fruitful collaboration between mathematical physicists from different parts of the world; its midwives did not suspect at the beginning that within just a couple of years their working conditions will change beyond any expectation. The series proved to have a strong enough motivation, however, to survive in the new conditions, with the periodicity which stabilized after some time to three years, and its meetings convened at different places, mostly in Europe but also once in Mexico.

The eleventh issue returned to the Czech Republic where the meeting was held twice before. This time the town of Hradec Králové was chosen as its site which gave the participants the opportunity to enjoy its historical center, a short walking distance from the new university building where the conference took place. The main sponsor of the meeting was *Doppler Institute for Mathematical Physics and Applied Mathematics*, a center of basic research supported by the Czech government and we also enjoyed support from the European project CZ.1.07/2.3.00/09.0044; we appreciate the financial help which made it possible to keep the registration fee at a reasonable level. We are also grateful to the Doppler Institute institutional constituents, Czech Technical University, Nuclear Physics Institute of the Czech Academy of Sciences, and in the first place, to University of Hradec Králové for the organizational support they provided.

The plenary lectures were devoted to the properties of quantum systems, both in the one-body and many-body situations, quantum information, and related mathematical problems. With three exceptions their contents are reflected in the papers collected in the first part of this book. The second part summarizes the topical sessions contents, featuring most of the invited talks. These six sessions were devoted to the spectral theory, many-body quantum systems, quantum chaos, quantum field theory, quantum information and, motivated by some recent intriguing observations, we have also included a session on the physics of social systems. The talks not included, both invited and contributed ones, are present through their abstracts, and

moreover, the volume is accompanied with a *dvd* containing most of the presentations as they appeared on the screen during the talks.

The seventh session was special, being devoted to the important jubilee of Ari Laptev in appreciation of his work for the mathematical physics community, both through his mathematical papers and by organizing numerous scientific events. We wished him good health, happiness, and many new interesting results.

I hope the reader of this volume will have no doubt that the *QMath11* conference offered a rich and interesting programme which its participants enjoyed. I want to thank here to those who made this possible: to the (other) members of the scientific and local organizing committees, to the topical session organizers, to the student volunteers and all the others who helped. With the eleventh issue of the series behind us, we firmly hope it will not be the last one.

Prague, January 2011

Pavel Exner

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PART A

Plenary Talks

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RELATIVE ENTROPIES AND ENTANGLEMENT MONOTONES

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We introduce two relative entropy quantities called the min- and max-relative entropies and discuss their properties and operational meanings. These relative entropies act as parent quantities for optimal one-shot rates of information-processing tasks such as data compression, information transmission and entanglement manipulation. Moreover, they lead us to define entanglement monotones which have interesting operational interpretations.

Keywords: Quantum relative entropy; entanglement monotone; smooth Rényi entropy.

1. Introduction

One of the fundamental quantities in Quantum Information Theory is the quantum relative entropy. Other entropic quantities, such as the von Neumann entropy, the conditional entropy and the mutual information, are obtainable from the relative entropy. Many basic properties of these entropic quantities can be derived from those of the relative entropy. The strong subadditivity of the von Neumann entropy, which is one of the most powerful results in Quantum Information Theory, follows easily from the monotonicity of the relative entropy under completely positive trace-preserving maps. Other than acting as a parent quantity for other entropic quantities, the relative entropy itself has an operational meaning. It serves as a measure of distinguishability between states.

The notion of relative entropy was introduced in 1951, in Mathematical Statistics, by Kullback and Leibler [1], as a means of comparing two different probability distributions. Its extension to the quantum setting was due to Umegaki [2]. The classical relative entropy plays a role similar to its quantum counterpart. Classical entropic quantities such as the Shannon entropy of a random variable, and the conditional entropy, the mutual information and the joint entropy of a pair of random variables, are all obtainable from it.

More recently, the concept of relative entropy has been generalized to sequences of states, in the so-called Information Spectrum Approach [3–8]. The latter is a powerful method which enables us to evaluate the optimal rates of various information theory protocols, without making any assumption on the structure of the sources, channels or (in the quantum case) the entanglement resources involved. In

particular, it allows us to eliminate the frequently-used, but often unjustified, assumption that sources, channels and entanglement resources are memoryless. The quantities arising from the generalizations of the relative entropy in this approach are referred to as *spectral divergence rates*. Like the relative entropy, they yield quantities which can be viewed as generalizations of entropy rates for sequences of states (or probability distributions, in the classical case). These quantities have been proved to be of important operational significance in Classical and Quantum Information Theory, as the optimal rates of protocols such as data compression, dense coding, entanglement concentration and dilution, transmission of classical information through a quantum channel and in the context of hypothesis testing [see e.g. [6, 7, 9–14]]. Hence, spectral divergence rates can be viewed as the basic tools of a unifying mathematical framework for studying information theoretical protocols.

A simultaneous but independent approach, developed to overcome the limitation of the memoryless criterion is the so-called *Smooth Entropy framework*, developed by Renner et al. (see e.g. [15], [16], [17], [18], [19]). This approach introduced new entropy measures called *smooth Rényi entropies* or *smoothed min- and max-entropies*. In contrast to the spectral entropy rates, the (unconditional and conditional) smooth min- and max-entropies are defined for individual states (or probability distributions) rather than sequences of states. They are non-asymptotic in nature but depend on an additional parameter ε, the smoothness parameter. Similar to the spectral entropies, the min- and max-entropies have various interesting properties e.g. chain rule inequalities and strong subadditivity. They are also of operational significance and have proved useful in the context of randomness extraction and cryptography.

It has been proved [20] that the two approaches discussed above, are related in the sense that the spectral entropy rates are obtained as asymptotic limits of the corresponding smoothed min- and max-entropies.

In this paper we introduce two new relative entropy quantities, namely the *min- and max-relative entropies* (and their smoothed versions), which act as parent quantities for the unconditional and conditional min- and max-entropies of Renner [15]. These new relative entropy quantities are seen to satisfy several interesting properties. Moreover, they have interesting operational interpretations in terms of probabilities of error in state discrimination (see Section 5 for details). Most importantly, the smoothed min- and max-relative entropies have been proved to act as parent quantities for optimal rates of various information-processing tasks, in the so-called "one-shot scenario", that is, when the resources (sources, channels and entanglement resources) employed in the tasks, are considered to be finite and correlated. The one-shot scenario therefore corresponds to the situation in which the (often unjustified) assumptions that resources are memoryless and that they are available for asymptotically many uses, is lifted. The optimal rates of transmission of information [21, 22], entanglement manipulation [23–25] and state splitting [26] in the one-shot scenario are all obtainable from the min- and max-relative entropies.

Just as one defines an important entanglement monotone, namely the relative

entropy of entanglement, in terms of the quantum relative entropy, the min- and max-relative entropies lead naturally to the definition of two entanglement monotones. We refer to these as the min-(max-) relative entropies of entanglement. They provide lower(upper) bounds on the relative entropy of entanglement. Smoothed versions of these entanglement monotones are also defined and these are shown to have interesting operational meanings.

We start with some mathematical preliminaries in Section 2. We define min- and max-relative entropies in Section 3, and state how the unconditional and conditional min- and max-entropies are obtained from them. We also define the min- and max-mutual informations. In Section 4 we investigate the properties of the new relative entropy quantities and in Section 5 we discuss their operational interpretations in relation to state discrimination. In Section 6 we define two entanglement monotones in terms of the min- and max-relative entropies and evaluate their properties, while in Section 7 we define the smoothed versions of these entanglement monotones and discuss their operational meanings in one-shot entanglement manipulation.

2. Mathematical preliminaries

Let $\mathcal{B}(\mathcal{H})$ denote the algebra of linear operators acting on a finite-dimensional Hilbert space $\mathcal{H}$, and let $\mathcal{D}(\mathcal{H}) \subset \mathcal{B}(\mathcal{H})$ denote the set of density matrices (i.e., positive semi-definite operators of unit trace). The von Neumann entropy of a state ρ, i.e., a positive operator of unit trace in $\mathcal{B}(\mathcal{H})$, is given by $S(\rho) = -\mathrm{Tr}\rho\log\rho$. Throughout this paper, we take the logarithm to base 2 and all Hilbert spaces considered are finite-dimensional. We denote the identity operator in $\mathcal{B}(\mathcal{H})$ by I.

In this paper we make use of spectral projections. Any self-adjoint operator A acting on a finite-dimensional Hilbert space may be written in its spectral decomposition $A = \sum_i \lambda_i P_i$, where P_i denotes the orthogonal projector onto the eigenspace of A spanned by eigenvectors corresponding to the eigenvalue λ_i. We define the non-negative spectral projection on A as $\{A \geq 0\} := \sum_{\lambda_i \geq 0} P_i$, the projector onto the eigenspace of A corresponding to non-negative eigenvalues. Corresponding definitions apply for the other spectral projections $\{A < 0\}, \{A > 0\}$ and $\{A \leq 0\}$. For two operators A and B, we can then define $\{A \geq B\}$ as $\{A - B \geq 0\}$. The following key lemmas are useful [8]:

Lemma 2.1. *For self-adjoint operators A, B and any positive operator $0 \leq P \leq I$, we have*

$$\mathrm{Tr}\big[P(A-B)\big] \leq \mathrm{Tr}\big[\big\{A \geq B\big\}(A-B)\big] \tag{1}$$

$$\mathrm{Tr}\big[P(A-B)\big] \geq \mathrm{Tr}\big[\big\{A \leq B\big\}(A-B)\big]. \tag{2}$$

Identical conditions hold for strict inequalities in the spectral projections $\{A < B\}$ and $\{A > B\}$.

Lemma 2.2. *Given a state ρ_n and a self-adjoint operator ω_n, for any real γ, we*

have

$$\mathrm{Tr}\big[\{\rho_n \geq 2^{n\gamma}\omega_n\}\omega_n\big] \leq 2^{-n\gamma}.$$

Lemma 2.3. *For self-adjoint operators A and B, and any completely positive trace-preserving (CPTP) map $\mathcal{T}$, the inequality*

$$\mathrm{Tr}\big[\{\mathcal{T}(A) \geq \mathcal{T}(B)\}\mathcal{T}(A-B)\big] \leq \mathrm{Tr}\big[\big\{A \geq B\big\}(A-B)\big] \tag{3}$$

holds.

The trace distance between two operators A and B is given by

$$||A-B||_1 := \mathrm{Tr}\big[\{A \geq B\}(A-B)\big] - \mathrm{Tr}\big[\{A < B\}(A-B)\big] \tag{4}$$

The fidelity of states ρ and ρ' is defined to be

$$F(\rho,\rho') := \mathrm{Tr}\sqrt{\rho^{\frac{1}{2}}\rho'\rho^{\frac{1}{2}}}.$$

3. Definitions of min- and max-relative entropies

In this section we define two new relative entropy quantities, namely, the min- and max-relative entropies.

Definition 3.1. The *max-relative entropy* of two operators ρ and σ, such that $\rho \geq 0$, $\mathrm{Tr}\rho \leq 1$ and $\sigma \geq 0$, is defined as [27]

$$D_{\max}(\rho||\sigma) := \log\min\{\lambda :\ \rho \leq \lambda\sigma\}. \tag{5}$$

Note that $D_{\max}(\rho||\sigma)$ is well-defined if $\mathrm{supp}\,\rho \subseteq \mathrm{supp}\,\sigma$. For ρ and σ satisfying $\mathrm{supp}\,\rho \subseteq \mathrm{supp}\,\sigma$, $D_{\max}(\rho||\sigma)$ is equivalently given by

$$D_{\max}(\rho||\sigma) := \log\mu_{\max}\big(\sigma^{-\frac{1}{2}}\rho\sigma^{-\frac{1}{2}}\big), \tag{6}$$

where the notation $\mu_{\max}(A)$ is used to denote the maximum eigenvalue of the operator A, and the inverses are generalized inverses defined as follows: A^{-1} is a generalized inverse of A if $AA^{-1} = A^{-1}A = P_A = P_{A^{-1}}$, where $P_A, P_{A^{-1}}$ denote the projectors onto the supports of A and A^{-1} respectively.

Another equivalent definition of $D_{\max}(\rho||\sigma)$ is:

$$D_{\max}(\rho||\sigma) := \log\min\{\lambda :\ \mathrm{Tr}\big[P_+^{\lambda}(\rho-\lambda\sigma)\big] = 0\}, \tag{7}$$

where $P_+^{\lambda} := \{\rho \geq \lambda\sigma\}$.

Definition 3.2. The *min-relative entropy* of two operators ρ and σ, such that $\rho \geq 0$, $\mathrm{Tr}\rho \leq 1$ and $\sigma \geq 0$, is defined as [27]

$$D_{\min}(\rho||\sigma) := -\log\mathrm{Tr}\big(\pi_\rho\sigma\big)\ , \tag{8}$$

where π_ρ denotes the projector onto $\mathrm{supp}\,\rho$, the support of ρ. It is well-defined if $\mathrm{supp}\,\rho$ has non-zero intersection with $\mathrm{supp}\,\sigma$.

Note that

$$D_{\min}(\rho||\sigma) = \lim_{\alpha\to 0^+} S_\alpha(\rho||\sigma), \tag{9}$$

where $S_\alpha(\rho||\sigma)$ denotes the *quantum relative Rényi entropy* of order α, with $0 < \alpha < 1$, defined by (see e.g. [28, 29]):

$$S_\alpha(\rho||\sigma) := \frac{1}{\alpha - 1} \log \mathrm{Tr}\rho^\alpha \sigma^{1-\alpha}. \tag{10}$$

Further if ρ and σ commute, and $\mathrm{supp}\,\rho \subseteq \mathrm{supp}\,\sigma$, then $D_{\max}(\rho||\sigma)$ is equal to

$$S_\infty(\rho||\sigma) := \lim_{\alpha\to\infty} S_\alpha(\rho||\sigma).$$

However, this is no longer true if ρ and σ do not commute. See [30] for counterexamples. Various properties of $D_{\min}(\rho||\sigma)$ and $D_{\max}(\rho||\sigma)$ are discussed in Section 4.

The min- and max- (unconditional and conditional) entropies, introduced by Renner in [15] can be obtained from $D_{\min}(\rho||\sigma)$ and $D_{\max}(\rho||\sigma)$ by making suitable substitutions for the positive operator σ. In particular, for $\sigma = I$, we obtain the min- and max-entropies of a state ρ, which are simply the Rényi entropies of order infinity and zero, respectively:

$$H_{\min}(\rho) = -D_{\max}(\rho||I) = -\log\|\rho\|_\infty, \tag{11}$$

$$H_{\max}(\rho) = -D_{\min}(\rho||I) = \log \mathrm{rank}(\rho). \tag{12}$$

The min- and max-entropies of a bipartite state, ρ_{AB}, relative to a state σ_B, are similarly obtained by setting $\sigma = I_A \otimes \sigma_B$:

$$\begin{aligned} H_{\min}(\rho_{AB}|\sigma_B) &:= -\log\min\{\lambda :\ \rho_{AB} \le \lambda \cdot I_A \otimes \rho_B\} \\ &= -D_{\max}(\rho_{AB}||I_A \otimes \sigma_B), \end{aligned} \tag{13}$$

and

$$\begin{aligned} H_{\max}(\rho_{AB}|\sigma_B) &:= \log \mathrm{Tr}\big(\pi_{AB}(I_A \otimes \sigma_B)\big) \\ &= -D_{\min}(\rho_{AB}||I_A \otimes \sigma_B). \end{aligned} \tag{14}$$

In the above, π_{AB} denotes the projector onto the support of ρ_{AB}.

In addition, by considering $\sigma = \rho_A \otimes \rho_B$, we obtain the following analogues of the quantum mutual information of a bipartite state $\rho = \rho_{AB}$:

Definition 3.3. For a bipartite state ρ_{AB}, the min- and max-mutual informations are defined by

$$\begin{aligned} D_{\min}(A:B) &:= D_{\min}(\rho_{AB}||\rho_A \otimes \rho_B) \\ D_{\max}(A:B) &:= D_{\max}(\rho_{AB}||\rho_A \otimes \rho_B). \end{aligned} \tag{15}$$

Smoothed min- and max-relative entropies are generalizations of the above-mentioned relative entropy measures, involving an additional *smoothness* parameter $\varepsilon \geq 0$. For $\varepsilon = 0$, they reduce to the *non-smooth* quantities.

Definition 3.4. For any $\varepsilon \geq 0$, the *ε-smooth min-* and *max-relative entropies* of a bipartite state ρ relative to a state σ are defined by

$$D^{\varepsilon}_{\min}(\rho||\sigma) := \sup_{\bar{\rho}\in B^{\varepsilon}(\rho)} D_{\min}(\bar{\rho}||\sigma)$$

and

$$D^{\varepsilon}_{\max}(\rho||\sigma) := \inf_{\bar{\rho}\in B^{\varepsilon}(\rho)} D_{\max}(\bar{\rho}||\sigma)$$

where $B^{\varepsilon}(\rho) := \{\bar{\rho} \geq 0 : \ \|\bar{\rho} - \rho\|_1 \leq \varepsilon, \mathrm{Tr}(\bar{\rho}) \leq \mathrm{Tr}(\rho)\}$.

As mentioned in the Introduction, the optimal rates of various information-processing tasks in the one-shot scenario are obtainable from the smoothed min- and max-relative entropies [21–23, 25, 26]. They hence act as parent quantities for these rates.

4. Properties of min- and max-relative entropies

The min- and max-relative entropies satisfy the following properties:

Lemma 4.1. *For a state ρ and a positive operator σ*

$$D_{\min}(\rho||\sigma) \leq D_{\max}(\rho||\sigma). \tag{16}$$

Proof. Let π_ρ denote the projector onto the support of ρ, and let $\lambda \geq 0$ such that $D_{\max}(\rho||\sigma) = \log\lambda$, i.e., $\lambda\sigma - \rho \geq 0$. Then, using the fact that for positive semi-definite operators A and B, $\mathrm{Tr}(AB) \geq 0$, we get

$$0 \leq \mathrm{Tr}\big((\lambda\sigma - \rho)\pi_\rho\big) = \lambda\mathrm{Tr}(\pi_\rho\sigma) - 1.$$

Hence,

$$D_{\min}(\rho||\sigma) := -\log\mathrm{Tr}(\pi_\rho\sigma) \leq \log\lambda = D_{\max}(\rho||\sigma).$$

□

Lemma 4.2. *The min- and max-relative entropies are non-negative when both ρ and σ are states. They are both equal to zero when ρ and σ are identical states. Moreover, $D_{\min}(\rho||\sigma) = 0$ when ρ and σ have identical supports.*

Proof. Due to Lemma 4.1, it suffices to prove that $D_{\min}(\rho||\sigma) \geq 0$, when ρ and σ are states. Note that $\mathrm{Tr}(\pi_\rho\sigma) \leq \mathrm{Tr}\sigma = 1$, where π_ρ denotes the projector onto the support of ρ. Hence,

$$D_{\min}(\rho||\sigma) := -\log\mathrm{Tr}(\pi_\rho\sigma) \geq 0.$$

The rest of the lemma follows directly from the definitions (6) and (8) of the max- and min-relative entropies, respectively.

□

Lemma 4.3. *The min- and max-relative entropies are monotonic under CPTP maps, i.e., for a state ρ, a positive operator σ, and a CPTP map $\mathcal{T}$:*

$$D_{\min}(\mathcal{T}(\rho)||\mathcal{T}(\sigma)) \leq D_{\min}(\rho||\sigma) \tag{17}$$

and

$$D_{\max}(\mathcal{T}(\rho)||\mathcal{T}(\sigma)) \leq D_{\max}(\rho||\sigma). \tag{18}$$

Proof. The monotonicity (17) follows directly from the monotonicity of the quantum relative Rényi entropy. For $0 < \alpha < 1$, we have [29]:

$$S_\alpha(\rho||\sigma) \leq S_\alpha(\mathcal{T}(\rho)||\mathcal{T}(\sigma)).$$

Taking the limit $\alpha \to 0^+$ on both sides of this inequality and using (9), yields (17).

The proof of (18) is analogous to Lemma 3.1.12 of [15]. Let $\lambda \geq 0$ such that $\log\lambda = D_{\max}(\rho||\sigma)$ and hence $(\lambda\sigma - \rho) \geq 0$. Since $\mathcal{T}$ is a CPTP map, $\mathcal{T}(\lambda\sigma - \rho) = \lambda\mathcal{T}(\sigma) - \mathcal{T}(\rho) \geq 0$. Hence,

$$\begin{aligned} D_{\max}(\mathcal{T}(\rho)||\mathcal{T}(\sigma)) &:= \log\min\{\lambda' : \mathcal{T}(\rho) \leq \lambda'\mathcal{T}(\sigma)\} \\ &\leq \log\lambda = D_{\max}(\rho||\sigma). \end{aligned} \tag{19}$$

□

Lemma 4.4. *The min-relative entropy is jointly convex in its arguments.*

Proof. The proof follows from the monotonicity of the min-relative entropy under CPTP maps (Lemma 4.3). Following [29], let $\rho_1, \ldots \rho_n$ be states acting on a Hilbert space $\mathcal{H}$, let $\sigma_1, \ldots \sigma_n$ be positive operators in $\mathcal{B}(\mathcal{H})$ such that $\operatorname{supp}\rho_{\rm i} \subseteq \operatorname{supp}\sigma_{\rm i}$, for $i = 1, \ldots, n$, and let $\{p_i\}_{i=1}^n$ denote a probability distribution. Let $\rho, \sigma \in \mathcal{B}(\mathcal{H})$.

Consider the following operators in $\mathcal{B}(\mathcal{H} \otimes \mathbf{C}^n)$

$$A := \sum_{i=1}^n p_i A_i = \sum_{i=1}^n p_i |i\rangle\langle i| \otimes \rho_i,$$

$$B := \sum_{i=1}^n p_i B_i = \sum_{i=1}^n p_i |i\rangle\langle i| \otimes \sigma_i.$$

Note that the operators $A_i, B_j, i, j \in \{1, 2, \ldots n\}$, have orthogonal support for $i \neq j$, i.e.,

$$\mathrm{Tr} A_i A_j = 0 = \mathrm{Tr} A_i B_j = \mathrm{Tr} B_i B_j \quad \text{for } i \neq j. \tag{20}$$

Let π_A and π_i denote the orthogonal projectors onto the support of A and ρ_i, respectively, with $i = 1, 2, \ldots n$. Then using (20) and the convexity of the function

$-\log x$, we obtain

$$\begin{aligned} D_{\min}(A||B) &= -\log \mathrm{Tr}\big(\pi_A B\big) = -\log\big(\sum_{i=1}^{n} p_i \mathrm{Tr}(\pi_i \sigma_i)\big) \\ &\leq \sum_{i=1}^{n} p_i \big[-\log \mathrm{Tr}(\pi_i \sigma_i)\big] \\ &= \sum_{i=1}^{n} p_i D_{\min}(\rho_i||\sigma_i). \end{aligned} \tag{21}$$

Taking the partial traces of A and B over $\mathbf{C}^n$ yields the operators

$$\mathrm{Tr}_{\mathbf{C}^n} A = \sum_i p_i \rho_i \quad ; \quad \mathrm{Tr}_{\mathbf{C}^n} B = \sum_i p_i \sigma_i.$$

However, since the partial trace over $\mathbf{C}^n$ is a CPTP map, we have by Lemma 4.3 that

$$D_{\min}\Big(\sum_{i=1}^{n} p_i \rho_i || \sum_{i=1}^{n} p_i \sigma_i\Big) \leq D_{\min}(A||B) \tag{22}$$

The inequalities (21) and (22) yield the joint convexities:

$$D_{\min}\Big(\sum_{i=1}^{n} p_i \rho_i || \sum_{i=1}^{n} p_i \sigma_i\Big) \leq \sum_{i=1}^{n} p_i D_{\min}(\rho_i||\sigma_i) \tag{23}$$

□

Lemma 4.5. *The max-relative entropy of two mixtures of states, $\rho := \sum_{i=1}^{n} p_i \rho_i$ and $\sigma := \sum_{i=1}^{n} p_i \sigma_i$, satisfies the following bound:*

$$D_{\max}(\rho||\sigma) \leq \max_{1 \leq i \leq n} D_{\max}(\rho_i||\sigma_i) \tag{24}$$

Proof. By definition (7):

$$D_{\max}(\rho||\sigma) = \log \min\{\lambda : \mathrm{Tr}\big[P_+^{\lambda}(\rho - \lambda\sigma)\big] = 0\},$$

where $P_+^{\lambda} = \{\rho \geq \lambda\sigma\}$. Consider the projection operators $P_+^{\lambda,i} := \{\rho_i \geq \lambda\sigma_i\}$ for $i = 1, 2, \ldots, n$. Then

$$\begin{aligned} 0 \leq \mathrm{Tr}\big[P_+^{\lambda}(\rho - \lambda\sigma)\big] &= \sum_i p_i \mathrm{Tr}\big[P_+^{\lambda}(\rho_i - \lambda\sigma_i)\big] \\ &\leq \sum_i p_i \mathrm{Tr}\big[P_+^{\lambda,i}(\rho_i - \lambda\sigma_i)\big], \end{aligned} \tag{25}$$

by Lemma 2.1. Set $\lambda = \max_{1 \leq i \leq n} \lambda_i$ where for each $i = 1, 2, \ldots, n$, λ_i is defined by

$$\log \lambda_i = D_{\max}(\rho_i||\sigma_i).$$

For this choice of λ, each term in the sum on the right hand side of (25) vanishes, implying that $\mathrm{Tr}\big[P_+^{\lambda}(\rho - \lambda\sigma)\big] = 0$, and hence $\lambda \geq D_{\max}(\rho||\sigma)$. □

Lemma 4.6. *The min- and max-relative entropies of two states ρ and σ are related to the quantum relative entropy $S(\rho||\sigma) := \mathrm{Tr}\big[\rho\log\rho - \rho\log\sigma\big]$ as follows:*

$$D_{\min}(\rho||\sigma) \leq S(\rho||\sigma) \leq D_{\max}(\rho||\sigma). \tag{26}$$

Proof. We first prove the upper bound $S(\rho||\sigma) \leq D_{\max}(\rho||\sigma)$:

Let $\rho \leq 2^{\alpha}\sigma$, with $\alpha = D_{\max}(\rho||\sigma)$. Then using the operator monotonicity of the logarithm [31], we have $\log\rho \leq \alpha + \log\sigma$. This in turn implies that $\rho\log\sigma \geq \rho\log\rho - \alpha\rho$. Hence, for a state ρ, $\mathrm{Tr}\rho\log\sigma \geq \mathrm{Tr}\rho\log\rho - \alpha$, and

$$\begin{aligned} S(\rho||\sigma) &:= \mathrm{Tr}\rho\log\rho - \mathrm{Tr}\rho\log\sigma \\ &\leq \mathrm{Tr}\rho\log\rho - \mathrm{Tr}\rho\log\rho + \alpha \\ &= D_{\max}(\rho||\sigma). \end{aligned} \tag{27}$$

We next prove the bound $D_{\min}(\rho||\sigma) \leq S(\rho||\sigma)$:

Consider the CPTP map, $\mathcal{T}$, defined by

$$\mathcal{T}(\omega) = \pi_\rho\omega\pi_\rho + \overline{\pi_\rho}\omega\overline{\pi_\rho},$$

where ω is any density matrix, π_ρ is the projector onto the support of ρ, and $\overline{\pi_\rho} = I - \pi_\rho$. Note that $\mathcal{T}(\rho) = \rho$.

Due to the monotonicity of $S(\rho||\sigma)$ under CPTP maps, we have

$$\begin{aligned} S(\rho||\sigma) &\geq S(\mathcal{T}(\rho)||\mathcal{T}(\sigma)) \\ &= \mathrm{Tr}\rho\log\rho - \mathrm{Tr}\rho\log(\pi_\rho\sigma\pi_\rho) \\ &= S(\rho||\pi_\rho\sigma\pi_\rho). \end{aligned} \tag{28}$$

Define the normalized state $\widetilde{\sigma} := \dfrac{1}{c}\pi_\rho\sigma\pi_\rho$ where $c = \mathrm{Tr}(\pi_\rho\sigma)$. Then

$$\begin{aligned} S(\rho||\pi_\rho\sigma\pi_\rho) &= S(\rho||c\widetilde{\sigma}) \\ &= \mathrm{Tr}\rho(\log\rho - \log\widetilde{\sigma}) - (\log c).\mathrm{Tr}\rho \\ &= S(\rho||\widetilde{\sigma}) - \log c \\ &\geq -\log c = D_{\min}(\rho||\sigma). \end{aligned} \tag{29}$$

From (28) and (29) we conclude that $D_{\min}(\rho||\sigma) \leq S(\rho||\sigma)$. □

Lemma 4.7. *The min-relative entropy of two states ρ and σ for which* $\mathrm{supp}\,\rho \subseteq \mathrm{supp}\,\sigma$*, satisfies the following bounds:*

$$D_{\min}(\rho||\sigma) \leq D_{\max}(\rho||\sigma) \leq -\log\mu_{\min}(\sigma), \tag{30}$$

where $\mu_{\min}(\sigma)$ denotes the minimum non-zero eigenvalue of σ.

Proof. The first inequality in (30) has been proved in Lemma 4.1. Since $\mathrm{supp}\,\rho \subseteq \mathrm{supp}\,\sigma$, we have $\pi_\rho \leq \pi_\sigma$, where π_ρ and π_σ, denote the projectors onto the supports

of ρ and σ respectively. Further, using the bounds $\rho \leq \pi_\rho$ and $\pi_\sigma \leq \mu_{\min}(\sigma)^{-1}\sigma$, where $\mu_{\min}(\sigma)$ denotes the minimum non-zero eigenvalue of σ, we obtain

$$\rho \leq \mu_{\min}(\sigma)^{-1}\sigma.$$

Using the definition of $D_{\max}(\rho||\sigma)$ we therefore infer that $D_{\max}(\rho||\sigma) \leq -\log \mu_{\min}(\sigma)$.

The following lemma is obtained easily from the definitions of the min- and max-relative entropies.

Lemma 4.8. *The min- and max-relative entropies are invariant under joint unitary transformations.*

5. Min- and max-relative entropies and state discrimination

Consider the scenario of state discrimination. Suppose it is known that that a finite quantum system is in one of two states ρ and σ, with equal apriori probability. To determine which state it is in, one does a binary Postive Operator-Valued Measurement (POVM) with elements E and $(I - E)$. If the outcome corresponding to E occurs then the system is inferred to be in the state ρ, whereas if the outcome corresponding to $(I - E)$ occurs, then the system is inferred to be in the state σ.

If the supports of the states ρ and σ are not mutually orthogonal, then there are two types of error which may occur. One might infer that the state is ρ when it is actually σ or vice versa. In the language of hypothesis testing, these are referred to as the *Type I error* and *Type II error* respectively, and their corresponding probabilties are given by

$$\alpha := \mathrm{Tr}\big((I - E)\rho\big)\,; \quad \beta := \mathrm{Tr}\big(E\sigma\big).$$

Moreover, the average probability of error is given by

$$p_e^{av} = \frac{1}{2}(\mathrm{Tr}(I - E)\rho + \mathrm{Tr}E\sigma). \tag{31}$$

Now consider a POVM in which $E = \pi_\rho$ (the projector onto the support of ρ). In this case, the *Type I error* vanishes and the *Type II error* is given by

$$\beta = \mathrm{Tr}(\pi_\rho\sigma) = 2^{-D_{\min}(\rho||\sigma)}.$$

Hence, $D_{\min}(\rho||\sigma)$ is equal to the negative of the logarithm of the *Type II error* when the *Type I error* is equal to zero.

Further, if $E = \pi_\rho$, the average probability of error is given by $p_e^{av} = \frac{1}{2}\mathrm{Tr}(\pi_\rho\sigma)$. However, by Helstrom's Theorem [32] the minimum possible value of p_e^{av} is given by

$$\frac{1}{2}\big[1 - \frac{1}{2}||\rho - \sigma||_1\big].$$

This yields the bound

$$\mathrm{Tr}(\pi_\rho\sigma) \geq \big[1 - \frac{1}{2}||\rho - \sigma||_1\big], \tag{32}$$

which in turn implies that

$$D_{\min}(\rho||\sigma) \leq -\log\big[1 - \frac{1}{2}||\rho - \sigma||_1\big].$$

Note that (32) can also be proved algebraically by a simple use of Lemma 2.1. □

It is known that if one has asymptotically many copies of two states ρ and σ, the error in discriminating between them decreases exponentially, and the error exponent is given by the so-called quantum Chernoff bound $\xi(\rho, \sigma)$ [33]. The latter has been shown to be given by $\xi(\rho, \sigma) = -\log\big(\min_{0\leq s\leq 1} \mathrm{Tr}\rho^s\sigma^{1-s}\big)$. From the expression (9) it follows that the min-relative entropy provides a lower bound to the quantum Chernoff bound, i.e.,

$$\xi(\rho, \sigma) \geq D_{\min}(\rho||\sigma).$$

The max-relative entropy, on the other hand is related to the optimal Bayesian error probability, in determining which one of a finite number (say M) of known states a given quantum system is prepared in. Suppose the quantum system is prepared in the k^{th} state, ρ_k, with apriori probability p_k, and the optimisation is over all possible choices of POVMs which could be made on the system to determine its state. Then the optimal Bayesian probability of error is given by

$$P_{av} = 1 - \inf_{\sigma} \max_{1\leq k\leq M} p_k 2^{D_{max}(\rho_k||\sigma)},$$

where the infimum is taken over all possible quantum states, σ, in the Hilbert space of the system. This operational interpretation, was first provided in [34] though in a somewhat different formalism. It is also explained in [30].

6. The min- and max-relative entropies of entanglement

An entanglement monotone is a measure of how entangled a state is*. There are certain properties which an entanglement monotone $E(\rho)$ of any bipartite state ρ should satisfy: (i) $E(\rho) = 0$ if ρ is separable; (ii) $E(\rho)$ is unchanged by a local change of basis and (iii) $E(\rho)$ does not increase under local operations and classical communication (LOCC). The property (iii) is a consequence of the fact that entanglement cannot be created or increased by LOCC.

In addition, an entanglement monotone is said to be a *full* entanglement monotone if it does not increase *on average* under LOCC, that is, if an LOCC map on a bipartite quantum state ρ results in a state ρ_i with probability p_i, then $E(\rho) \geq \sum_i p_i E(\rho_i)$.

One possible way of defining an entanglement monotone of a bipartite state ρ is in terms of its "distance" from the set of separable states. An important entanglement monotone is the relative entropy of entanglement $E_R(\rho)$ [35] in which the

*In this paper we will restrict our attention to bipartite states alone.

"distance" is measured in terms of the quantum relative entropy:

$$E_R(\rho) := \min_{\sigma \in \mathcal{S}} S(\rho||\sigma),$$

the minimum being taken over the set $\mathcal{S}$ of all separable states (see also [36]).

Analogously, the min- and max-relative entropies lead us to the define two new quantities, namely, the min- and max-relative entropies of entanglement, which can indeed be proved to be entanglement monotones.

Definition 6.1. For a bipartite state $\rho \in \mathcal{D}(\mathcal{H}_A \otimes \mathcal{H}_B)$, the min-relative entropy of entanglement is defined as [37]

$$E_{\min}(\rho) := \min_{\sigma \in \mathcal{S}} D_{\min}(\rho||\sigma), \tag{33}$$

where the minimum is taken over the set $\mathcal{S}$ of all separable states.

Definition 6.2. For a bipartite state $\rho \in \mathcal{D}(\mathcal{H}_A \otimes \mathcal{H}_B)$, the max-relative entropy of entanglement is defined as [27, 37]

$$E_{\max}(\rho) := \min_{\sigma \in \mathcal{S}} D_{\max}(\rho||\sigma), \tag{34}$$

where the minimum is taken over the set $\mathcal{S}$ of all separable states.

To prove properties (i) and (ii) above, it suffices to prove that $D_{\min}(\rho||\sigma)$ and $D_{\max}(\rho||\sigma)$ satisfy the following properties: for $* \in \{\min, \max\}$

(1) $D_*(\rho||\sigma) \geq 0$ with equality if $\rho = \sigma$.
(2) $D_*(\rho||\sigma) = D_*(U\rho U^\dagger||U\sigma U^\dagger)$ for any unitary operator U.
(3) $D_*(\Lambda(\rho)||\Lambda(\sigma)) \leq D_*(\rho||\sigma)$ for any LOCC map Λ

Proof of (1): It is evident from the definition (8) of $D_{\min}(\rho||\sigma)$ that if $\rho = \sigma$ then $D_{\min}(\rho||\sigma) = 0$, since then the projections on the supports of ρ and σ are identical.

For the case of $D_{\max}(\rho||\sigma)$ we have the stronger property that $D_{\max}(\rho||\sigma) = 0$ if and only if $\rho = \sigma$. This can be seen as follows: From Lemma 4.2 we have that if $\rho = \sigma$ then $D_{\max}(\rho||\sigma) = 0$. To prove the converse, i.e., $D_{\max}(\rho||\sigma) = 0$ implies that $\rho = \sigma$, note that $D_{\max}(\rho||\sigma) = 0 \implies (\sigma - \rho) \geq 0$. On the other hand, since ρ and σ are states, we have $\mathrm{Tr}(\sigma - \rho) = 0$, which in turn implies that $(\sigma - \rho) = 0$.

Proof of (2): This follows simply from Lemma 4.8.

Proof of (3): This follows from Lemma 4.3, since the partial trace is a CPTP map.

In addition, $E_{\max}(\rho)$ is a full entanglement monotone as is proved here: let an LOCC map Λ have the following Kraus representation

$$\Lambda(\rho) = \sum_i A_i \rho A_i^\dagger, \tag{35}$$

where ρ denotes a bipartite state. To prove that $E_{\max}(\rho)$ is a full entanglement monotone it suffices to prove that for bipartite states ρ and σ

$$\sum_i p_i D_{\max}\Big(\frac{\rho_i}{p_i}||\frac{\sigma_i}{q_i}\Big) \leq D_{\max}(\rho||\sigma), \tag{36}$$

where

$$\rho_i = A_i \rho A_i^\dagger \quad ; \quad \sigma_i = A_i \sigma A_i^\dagger \quad ; \quad p_i := \mathrm{Tr}\rho_i, \quad ; \quad q_i := \mathrm{Tr}\sigma_i. \tag{37}$$

This is because of the following. Let $E_{\max}(\rho) = D_{\max}(\rho||\sigma^*)$, i.e., let the minimum of $D_{\max}(\rho||\sigma)$, over all separable states σ, be attained at σ^*. Then from (36) we have

$$\begin{aligned} E_{\max}(\rho) = D_{\max}(\rho||\sigma^*) &\geq \sum_i p_i D_{\max}\Big(\frac{\rho_i}{p_i}||\frac{A_i^\dagger \sigma^* A_i}{\mathrm{Tr}(A_i^\dagger \sigma^* A_i)}\Big) \\ &\geq \sum_i p_i E_{\max}\Big(\frac{\rho_i}{p_i}\Big), \end{aligned}$$

since for each i, $(A_i^\dagger \sigma^* A_i)/\mathrm{Tr}(A_i^\dagger \sigma^* A_i)$ is a normalized, separable state.

Proof of (36): From (6) it follows that

$$\begin{aligned} D_{\max}\Big(\frac{\rho_i}{p_i}||\frac{\sigma_i}{q_i}\Big) &= \log \lambda_{\max}\Big(\big(\frac{\sigma_i}{q_i}\big)^{-\frac{1}{2}} \frac{\rho_i}{p_i} \big(\frac{\sigma_i}{q_i}\big)^{-\frac{1}{2}}\Big) \\ &= \log\Big(\frac{q_i}{p_i}\lambda_{\max}\big(\sigma_i^{-\frac{1}{2}} \rho_i \sigma_i^{-\frac{1}{2}}\big)\Big) \\ &= -\log\frac{p_i}{q_i} + D_{\max}(\rho_i||\sigma_i) \end{aligned} \tag{38}$$

Hence, denoting the Kullback-Leibler divergence of the probability distributions $\{p_i\}$ and $\{q_i\}$ as

$$D\Big(\{p_i\}||\{q_i\}\Big) := \sum_i p_i \log\frac{p_i}{q_i},$$

we have

$$\begin{aligned} \text{LHS of (36)} &= -D\big(\{p_i\}||\{q_i\}\big) + \sum_i p_i D_{\max}(\rho_i||\sigma_i) \\ &\leq \max_i D_{\max}(\rho_i||\sigma_i) \\ &\leq D_{\max}(\rho||\sigma). \end{aligned} \tag{39}$$

The first inequality follows from the non-negativity of the Kullback-Leibler divergence. The last inequality follows from the fact that $D_{\max}(\rho_i||\sigma_i) \leq D_{\max}(\rho||\sigma)$ $\forall$ i. This is because for $\lambda = D_{\max}(\rho||\sigma)$ we have $\rho \leq \lambda\sigma$, and this implies $A_i \rho A_i^\dagger \leq \lambda A_i \sigma A_i^\dagger$ for this value of λ. Hence, $D_{\max}(\rho_i||\sigma_i) \leq D_{\max}(\rho||\sigma)$.

Note, however, that $E_{\min}(\rho)$ is not a full entanglement monotone. This can be proved by showing that $E_{\min}(\rho)$ violates the requirement (Lemma 1 of [38]) that any full entanglement monotone, when evaluated on a pure state, should be a concave function of its partial trace. This can be seen as follows. For a pure state $\rho = |\psi\rangle\langle\psi| \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$, $E_{\min}(\rho) = -\log\lambda_{\max}(\rho_\psi^A)$, where $\rho_\psi^A = \mathrm{Tr}_B|\psi\rangle\langle\psi|$, and $\lambda_{\max}(\rho_\psi^A)$ denotes its maximum eigenvalue. Since the maximum eigenvalue of a density matrix is a convex function, as is the negative of the logarithm, $E_{\min}(\rho)$ is a *convex* function of ρ_ψ^A.

The min- and max-relative entropies of entanglement are both equal to 1 for a Bell state. This follows simply from the definitions of $E_{\min}(\rho)$ and $E_{\max}(\rho)$.

In [37] we proved that for a bipartite pure state $\rho = |\psi_{AB}\rangle\langle\psi_{AB}|$, $E_{\max}(\rho)$ is equal to the logarithmic negativity [39], which is defined as follows

$$LN(\rho) := \log ||\rho^{\Gamma}||_1,$$

where ρ^{Γ} denotes the partial transpose of ρ with respect to the subsystem A, and $||\omega||_1 = \mathrm{Tr}\sqrt{w^{\dagger}\omega}$. Further, it was proved in [37] that for an arbitrary bipartite state $\rho \in \mathcal{D}(\mathcal{H})$, where $\mathcal{H} \simeq \mathcal{H}_A \otimes \mathcal{H}_B$, $E_{\max}(\rho)$ is equal to its *global log robustness* of entanglement [40], which is defined as follows:

$$LR_g(\rho) := \log\big(1 + R_g(\rho)\big), \tag{40}$$

where $R_g(\rho)$ is the *global robustness of entanglement* [41], given by

$$R_g(\rho) = \min_{s\in\mathbb{R}}\Big(s : \exists\, \omega \in \mathcal{D}(\mathcal{H}) \text{ s.t. } \frac{1}{1+s}\rho + \frac{s}{1+s}\omega \in \mathcal{S}(\mathcal{H})\Big),$$

with $\mathcal{S}(\mathcal{H}) \subset \mathcal{D}(\mathcal{H})$ denoting the set of separable states.

7. Smoothed min- and max-relative entropies of entanglement and their operational interpretations

We define smoothed versions of $E_{\min}(\rho)$ and $E_{\max}(\rho)$ as follows:

Definition 7.1. For any $\varepsilon > 0$, the smoothed max-relative entropy of entanglement of a bipartite state $\rho \in \mathcal{D}(\mathcal{H}_A \otimes \mathcal{H}_B)$ is given by

$$E^{\varepsilon}_{\max}(\rho) := \min_{\bar{\rho}\in B^{\varepsilon}(\rho)} E_{\max}(\bar{\rho}), \tag{41}$$

where $B^{\varepsilon}(\rho) := \{\bar{\rho} \in \mathcal{D}(\mathcal{H}) : F(\bar{\rho}, \rho) \geq 1 - \varepsilon\}$.

The smoothed min-relative entropy of entanglement of $\rho \in \mathcal{D}(\mathcal{H}_A \otimes \mathcal{H}_B)$ is defined as

$$E^{\varepsilon}_{\min}(\rho) := \max_{\substack{0\leq A\leq I \\ \mathrm{Tr}(A\rho)\geq 1-\varepsilon}} \min_{\sigma\in\mathcal{S}} \left(-\log \mathrm{Tr}(A\sigma)\right). \tag{42}$$

The smoothed min- and max-relative entropies of entanglement have interesting operational significances in entanglement manipulation under the so-called *separability preserving maps* (which are defined below) [42]. Entanglement manipulation is the process by which Alice and Bob convert an initial bipartite state ρ_{AB} which they share, to a desired target state σ_{AB} using local operations and classical communication (LOCC). If the target state σ_{AB} is a maximally entangled state, then the protocol is called entanglement distillation, whereas if the initial state ρ_{AB} is a maximally entangled state, then the protocol is called entanglement dilution. Optimal rates of these protocols (which are referred to as the *distillable entanglement* and the *entanglement cost*, respectively) were originally evaluated under the assumption that the entanglement resource accessible to Alice and Bob consist of

multiple copies, i.e., tensor products $\rho_{AB}^{\otimes n}$, of the initial bipartite state ρ_{AB}, and the requirement that the final state of the protocol is equal to n copies of the desired target state $\sigma_{AB}^{\otimes n}$ with asymptotically vanishing error in the limit $n \to \infty$.

The smoothed min- and max-relative entropies of entanglement are related to the optimal rates of entanglement manipulation under *separability preserving maps* (as opposed to LOCC) in the *single copy* (or one-shot) regime. Separability preserving maps maps constitute the largest class of CPTP maps which yield a separable state when acting on a separable state. Every LOCC map is separability preserving but the converse is not true.

Definition 7.2. A CPTP map Λ is said to be a separability preserving map if $\Lambda(\sigma)$ is separable for any separable state σ. We denote the class of such maps as SEPP. (The acronym comes from the name *separability preserving.*)

Definition 7.3. For any given $\delta > 0$ we say a map Λ is a δ-separability preserving map if $R_G(\Lambda(\sigma)) \leq \delta$ for every separable state σ. We denote the class of such maps as δ-SEPP.

Entanglement manipulation (under SEPP) in the one-shot scenario, is the process by which Alice and Bob convert an initial bipartite state which they share, to a desired target state using separability-preserving maps. As in the case of LOCC, the process is referred to as entanglement dilution (under SEPP) if the initial state is maximally entangled, and as entanglement distillation (under SEPP) if the final state is maximally entangled.

In the sequel, we denote the pure state density matrix corresponding to a maximally entangled state of rank M by Ψ_M, i.e., $\Psi_M = |\Psi_M\rangle\langle\Psi_M|$, with

$$|\Psi_M\rangle := \frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i_A\rangle \otimes |i_B\rangle, \tag{43}$$

where $\{|i_A\rangle\}$ and $\{|i_B\rangle\}$ denote orthonormal bases in isomorphic Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$.

We first give the definitions of one-shot entanglement cost and distillable entanglement under SEPP.

Definition 7.4. The one-shot entanglement cost of a bipartite state ρ under SEPP maps is defined as

$$E_{C,\mathrm{SEPP}}^{(1),\varepsilon}(\rho) := \min_{M,\Lambda} \{\log M : F(\rho, \Lambda(\Psi_M)) \geq 1 - \varepsilon, \Lambda \in \mathrm{SEPP}, M \in \mathbb{Z}^+\}. \tag{44}$$

Definition 7.5. The one-shot distillable entanglement of a bipartite state ρ under SEPP maps is defined as

$$E_{D,\mathrm{SEPP}}^{(1),\varepsilon}(\rho) := \max_{M,\Lambda} \{\log M : F(\Lambda(\rho), \Psi_M) \geq 1 - \varepsilon, \Lambda \in \mathrm{SEPP}, M \in \mathbb{Z}^+\}. \tag{45}$$

We also consider a *catalytic* version of entanglement dilution under δ-SEPP. This is the entanglement dilution process in which Alice and Bob initially share an *extra* maximally entangled state Ψ_K (say of rank K) which is not consumed in the process but instead is retrieved unchanged at the end of the protocol. It therefore acts as a catalyst.

Definition 7.6. For any $\delta > 0$, the one-shot catalytic entanglement cost of ρ under $\delta -$ SEPP maps is defined as

$$\tilde{E}^{(1),\varepsilon}_{C,\mathrm{SEPP}}(\rho) := \min_{M,K,\Lambda}\{\log M : \Lambda(\Psi_M \otimes \Psi_K) = \rho' \otimes \Psi_K, \\ F(\rho,\rho') \geq 1-\varepsilon, \Lambda \in \mathrm{SEPP}, M, K \in \mathbb{Z}^+\}. \tag{46}$$

As proved in [42] the one-shot distillable entanglement of ρ under SEPP can be identified with its smoothed min-relative entropy of entanglement, whereas bounds on the one-shot catalytic entanglement cost of ρ under $\delta -$ SEPP, for any $\delta > 0$, are given in terms of the smoothed max-relative entropy of entanglement. For sake of completeness, we give the statements of the relevant theorems (which were proved in [42]) below:

The first theorem relates the smoothed min-relative entropy of entanglement to the one-shot distillable entanglement under SEPP.

Theorem 7.1. *For any state ρ and any $\varepsilon \geq 0$,*

$$\lfloor E^{\varepsilon}_{\min}(\rho) \rfloor \leq E^{(1),\varepsilon}_{D,SEPP}(\rho) \leq E^{\varepsilon}_{\min}(\rho). \tag{47}$$

The next theorem relates the smoothed max-relative entropy of entanglement to the one-shot catalytic entanglement cost under δ-SEPP.

Theorem 7.2. *For any $\delta, \varepsilon > 0$ there exists a positive integer K, such that for any state ρ*

$$E^{\varepsilon}_{\max}(\rho \otimes \Psi_K) - \log K - \log(1+\delta) \leq \widetilde{E}^{(1),\varepsilon}_{C,\delta-SEPP}(\rho) \\ \leq E^{\varepsilon}_{\max}(\rho \otimes \Psi_K) - \log(1-\varepsilon) - \log K + 1. \tag{48}$$

In particular, we can take $K = \lceil 1 + \delta^{-1} \rceil$.

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BINDING, STABILITY, AND NON-BINDING OF MULTI-POLARON SYSTEMS

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To Ari Laptev, friend and mentor, on the occasion of his 60th birthday

The binding of polarons, or its absence, is an old and subtle topic. After defining the model we state some recent theorems of ours. First, the transition from many-body collapse to the existence of a thermodynamic limit for N polarons occurs precisely at $U = 2\alpha$, where U is the electronic Coulomb repulsion and α is the polaron coupling constant. Second, if U is large enough, there is no multi-polaron binding of any kind. We also discuss the Pekar-Tomasevich approximation to the ground state energy, which is valid for large α. Finally, we derive exact results, not reported before, about the one-dimensional toy model introduced by E. P. Gross.

Keywords: Polaron; binding energies; stability; Coulomb system; Lieb-Thirring inequality.

1. Definition and previous rigorous results

The large polaron, first considered by H. Fröhlich [6] in 1937, is a model of an electron moving in three dimensions and interacting with the quantized optical

modes of a polar crystal. (It is called 'large' because the size of the electronic wave function is large compared to the crystal lattice spacing, so a continuum approximation is appropriate.) It is also a simple quantum field theory model and over the years has been used as a testing ground for various approximations.

In suitable units, its Hamiltonian is

$$H^{(1)} = \mathbf{p}^2 + \int_{\mathbb{R}^3} a^\dagger(\mathbf{k}) a(\mathbf{k})\, d\mathbf{k} + \frac{\sqrt{\alpha}}{\sqrt{2}\,\pi} \int_{\mathbb{R}^3} \frac{1}{|\mathbf{k}|} [a(\mathbf{k}) \exp(i\mathbf{k}\cdot\mathbf{x}) + h.c.]\, d\mathbf{k}\,. \qquad (1)$$

This Hamiltonian acts in the Hilbert space $L^2(\mathbb{R}^3) \otimes \mathcal{F}$, where $\mathcal{F}$ is the bosonic Fock space for the longitudinal optical modes of the crystal, with scalar creation and annihilation operators $a^\dagger(\mathbf{k})$ and $a(\mathbf{k})$ satisfying $[a(\mathbf{k}), a^\dagger(\mathbf{k}')] = \delta(\mathbf{k}-\mathbf{k}')$. The momentum of an electron is $\mathbf{p} = -i\nabla$, and the coupling constant is $\alpha > 0$. (Other authors have used a different convention, where α is replaced by $\alpha/\sqrt{2}$ [1, 6].)

The ground state energy $E^{(1)}(\alpha)$ is the infimum of the spectrum of $H^{(1)}$. Because of translation invariance, $E^{(1)}(\alpha)$ cannot be expected to be an eigenvalue, and indeed it is not [7, 8]. The following rigorous results concerning $E^{(1)}(\alpha)$ will be important in our analysis.

(i) For all α,

$$-\alpha - \alpha^2/3 \leq E^{(1)}(\alpha) \leq -\alpha\,.$$

These upper and lower bounds are in [11, 14, 15] and [23], respectively. As a consequence, $E^{(1)}(\alpha) \sim -\alpha$ for α small.

(ii) Pekar [25], using a product function, showed that

$$E^{(1)}(\alpha) \leq -C_P \alpha^2\,,$$

for all α. The lower bound

$$E^{(1)}(\alpha) \geq -C_P \alpha^2 - \text{const}\ \alpha^{9/5}$$

for large α was proved in [21]. It was proved earlier in [2], but without the $\alpha^{9/5}$-error estimate. Here, $C_P = 0.109$ [24] is the number determined by Pekar's variational problem for the electron density,

$$C_P = \inf \left\{ \int_{\mathbb{R}^3} |\nabla\psi|^2\, d\mathbf{x} - \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\psi(\mathbf{x})|^2\, |\psi(\mathbf{y})|^2}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{x}\, d\mathbf{y} : \|\psi\|_2 = 1 \right\}. \qquad (2)$$

The minimizing ψ is unique up to translations (and a trivial phase) [16].

(iii) There is a representation for $E^{(1)}(\alpha)$ in terms of path integrals. In terms of the partition function $Z^{(1)}(T) = \text{Tr}\exp\big(-TH^{(1)}\big)$, one has $E^{(1)}(\alpha) = -\lim_{T\to\infty} T^{-1} \log Z^{(1)}(T)$. (Strictly speaking, $Z^{(1)}(T)$ does not exist because of the translation invariance of $H_0^{(1)}$ and the infinite number of phonon modes. These technicalities can be handled by inserting appropriate cutoffs, to be removed at the end of the calculation [26, 31].) It was shown in [3] that after one

integrates out the phonon variables, $Z^{(1)}(T)$ has a functional integral representation

$$Z^{(1)}(T) = \int d\mu \exp\left[\frac{\alpha}{2}\int_0^T\int_0^T \frac{e^{-|t-s|}\,dt\,ds}{|\mathbf{x}(t)-\mathbf{x}(s)|}\right], \tag{3}$$

where $d\mu$ is Wiener measure on all T-periodic paths $\mathbf{x}(t)$. (In physics notation $d\mu = \exp(-\int_0^T \dot{\mathbf{x}}(t)^2\,dt)\,d\,\text{path}$. Strictly speaking, $t-s$ has to be understood modulo T, but this is irrelevant as $T\to\infty$.)

2. The multi-polaron problem and new results

Of great physical interest is the binding energy of N polarons, with Hamiltonian

$$H_U^{(N)} = \sum_{j=1}^N \mathbf{p}_j^2 + \int a^\dagger(\mathbf{k})a(\mathbf{k})\,d\mathbf{k} + \frac{\sqrt{\alpha}}{\sqrt{2}\,\pi}\sum_{j=1}^N \int \frac{1}{|\mathbf{k}|}[a(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{x}_j) + h.c.]\,d\mathbf{k} + U\sum_{1\le i<j\le N}|\mathbf{x}_i-\mathbf{x}_j|^{-1} \tag{4}$$

and ground state energy $E_U^{(N)}(\alpha)$. We ignore Fermi statistics for the electrons, because its imposition changes things only quantitatively, not qualitatively. The Coulomb repulsion parameter $U\ge 0$ is equal to e^2. The derivation of $H_U^{(N)}$ in [6] implies that $U > 2\alpha$, and this is crucial for thermodynamic stability, as we shall see.

The generalization of (3) is

$$Z_U^{(N)}(T) = \int d\mu^{(N)} \exp\Big(\frac{\alpha}{2}\sum_{i,j}\int_0^T\int_0^T \frac{e^{-|t-s|}\,dt\,ds}{|\mathbf{x}_i(t)-\mathbf{x}_j(s)|} - U\sum_{i<j}\int_0^T \frac{dt}{|\mathbf{x}_i(t)-\mathbf{x}_j(t)|}\Big), \tag{5}$$

where $d\mu^{(N)}$ is Wiener measure on all T-periodic paths $(\mathbf{x}_1(t),\dots,\mathbf{x}_N(t))$. This is relevant for us since $E_U^{(N)}(\alpha) = -\lim_{T\to\infty} T^{-1}\log Z_U^{(N)}(T)$.

The generalization of the Pekar approximation (2) to the N-electron case is the minimization of the following Pekar-Tomasevich functional for normalized functions ψ on $\mathbb{R}^{3N}$,

$$\sum_{i=1}^N \int_{\mathbb{R}^{3N}} |\nabla_i\psi|^2\,dX + U\sum_{i<j}\int_{\mathbb{R}^{3N}} \frac{|\psi(X)|^2}{|\mathbf{x}_i-\mathbf{x}_j|}\,dX - \alpha\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_\psi(\mathbf{x})\,\rho_\psi(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}\,d\mathbf{y}\,,$$

where $dX = \prod_{k=1}^N d\mathbf{x}_k$. The density ρ_ψ of ψ is defined as usual by

$$\rho_\psi(\mathbf{x}) = \sum_{i=1}^N \int_{\mathbb{R}^{3(N-1)}} |\psi(\mathbf{x}_1,\dots,\mathbf{x},\dots,\mathbf{x}_N)|^2\,d\mathbf{x}_1\cdots\widehat{d\mathbf{x}_i}\cdots d\mathbf{x}_N$$

with $\mathbf{x}$ at the i-th position, and $\widehat{d\mathbf{x}_i}$ meaning that $d\mathbf{x}_i$ has to be omitted in the product $\prod_{k=1}^N d\mathbf{x}_k$. This minimization problem is obtained from the original problem of minimizing $\langle\Psi, H_U^{(N)}\Psi\rangle$ by restricting the allowed Ψ's to be of the form $\psi\otimes\Phi$,

where $\psi \in L^2(\mathbb{R}^{3N})$, $\Phi \in \mathcal{F}$, and both ψ and Φ are normalized. Since the Pekar-Tomasevich functional is the result of a variational calculation, its energy gives an upper bound to the ground state energy $E_U^{(N)}(\alpha)$.

2.1. *Binding of multi-polaron systems*

We first consider the bipolaron binding energy $\Delta E_U(\alpha) = 2E^{(1)}(\alpha) - E_U^{(2)}(\alpha)$. For some time this was thought to be zero for all $U \geq 2\alpha$, on the basis of an inadequate variational calculation, but it is now known [1] to be positive for some $U > 2\alpha$. The first question we address is whether $\Delta E_U(\alpha) = 0$ for U sufficiently large. It is understood that the effective interaction induced by the phonon field for two polarons at large distances d is approximately Coulomb-like $-2\alpha/d$, but this alone does not preclude binding. (The reason for $2\alpha \cdot \text{distance}^{-1}$ can be seen from the Wiener integral representation (5), where there is a factor $\alpha/2$, but the pair (i, j) appears twice, and the integral $\int_{\mathbb{R}} e^{-|t-s|}\, ds = 2$.) The known existence of bipolarons for some $U > 2\alpha$ is an effect of correlations. It is *a priori* conceivable that correlations lead to an effective attraction that is stronger than Coulomb at large distances. If it were, for example, equal to $(2\alpha/d)\log(\log(\log(d)))$, then this minuscule perturbation of Coulomb's law, which would be virtually undetectable by a variational calculation, would result in binding for *all* U. The absence of binding is a problem that has resisted a definitive resolution for many years. The following was proved in [4, 5]:

Theorem 2.1 (Absence of binding for bipolarons). *Let $N = 2$. For some constant $C < 26.6$,*

$$E_U^{(2)}(\alpha) = 2E^{(1)}(\alpha) \tag{6}$$

whenever $U \geq 2C\alpha$.

The constant 26.6 vastly exceeds the current, non-rigorous estimates of about 1.15 [27, 33], so it is an *open problem* to find a more accurate rigorous bound.

The existence of a critical repulsion strength for a bipolaron is consistent with the idea that the attractive interaction induced by the field is Coulomb-like, and therefore one expects that there is an N-independent $U_c(\alpha)$ such that there is no binding of any kind when $U > U_c(\alpha)$. This was proved in [4, 5] as well.

Theorem 2.2 (Absence of binding for N polarons). *For given $\alpha > 0$ there is a finite $U_c(\alpha) > 2\alpha$ such that*

$$E_U^{(N)}(\alpha) = NE^{(1)}(\alpha) \quad \textit{for all } N \geq 2 \tag{7}$$

whenever $U \geq U_c(\alpha)$.

Remark 2.1. If $U > U_c(\alpha)$, then given (7) and any normalized ψ

$$\left\langle \psi \middle| H_U^{(N)} \middle| \psi \right\rangle \geq NE^{(1)}(\alpha) + (U - U_c(\alpha)) \left\langle \psi \middle| \sum_{i<j} |\mathbf{x}_i - \mathbf{x}_j|^{-1} \middle| \psi \right\rangle. \tag{8}$$

This inequality gives a quantitative estimate of the energy penalty needed to bring two or more particles within a finite distance of each other. In particular, it implies that for $U > U_c(\alpha)$ there cannot be a normalizable ground state, even in a fixed momentum sector. Inequality (8) is not only true for our bound on $U_c(\alpha)$, but also for the (unknown) exact value of the critical repulsion parameter.

We state Theorem 2.1 separately for two reasons: One is that the proof is easier than for the general N case. The second is that we have an upper bound on $U_c(\alpha)$ that is linear in α. While our N-polaron bound is linear in α for large α, we have not achieved this linear bound for small α and this remains an *open problem*.

2.2. *Thermodynamic stability of multi-polaron systems*

The second problem we consider is the existence of the thermodynamic limit. For large N, physical intuition suggests that $E_U^{(N)}(\alpha) \sim -\text{const } N$. This supposition is known to be false if $U < 2\alpha$. Indeed, it was shown in [9] that, even with the Pauli principle, $E_U^{(N)}(\alpha) \sim -\text{const } N^{7/3}$ when $U < 2\alpha$. Absent the Pauli principle, $E_U^{(N)}(\alpha)$ would behave even worse, as $-\text{const } N^3$. It is also known [9] that $E_U^{(N)}(\alpha) \geq -\text{const } N^2$ if $U > 2\alpha$. The latter bound ought to be $-\text{const } N$ instead, and in [4, 5] we proved that this is indeed the case for all $U > 2\alpha$.

Theorem 2.3 (Thermodynamic stability for $U > 2\alpha$). *For given $U > 2\alpha > 0$, $N^{-1}E_U^{(N)}(\alpha)$ is bounded independently of N.*

Our lower bound on $N^{-1}E_U^{(N)}(\alpha)$ goes to $-\infty$ as $U \searrow 2\alpha$, but we are not claiming that this reflects the true state of affairs. Whether $\lim_{N\to\infty} N^{-1}E_{2\alpha}^{(N)}(\alpha)$ is finite or not remains an *open problem*. There are partial results in the Pekar-Tomasevich approximation [9].

The linear lower bound from Theorem 2.3, together with the sub-additivity of the energy [9], [20, Sec. 14.2], i.e.,

$$E_U^{(N+M)}(\alpha) \leq E_U^{(N)}(\alpha) + E_U^{(M)}(\alpha)\,, \tag{9}$$

implies:

Corollary 2.1 (Thermodynamic limit for $U > 2\alpha$). *For given $U > 2\alpha > 0$, $\lim_{N\to\infty} N^{-1}E_U^{(N)}(\alpha)$ exists.*

For U in the range $2\alpha < U < U_c(\alpha)$, there are bound states of an undetermined nature. Does the system become a gas of bipolarons, or does it coalesce into a true N-particle bound state? If the latter, does this state exhibit a periodic structure, thereby forming a super-crystal on top of the underlying lattice of atoms? This is perhaps the physically most interesting *open problem*. While particle statistics does not play any role for our main results, the answer to this question will crucially depend on particle statistics (Bose or Fermi) [29, 30].

3. Absence of bipolaron binding

In order to give the flavor of our methods, we sketch the proof of Theorem 2.1, as given in [4], ©Amer. Phys. Soc. The proofs of the other two theorems are also sketched in [4].

The proof of Theorem 1 is conveniently structured in 4 steps.

Step 1. Partition of the interparticle distance: We fix a length ℓ, whose value will later be chosen proportional to α^{-1}, and partition the relative distance $r = |\mathbf{x}_1 - \mathbf{x}_2|$ between the particles into spherical shell-like regions of radial size $2^{k-1}\ell \leq r \leq 2^k\ell$ with $k = 1, 2, \ldots$. This partitioning is one of the key points of our analysis. In addition there is the $k = 0$ region, where the particle separation is between zero and ℓ. Because of the uncertainty principle these regions have to overlap a bit, but this can be easily handled, and we ignore it for the sake of simplicity. There is a kinetic energy cost for localizing the particles according to this partition, which is $c_1 2^{-2k}\ell^{-2}$ in the shell k. In the next step we look at the energy of the particles localized to one of these shell-like regions.

Step 2. Further localization for well-separated particles: For $k \geq 1$ we further localize the particles into individual boxes of size $2^{k-3}\ell$. This costs another localization error $c_2 2^{-2k}\ell^{-2}$. Because the separation exceeds $2^{k-1}\ell$, the two particles cannot be in the same or neighboring boxes. From the path integral (5), but now with the $\mathbf{x}_i(t)$'s constrained to their respective boxes, we see that *the separated particles feel an effective Coulomb-like attractive potential.* However, this can contribute at worst $-c_3\alpha 2^{-k}\ell^{-1}$ to the energy. But the Coulomb repulsion is at least $U2^{-k}\ell^{-1}$, which implies that the total energy exceeds $2E^{(1)}$ if

$$U2^{-k}\ell^{-1} > c_3\alpha 2^{-k}\ell^{-1} + (c_1 + c_2)2^{-2k}\ell^{-2}\,.$$

If this inequality holds for $k = 1$, it holds for all $k \geq 2$ as well. Thus, if we can deal with the $k = 0$ region, we will establish that binding is not possible if

$$U\alpha^{-1} > c_3 + (c_1 + c_2)/(2\ell\alpha)\,. \tag{10}$$

Step 3. The region of no minimal separation: In the $k = 0$ region, the Coulomb repulsion is at least $U\ell^{-1}$, but since there is no minimal separation, we have no direct handle on the possible attraction due to the field. We need a lemma, which we will prove in Step 4. It concerns $E_0^{(2)}(\alpha)$, the energy of the bipolaron with no Coulomb repulsion, i.e., $U = 0$;

$$E_0^{(2)}(\alpha) \geq 2E^{(1)}(\alpha) - 7\alpha^2/3 \quad \text{for all } \alpha\,. \tag{11}$$

Assuming this, the total energy in the $k = 0$ region exceeds $2E^{(1)}(\alpha)$ provided

$$U\ell^{-1} > 7\alpha^2/3 + c_1\ell^{-2}\,,$$

that is, no binding occurs if

$$U\alpha^{-1} > 7\ell\alpha/3 + c_1/(\ell\alpha)\,. \tag{12}$$

Setting the right sides of (10) and (12) equal leads to the choice $\ell = c_4/\alpha$ and to absence of binding if $U > C\alpha$, as asserted.

Step 4. The universal lower bound (11)*:* In this step, $U = 0$. We first note that

$$E^{(1)}(2\alpha) \geq 2E^{(1)}(\alpha) - 4\alpha^2/3\,.$$

This follows from the lower bound $E^{(1)}(\alpha) \geq -\alpha - \alpha^2/3$ in [23] and the upper bound $E^{(1)}(\alpha) \leq -\alpha$ in [11, 14, 15], stated above. So (11) will follow if we can prove that

$$E_0^{(2)}(\alpha) \geq E^{(1)}(2\alpha) - \alpha^2\,. \tag{13}$$

For this purpose we go back to the functional integral (5) and use Schwarz's inequality $\langle e^{a+b}\rangle \leq \langle e^{2a}\rangle^{1/2}\langle e^{2b}\rangle^{1/2}$, where $\langle\cdot\rangle$ now denotes expectation with respect to Wiener measure. We choose a to be the sum of the two terms $i = j = 1$ and $i = j = 2$ in (5), and b to be the mixed terms $i \neq j$. Since $\langle e^{2a}\rangle^{1/2} \sim e^{-TE^{(1)}(2\alpha)}$ for large T, inequality (13) will be achieved if we can show that $\langle e^{2b}\rangle^{1/2} \sim e^{T\alpha^2}$. At first sight, the double path integral $\langle e^{2b}\rangle$ looks like that for a positronium-like atom, i.e., two particles attracting each other through a Coulomb force with coupling constant 4α. The trouble is that the interaction in (3) is at different times, i.e., $|\mathbf{x}_1(t) - \mathbf{x}_2(s)|^{-1}$. A simple application of Jensen's inequality, however, shows that we can fix the time difference $u = t - s$ and obtain the bound

$$\langle e^{2b}\rangle \leq \int_{-\infty}^{\infty} \frac{e^{-|u|}du}{2} \int d\mu^{(2)} \exp\left[4\alpha \int_0^T \frac{dt}{|\mathbf{x}_1(t) - \mathbf{x}_2(t-u)|}\right].$$

Because of the T-periodic time translation invariance of the Wiener measure, the path integral is, in fact, independent of u. Hence we get the positronium-like answer as a bound. This completes our argument for the universal bound (11) and hence the absence of bipolaron binding for sufficiently large U/α.

4. Polarons in one dimension

In 1976 E. P. Gross [10] wrote a seminal paper on the polaron in which he discussed a one-dimensional version. Even though it is not very physical, this model has been widely studied [28, 31, 32] and we are able to prove an interesting theorem about it which we report here for the first time. While we have ignored the Fermi statistics up to now, it will play an important role in this section.

There are N particles on the real line at $x_1, \ldots, x_N \in \mathbb{R}$. We assume they are fermions, but with q spin states for each particle. The case $q = N$ is equivalent to saying that Fermi statistics is irrelevant, i.e., one is dealing with boltzons. The Hamiltonian is as in (4), except that $|\mathbf{k}|^{-1}$ is replaced by 1; the Coulomb repulsion is thus replaced by the delta function, and the corresponding pair potential is replaced by $U\sum_{i<j}\delta(x_i - x_j)$. In one dimension the delta function is a perfectly good potential of a Schrödinger operator.

In this case we can also consider the Pekar approximation, whereby only variational functions of the form $\Psi = \psi(z_1, \ldots, z_N)\cdot\Phi$ are allowed. Here Φ is a vector

in Fock space and $z_j = (x_j, \sigma_j) \in \mathbb{R} \times \{1, \dots, q\}$ is a space-spin coordinate for an electron.

After minimizing the energy with respect to Φ, one obtains the N-particle Pekar-Tomasevich functional (with spin)

$$\sum_{i=1}^{N} \int |\nabla_i \psi|^2 \, dZ + U \sum_{i<j} \int \delta(x_i - x_j) |\psi(Z)|^2 \, dZ - \alpha \int_{\mathbb{R}} \rho_\psi(x)^2 \, dx \,. \qquad (14)$$

Here $\int dZ = \sum_{\sigma_1,\dots,\sigma_N} \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} dx_1 \cdots dx_N$, and the density ρ_ψ is defined by

$$\rho_\psi(x) = N \sum_{\sigma_1,\dots,\sigma_N} \int_{\mathbb{R}^{N-1}} |\psi(x_1, \sigma_1, \dots, x_{N-1}, \sigma_{N-1}, x, \sigma_N)|^2 \, dx_1 \cdots dx_{N-1} \,.$$

We denote by $E_U^{(N)}(\alpha, q)$ the infimum of (14) over all antisymmetric q-state functions ψ with $\int |\psi|^2 dZ = 1$. This minimization problem also makes sense for $U = \infty$, where any finite energy wave function $\psi(z_1, \dots, z_N)$ must vanish if $x_i = x_j$ for any $i \neq j$. We shall prove two facts about this minimization problem.

Theorem 4.1. *If $U = 0$ and N/q is an integer, then*

$$E_0^{(N)}(\alpha, q) = (N/q) E_0^{(q)}(\alpha, q) \,.$$

If $U = \infty$, then

$$E_\infty^{(N)}(\alpha, q) = N E_0^{(1)}(\alpha, 1) \,.$$

The field can cause multi-particle binding. A corollary of our first result is that, in the absence of repulsion, the energy per particle in the q-on state is at least as low as in any other state. That is, for any N (not necessarily divisible by q)

$$N^{-1} E_0^{(N)}(\alpha, q) \geq q^{-1} E_0^{(q)}(\alpha, q) \,.$$

To see this, consider the particle number $M = Nq$ and apply Theorem 4.1 to this case. As a variational candidate for $E_0^{(M)}(\alpha, q)$ we can take q lowest energy N-particle states infinitely separated from each other. Then we have $E_0^{(M)}(\alpha, q) \leq q E_0^{(N)}(\alpha, q)$. On the other hand, by Theorem 4.1, $E_0^{(M)}(\alpha, q) = N E_0^{(q)}(\alpha, q)$, and this proves our assertion. Thus the q-on plays a similar role to that of nickel-62 in the curve of nuclear binding energies.

When $U = \infty$, the situation is even more dramatic; there is no binding of any kind.

One may say that in one-dimension antisymmetry trumps the attraction caused by the field. (This is not true in higher dimensions.) Presumably there are finite critical values of U such that *p-ons* break apart into *r-ons* with $p > r \geq 1$, but we are not able to prove this. There should also be a finite critical value of U above which there is no binding of any kind.

We now turn to the proof of Theorem 4.1. We observe that the energy of a *q-on* can be computed explicitly, as follows.

Lemma 4.1. *If $N = q$, then*

$$E_0^{(q)}(\alpha, q) = -\alpha^2 q^3/12\,.$$

Proof of Lemma 4.1. Whatever ρ_ψ might be, the minimum kinetic energy is realized by the product function $\psi(x_1, \ldots, x_q) = \varphi(x_1)\cdots\varphi(x_q)$, where $\varphi(x) = \sqrt{\rho_\psi(x)/q}$. Thus [12]

$$\sum_{i=1}^{N} \int |\nabla_i \psi|^2 \, dZ \geq \int_{\mathbb{R}} |\nabla \sqrt{\rho_\psi}|^2 \, dx\,. \tag{15}$$

Because there are q spin states, there is an antisymmetric spin function of q variables with which this product function can be multiplied to yield a valid antisymmetric space-spin function. Equality in (15) is then achievable.

To evaluate $E_0^{(q)}(\alpha, q)$ we have to find

$$E_0^{(q)}(\alpha, q) = \inf \left\{ \int_{\mathbb{R}} \left(q|\varphi'|^2 - \alpha q^2 |\varphi|^4 \right) \, dx : \|\varphi\|_2 = 1 \right\}.$$

The function $\varphi(x) = (\alpha q/4)^{1/2}(1/\cosh(\alpha q x/2))$ is easily seen to be a solution to the corresponding Euler-Lagrange equation and, indeed, one can prove that it is the unique solution of the above minimization problem (up to translations and a complex phase) [13, 22]. This leads to the desired expression for the energy. □

We need a slightly unorthodox version of a Lieb-Thirring inequality, which has been used before in [17]:

Lemma 4.2. *Assume that N/q is an integer and let ψ be a normalized, antisymmetric q-state function. Then*

$$\sum_{i=1}^{N} \int |\nabla_i \psi|^2 \, dZ \geq \frac{3}{Nq^2} \left(\int_{\mathbb{R}} \rho_\psi(x)^2 \, dx \right)^2 . \tag{16}$$

Proof of Lemma 4.2. Let $V = -W$ be a negative potential in $L^2(\mathbb{R})$ and denote the eigenvalues of the one-dimensional Schrödinger operator $-\frac{d^2}{dx^2} - W$ by $\lambda_1 \leq \lambda_2 \leq \ldots$. If there is only a finite number M of negative eigenvalues, we set $\lambda_{M+1} = \lambda_{M+2} = \ldots = 0$. By the variational principle (see, e.g., [18, Thm. 12.5]) we have

$$\sum_{i=1}^{N} \int \left(|\nabla_i \psi|^2 - W(x_i)|\psi(Z)|^2 \right) \, dZ \geq q \sum_{j=1}^{N/q} \lambda_j\,.$$

By Hölder's inequality and the sharp Lieb-Thirring inequality [22] for 3/2-moments of the eigenvalues, we find

$$\sum_{j=1}^{N/q} |\lambda_j| \leq \left(\frac{N}{q}\right)^{1/3} \left(\sum_{j=1}^{\infty} |\lambda_j|^{3/2} \right)^{2/3} \leq \left(\frac{N}{q}\right)^{1/3} \left(\frac{3}{16} \int_{\mathbb{R}} W(x)^2 \, dx \right)^{2/3} .$$

To summarize, we have shown that

$$\sum_{i=1}^{N} \int |\nabla_i \psi|^2 \, dZ \geq \int_{\mathbb{R}} W(x) \rho_\psi(x) \, dx - N^{1/3} q^{2/3} \left(\frac{3}{16} \int_{\mathbb{R}} W(x)^2 \, dx \right)^{2/3}$$

for any $0 \leq W \in L^2(\mathbb{R})$. By choosing $W = c\rho_\psi$ and optimizing over the constant c, we obtain the desired bound (16). □

Proof of Theorem 4.1. *The case $U = 0$.* We substitute the bound (16) into the expression (14) for the energy. This lower bound only depends on the unknown quantity $I = \int \rho_\psi(x)^2 \, dx$. By minimizing this expression with respect to I we arrive at the lower bound $E_0^{(N)}(\alpha, q) \geq -\alpha^2 N q^2/12$. According to Lemma 4.1 this coincides with $N E_0^{(q)}(\alpha, q)/q$.

To conclude the proof, we need an upper bound of the same kind. This is easily done by noting that we can make a state of N/q widely separated *q-ons*. In the limit that the separation goes to infinity we obtain the upper bound of N/q times the energy of a single *q-on*.

The case $U = \infty$. This case is easy in view of what we just proved. The electrons, regardless of their spin, cannot get past each other, i.e., the N-particle wave function vanishes whenever $x_i = x_j$ for some $i \neq j$. The configuration space is thus decomposed into a union of simplices of which $S = \{x_1 < x_2 < \ldots < x_N\}$ is representative.

Given a normalized q-state wave function ψ we define a normalized, antisymmetric 1-state wave function $\tilde{\psi}$ as follows: For $x \in S$ we set

$$\tilde{\psi}(x) := \left(\frac{1}{N!} \sum_{\sigma_1, \ldots, \sigma_N} \sum_{\pi} |\psi(z_{\pi(1)}, \ldots, z_{\pi(N)})|^2 \right)^{1/2}$$

and we extend $\tilde{\psi}$ *antisymmetrically* to the other simplices. A similar construction is used in [19]. The crucial point is that if ψ has finite kinetic energy and vanishes on the boundaries of the simplices, then $\tilde{\psi}$ has finite kinetic energy as well and vanishes on the boundaries of the simplices. Moreover, by the convexity inequality for gradients [18, Thm. 7.8] we have

$$\sum_{i=1}^{N} \int_{\mathbb{R}^N} |\nabla_i \tilde{\psi}|^2 \, dx \leq \sum_{i=1}^{N} \int |\nabla_i \psi|^2 \, dZ \, .$$

On the other hand, $\rho_{\tilde{\psi}} = \rho_\psi$, and therefore the total energy of ψ is bounded from below by that of $\tilde{\psi}$. Note that these two energies coincide if the original ψ was an antisymmetric function of space times a symmetric function of spin. To summarize, we have shown that $E_\infty^{(N)}(\alpha, q) = E_\infty^{(N)}(\alpha, 1)$. Note that in the $q = 1$ case, the repulsion energy vanishes because the antisymmetry forces the wave function to vanish on the boundaries of the simplices. Thus $E_\infty^{(N)}(\alpha, 1) = E_0^{(N)}(\alpha, 1)$, and the conclusion follows from the first part of the theorem. □

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INTERACTING ELECTRONS ON THE HONEYCOMB LATTICE

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In this talk I review recent advances on the understanding of the ground state properties of interacting electrons on the honeycomb lattice. In the case of weak short range interactions, renormalization group methods allowed us to give a complete construction of the ground state of the half-filled system and to prove analyticity in the coupling constant of the thermodynamic functions and of the equilibrium correlations. In the case that the electrons interact with a three-dimensional quantum electromagnetic field, the ground state can be constructed order by order in renormalized perturbation theory, with the n-th order admitting $n!$-bounds. Ward Identities are needed in order to control the flow of the effective charges. Lorentz invariance is dynamically restored, thanks to lattice gauge invariance. This talk is based on joint work with V. Mastropietro and M. Porta.

Keywords: Graphene; Hubbard model; honeycomb lattice; renormalization group; lattice gauge theory; Ward identities; Peierls' instability; Kekulé pattern.

1. Introduction

Graphene is a truly two-dimensional (2D) material, consisting of a one-atom-thick layer of graphite. Its crystalline structure is that of an hexagonal lattice of carbon atoms. Since its experimental realization in 2004 [1, 2] graphene has become the center of a very intense experimental and theoretical research. For its discovery, A. Geim and K. Novoselov were recently awarded the Nobel prize in physics 2010.

Among the unusual and exciting features of graphene, which make it a promising material for possible technological applications, are its very high electron mobility and mechanical rigidity and, more in general, the remarkably high quality of its crystalline and electronic properties in a wide range of temperatures, from a few Kelvins to room temperature. See [3] for a complete and up-to-date review of the most relevant properties of graphene.

From the microscopic point of view, what distinguishes graphene from most conventional 2D electron gases is that at half-filling the density of charge carriers vanishes and, correspondingly, the Fermi surface degenerates into two isolated points, at the tips of two conical cusps, known as *Fermi points*, see Figure 1.

In the absence of interactions, the ground state simply consists of a Fermi sea, with all the energy states of the lower band occupied, and all the states of the upper

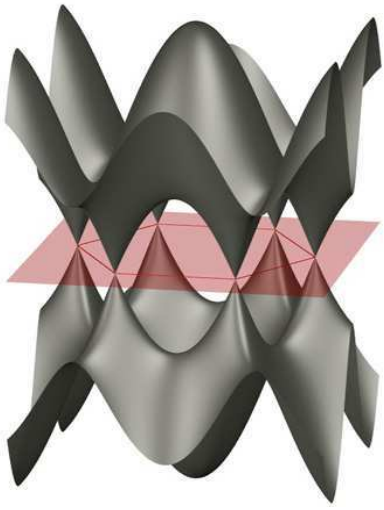

Fig. 1. A sketch of the energy bands of the free electron gas with nearest neighbor hopping on the honeycomb lattice. The red plane corresponds to the Fermi energy at half-filling. It cuts the bands at a discrete set of points, known as the Fermi points or Dirac points. From the picture, it seems that there are six distinct Fermi points. However, after identification of the points modulo vectors of the reciprocal lattice, it turns out that only two of them are independent.

band empty. At low energies, the dominant excitations consist of particle-hole pairs around the two Fermi points. Their dispersion relation is approximately linear at low energies and closely resembles the one of massless 2D Dirac particles [4, 5] with effective speed of light proportional to the hopping strength (300 times smaller than the speed of light, in physical units).

For these reasons, the interacting system should display some analogies with quantum electrodynamics: in this sense, graphene provides an ideal laboratory for simulating QED_{2+1} at low energies and to possibly observe the condensed matter analogues of several high energy exotic phenomena, such as the axial anomaly, chiral symmetry breaking and spontaneous mass generation [5–7].

In the following, I will review some recent developments in the mathematical understanding of the ground state properties of this system, both in the case of short- and long-ranged interactions. The plan of the talk is the following: in the first part I will discuss the case of short-range interactions and more precisely, (i) I will first introduce a natural model for single layer graphene with screened electron-electron interactions, (ii) then I will review the theory of the free gas on the honeycomb lattice, (iii) next I will state a theorem about the analyticity of the ground state at weak coupling and half-filling [8, 9]; in the second part I will discuss the case of electromagnetic interactions and, in particular, (iv) I will introduce a lattice gauge theory model describing hopping electrons on the honeycomb lattice coupled to a $U(1)$ gauge field living in the three-dimensional continuum, (v) then I will state a theorem about the order by order construction of the ground state

including explicit $n!$-bounds on the generic n-th order contribution in perturbation theory, (vi) finally discuss the effect of lattice distortions on the infrared properties of the system, as well as a possible mechanism for the spontaneous formation of a Peierls-Kekulé instability.

2. Short range interactions

A basic model for half-filled single-layer graphene with screened Coulomb interactions is the **2D Hubbard model** on the honeycomb lattice, whose Hamiltonian, in the grand canonical ensemble, reads

$$\begin{aligned} H_\Lambda = & -t \sum_{\substack{\vec{x}\in\Lambda_A \\ i=1,2,3}} \sum_{\sigma=\uparrow\downarrow} \left(a^+_{\vec{x},\sigma} b^-_{\vec{x}+\vec{\delta}_i,\sigma} + b^+_{\vec{x}+\vec{\delta}_i,\sigma} a^-_{\vec{x},\sigma} \right) \\ & + U \sum_{\vec{x}\in\Lambda_A} \left(a^+_{\vec{x},\uparrow} a^-_{\vec{x},\uparrow} - \frac{1}{2} \right) \left(a^+_{\vec{x},\downarrow} a^-_{\vec{x},\downarrow} - \frac{1}{2} \right) \\ & + U \sum_{\vec{x}\in\Lambda_B} \left(b^+_{\vec{x},\uparrow} b^-_{\vec{x},\uparrow} - \frac{1}{2} \right) \left(b^+_{\vec{x},\downarrow} b^-_{\vec{x},\downarrow} - \frac{1}{2} \right) . \end{aligned} \tag{1}$$

Here $a^\pm$ and $b^\pm$ are creation/annihilation operators associated to the two (finite and periodic) triangular sublattices $\Lambda_A = \Lambda$ and $\Lambda_B = \Lambda + \vec{\delta}_i$, see Fig.2. The vectors

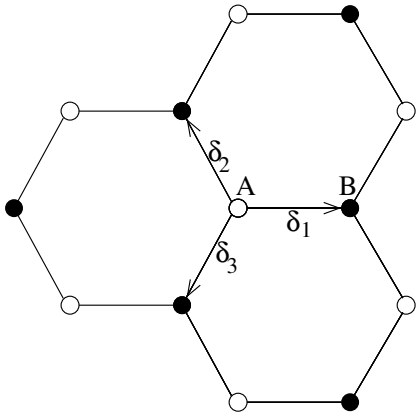

Fig. 2. A portion of the honeycomb lattice Λ. The white and black dots correspond to the sites of the Λ_A and Λ_B triangular sublattices, respectively. These two sublattices are one the translate of the other. They are connected by nearest neighbor vectors $\vec{\delta}_1, \vec{\delta}_2, \vec{\delta}_3$ that, in our units, are of unit length.

$\vec{\delta}_1, \vec{\delta}_2, \vec{\delta}_3$ are the nearest neighbor vectors (of unit length, in our units); moreover, t is a real number, representing the hopping strength. Therefore, the term in the first line of Eq.(1) describes nearest neighbor hopping from the sites of the B sublattice to those of the A sublattice, and viceversa. The parameter U is the strength of

the on-site density-density interaction, which may be either positive or negative. In the following, it should be thought of as a small number. Note that the terms in the second and third line of Eq.(1) can be rewritten as the sum of a truly quartic term in the creation/annihilation operators (the density-density interaction), plus a quadratic term (a chemical potential term, of the form $-\mu N$, with $\mu = U/2$ the chemical potential and N the total particles number operator), plus a constant (which plays no role in the thermodynamic properties of the system). The system is symmetric under hole-particle symmetry (i.e., $a^{\pm} \to a^{\mp}$, $b^{\pm} \to -b^{\mp}$), which implies that the average electron density is exactly one, for all inverse temperatures β and all lattice sizes $|\Lambda|$; in other words, the grand-canonical Hamiltonian Eq.(1) describes the system at half-filling, for all U, β, Λ.

If $U = 0$, the Hamiltonian is quadratic and translation invariant (thanks to the periodic boundary conditions); therefore, it can be easily diagonalized by Fourier transform:

$$H_\Lambda = H^0_\Lambda = -t \sum_{\substack{\vec{x}\in\Lambda_A \\ i=1,2,3}} \sum_{\sigma=\uparrow\downarrow} \left(a^+_{\vec{x},\sigma} b^-_{\vec{x}+\vec{\delta}_i,\sigma} + b^+_{\vec{x}+\vec{\delta}_i,\sigma} a^-_{\vec{x},\sigma} \right)$$

$$= -\frac{v_0}{|\Lambda|} \sum_{\vec{k}} \sum_{\sigma=\uparrow\downarrow} (\hat{a}^+_{\vec{k},\sigma}, \hat{b}^+_{\vec{k},\sigma}) \begin{pmatrix} 0 & \Omega^*(\vec{k}) \\ \Omega(\vec{k}) & 0 \end{pmatrix} \begin{pmatrix} \hat{a}^-_{\vec{k},\sigma} \\ \hat{b}^-_{\vec{k},\sigma} \end{pmatrix}$$

with $v_0 = \frac{3}{2}t$ the non-interacting **Fermi velocity** and $\Omega(\vec{k})$ the **complex dispersion relation**:

$$\Omega(\vec{k}) = \frac{2}{3} \sum_{i=1}^{3} e^{i\vec{k}(\vec{\delta}_i - \vec{\delta}_1)} = \frac{2}{3}(1 + 2e^{-i3k_1/2} \cos \frac{\sqrt{3}}{2} k_2) \ .$$

Note that the natural creation/annihilation operator is a 2D spinor of components a and b. In order to fully diagonalize the theory, one is left with diagonalizing the 2×2 matrix $\begin{pmatrix} 0 & \Omega^*(\vec{k}) \\ \Omega(\vec{k}) & 0 \end{pmatrix}$: the result is that the energy bands are $\pm v_0 |\Omega(\vec{k})|$, plotted in Fig.1 above and vanishing linearly only at the two Fermi points

$$\vec{p} = \vec{p}_F^{\ \pm} = (\frac{2\pi}{3}, \pm \frac{2\pi}{3\sqrt{3}})$$

The ground state consists of a Fermi sea, with all the states of negative energies filled up, and all the positive energy states empty.

In the absence of interactions, we can also compute exactly a complete set of correlation functions: in fact, being the Hamiltonian quadratic, the $2n$-points correlation functions can be all computed in terms of the two-point fucntion, via the fermionic Wick rule. The two-point function is defined as:

$$S_0(\mathbf{x} - \mathbf{y}) = \langle \mathbf{T} \big(\Psi^-_{\mathbf{x},\sigma} \Psi^+_{\mathbf{y},\sigma} \big) \rangle \big|_{U=0} \ , \tag{2}$$

where: $\mathbf{x} = (x_0, \vec{x})$, with $x_0 \in [0, \beta)$ an imaginary time; $\mathbf{T}$ is the fermionic time-ordering operator; $\Psi^{\pm}_{\vec{x},\sigma} = \left(a^{\pm}_{\vec{x},\sigma}, b^{\pm}_{\vec{x}+\vec{\delta}_1,\sigma}\right)$ and

$$\Psi^{\pm}_{\mathbf{x},\sigma} = e^{H_\Lambda x_0} \Psi^{\pm}_{\vec{x},\sigma} e^{-H_\Lambda x_0} \ , \quad \text{with} \quad \mathbf{x} = (x_0, \vec{x}) \ .$$

The *propagator* $S_0(\mathbf{x})$, a priori defined in $(-\beta, \beta) \times \Lambda$, can be extend periodically in the imaginary time and conveniently re-expressed in Fourier space as (k_0 is the *Matsubara frequency*, i.e., the Fourier dual variable of x_0):

$$\hat{S}_0(\mathbf{k}) = - \begin{pmatrix} ik_0 & v_0 \Omega^*(\vec{k}) \\ v_0 \Omega(\vec{k}) & ik_0 \end{pmatrix}^{-1} \ .$$

If $\vec{k}' = \vec{k} - \vec{p}^{\pm}_F$ is small, the dispersion relation is

$$\Omega(\vec{k}' + \vec{p}^{\pm}_F) \simeq i k'_1 \pm k'_2 \ ,$$

and the propagator is asymptotically the same as the one for massless Dirac fermions:

$$\hat{S}_0(k_0, \vec{k}' + \vec{p}^{\pm}_F) \simeq \begin{pmatrix} -ik_0 & v_0(ik'_1 \mp k'_2) \\ v_0(-ik'_1 \mp k'_2) & -ik_0 \end{pmatrix}^{-1}$$

In particular, the two quasi-particle spinors describing the excitations around $\vec{p}^{\pm}_F$ can be combined to form a single four-components spinor $\psi_{\mathbf{q}}$, with propagator

$$\langle \psi_{\mathbf{q}} \bar{\psi}_{\mathbf{q}} \rangle \simeq \frac{1}{i \not{\mathbf{q}}} \ ,$$

where $\not{\mathbf{q}} := q_\mu \gamma_\mu$, $\mu = 0, 1, 2$, and γ_μ are euclidean gamma matrices [5].

The Dirac-like behavior of the quasi-particles is responsible for most observed anomalous features of graphene. It is then natural to ask what is the effect of interactions on the ground (or low) temperature properties of graphene. The question has been first investigated by power counting arguments, suggesting that **the local Hubbard interaction is irrelevant**, see for instance [10] and references therein. Of course, power counting is not enough to conclude that the ground state interacting correlations are asymptotically close to those of the free gas, a notoriously difficult question, which is still open for most physically relevant quantum many body systems, with the exception of a few one-dimensional cases [11–14].

Quite remarkably, in the case of graphene with short ramge interactions, we have a theorem guaranteeing the analyticity of the ground state at weak coupling and half-filling, see [9] for a proof.

THEOREM (Giuliani-Mastropietro [8, 9]):
There exists a positive constant U_0 such that the specific ground state energy and the zero temperature correlation functions of the half-filled 2D Hubbard model

on the honeycomb lattice are ***analytic*** *in U, for $|U| \le U_0$. In particular,*

$$S(k_0, \vec{k}' + \vec{p}_F^{\pm}) \simeq \frac{1}{Z} \begin{pmatrix} -ik_0 & v(ik'_1 \mp k'_2) \\ v(-ik'_1 \mp k'_2) & -ik_0 \end{pmatrix}^{-1} ,$$

where $Z = 1 + O(U^2)$ and $v = v_0 + O(U)$ are analytic functions of U, for $|U| \le U_0$.

Remarks.

(1) This is the first complete (non-perturbative) construction of the ground state of a 2D system of interacting electrons.

(2) The interacting correlations have the same long distance behavior as the free ones, modulo a finite renormalization of the quasi-particle weight Z^{-1} and of the Fermi velocity v. In particular,

$$|\langle \vec{S}_{\vec{x}} \cdot \vec{S}_{\vec{y}} \rangle| \le \frac{\text{const.}}{1 + |\vec{x} - \vec{y}|^4} ,$$

which rigorously excludes magnetic long range order (LRO) in the ground state. Similarly, we can rigorously exclude superconducting LRO and the presence of a mass gap.

(3) The proof is based on a multiscale integration of the partition function

$$\begin{aligned} \mathrm{Tr}\{e^{-\beta H^0_\Lambda - \beta V_\Lambda}\} &= \int P(d\psi) e^{-V(\psi)} \\ &= \int P(d\psi^{(\le h)}) e^{-\mathcal{V}^{(h)}(\psi^{(\le h)})} \end{aligned}$$

and fermionic cluster expansion methods due to a large community of researchers and developed starting from the beginning of the eighties, using constructing field theory techniques. Some of the key names involved in these developments are: K. Gawedski and A. Kupiainen [11]; A. Lesniewski [15]; G. Battle, D. Brydges and P. Federbush [16]; G. Benfatto and G. Gallavotti [17]; J. Feldman, J. Magnen, V. Rivasseau and E. Trubowitz [18]; ...

3. Coulomb interactions

The case of Coulomb interactions is the most interesting one for physical applications to clean suspended graphene: in fact, at half-filling and in the absence of defects, the electrostatic repulsion among electrons is supposed to be **unscreened**.

The effects of Coulomb interactions have been first analyzed by Hartree-Fock and approximate Renormalization Group methods by several people, including A. H. Castro Neto, J. Gonzalez, F. Guinea, V. P. Gusynin, I. F. Herbut, E. G. Mischenko, S. G. Sharapov, O. Vafek, M. A. H. Vozmediano and many many others, see e.g. [3, 10, 19–24].

Power counting and the computation of the one- and two-loops beta function suggest that:

(1) the Coulomb interaction is marginal but gives rise to a controlled flow;
(2) the effective Fermi velocity diverges logarithmically at the Fermi points (without critical exponents).

However, it is not clear whether the theory is renormalizable at all orders and what is the physical meaning of an infinite Fermi velocity. Moreover, the uncontrolled approximations used to perform the computations lead to ambiguities that are still under debate. It has been proposed that the model should be considered reliable only at energy scales such that the effective Fermi velocity remains smaller than the speed of light. At lower energies, the model loses its significance and finite speed of light propagation has to be taken into account [10].

Building on this proposal, we introduced a new lattice gauge theory model, which describes graphene with e.m. interactions and defined by the following Hamiltonian [26]:

$$H_\Lambda = -t \sum_{\substack{\vec{x}\in\Lambda \\ i=1,2,3}} \sum_{\sigma=\uparrow\downarrow} \left(a^+_{\vec{x},\sigma} b^-_{\vec{x}+\vec{\delta}_i,\sigma} e^{ie\int_0^1 \vec{A}(\vec{x}+s\vec{\delta}_i)\cdot\vec{\delta}_i\, ds} + c.c. \right)$$
$$+ \frac{e^2}{2} \sum_{\vec{x},\vec{y}\in\Lambda_A\cup\Lambda_B} (n_{\vec{x}}-1)\varphi(\vec{x}-\vec{y})(n_{\vec{y}}-1) + \mathcal{H}_A^{(\le M_0)} \ ,$$

where $n_{\vec{x}}$ is the electronic density at site $\vec{x}$;

$$\varphi(\vec{x}) = \int_{|\underline{p}|\le M_0} \frac{d^3\underline{p}}{(2\pi)^3} \frac{e^{-i\vec{p}\cdot\vec{x}}}{|\underline{p}|^2} \ ,$$

with $\underline{p} := (\vec{p}, p_3)$ and M_0 a fixed ultraviolet cut-off. Moreover, $\underline{A}(\underline{x})$ is a quantized e.m. vector potential in the Coulomb gauge, living in the 3D continuum and $\mathcal{H}_A^{(\le M_0)}$ is its field energy, in the presence of the ultraviolet cutoff M_0. Note that the third component of the vector potential propagates freely in 3D space and can be explicitly integrated out. After integration of these free modes, the resulting effective model is a lattice QED_{2+1} theory, with a modified photon propagator scaling like $|\mathbf{p}|^{-1}$ at small transferred momenta.

Remarkably, the theory is renormalizable at all orders in the electric charge, contrary to what appears to be the theory with electrostatic interactions. After systematic resummations of the original perturbative expansion, we get an explicit formula for the ground state two-point function $S_{\mathbf{k}} = \langle \psi^+_{\mathbf{k},\sigma} \psi^-_{\mathbf{k},\sigma} \rangle$, which is singular only at the Fermi points $\mathbf{p}_F^\pm = (0, \frac{2\pi}{3}, \pm\frac{2\pi}{3\sqrt{3}})$.

THEOREM (Giuliani-Mastropietro-Porta, [25, 26]):
As an identity between formal power series in e^2,

$$S_{\mathbf{k}}^{-1} = -Z(\mathbf{k}) \begin{pmatrix} ik_0 & v(\mathbf{k})\Omega^*(\vec{k}) \\ v(\mathbf{k})\Omega(\vec{k}) & ik_0 \end{pmatrix} (1 + B(\mathbf{k})) \ ,$$

where $B(\mathbf{k}) = \sum_{n\geq 1} b_n(\mathbf{k})e^{2n}$ *has coefficients of order* n *bounded as* $|b_n(\mathbf{k})| \leq c^n n!|\mathbf{k} - \mathbf{p}_F^{\pm}|^{1/2}$. *Moreover:*

$$Z(\mathbf{k}) \sim |\mathbf{k} - \mathbf{p}_F^{\pm}|^{-\eta} , \qquad 1 - v(\mathbf{k}) \sim |\mathbf{k} - \mathbf{p}_F^{\pm}|^{\tilde{\eta}}$$

where

$$\eta = \frac{e^2}{12\pi^2} + \cdots \quad \text{and} \quad \tilde{\eta} = \frac{2e^2}{5\pi^2} + \cdots$$

The higher order corrections to η *and* $\tilde{\eta}$ *are given by formal power series in* e^2, *of the form* $\sum_{n\geq 0} a_n e^{2n}$, *with coefficients of order* n *bounded by* $|a_n| \leq c^n n!$.

Remarks.

(1) The long distance decay of the interacting correlations depends on the **anomalous critical exponents** η and $\tilde{\eta}$, describing the behavior of the effective quasi-particle weight $Z^{-1}(\mathbf{k})$ and of the effective Fermi velocity $v(\mathbf{k})$ close to the Fermi points.
(2) Lorentz symmetry dynamically emerges, thanks to lattice gauge invariance.
(3) The vertex interaction $e\int A\psi^+\psi^-$ is marginal. The beta function governing the flow of the effective charge can be proved to be asymptotically vanishing, thanks to an exact lattice Ward Identity (WI).
(4) Similarly, the dressed mass of the photon is zero (no screening), again by an exact lattice WI.
(5) This is the first systematic analysis of the thermodynamic and correlation functions of the ground state of graphene in the presence of electromagnetic interactions, with explicit bound at all orders in perturbation theory. The proof is again based on fermionic Renormalization Group methods. Unfortunately, contrary to the case of short range interactions, we are not able to prove convergence of the resummed series yet. Such a proof would be very important: it would provide the first construction of the ground state of a quantum Coulomb system and the first explicit example of a 2D Luttinger liquid.
(6) The proof of convergence will require a combination of determinant bounds for the fermionic sector and cluster expansion for the bosonic one. It is presumably doable, but an extensions of present techniques is required.

4. Peierls-Kekulé instability

The previous discussion suggests that at weak coupling, in the absence of lattice defects or of an underlying periodic potential, the spectrum of the interacting quasi-particles is gapless. This is a serious drawback for possible technological applications of graphene: therefore, people started to investigate possible mechanisms for the generation of a mass gap. One way to induce a gap is by adding an interaction with an external periodic field, which can be generated, e.g., by the presence of a substrate [27]. In the absence of a substrate, Ref. [28–31] proposed a mechanism similar to

the one at the basis of spontaneous chiral symmetry breaking in strongly-coupled QED_3; the applicability of these proposals to real graphene is a delicate issue, due to the uncontrolled approximations related to a large-N expansions. Another possible mechanism for gap generation is based on a Peierls-Kekulé distortion of the honeycomb lattice, which is a prerequisite for electron fractionalization [7, 32]. One optimizes over the distortion pattern, by minimizing the corresponding electronic energy. In the absence of electron-electron interactions, a rather strong coupling with the classical phonon field is needed for the formation of a non-trivial distortion [32], while the effects of the electron interactions is still poorly understood.

Interestingly, the Renormalization Group approach we developed allowed us to investigate the possible emergence of a Peierls instability in the presence of electromagnetic repulsion among the electrons and the corresponding opening of a mass gap [26]. If we allow distortions of the honeycomb lattice, the hopping becomes a function of the bond length $\ell_{\vec{x},j}$ that, for small deformations, can be approximated by the linear function $t_{\vec{x},j} = t + \phi_{\vec{x},j}$, where $\bar{\ell}$ is the equilibrium length of the bond. In the Born-Oppenheimer approximation the phonon field $\phi_{\vec{x},j} = g(\ell_{\vec{x},j} - \bar{\ell})$ is picked in such a way that the sum of the electronic energy $E_0(\{\phi_{\vec{x},j}\})$ and the elastic energy $\frac{\kappa}{2g^2}\sum_{\vec{x},j}\phi^2_{\vec{x},j}$ is minimal. The extremality condition for the energy reads

$$\kappa\phi_{\vec{x},j} = g^2 \sum_{\sigma} \langle \big(a^+_{\mathbf{x},\sigma} b^-_{\mathbf{x}+(0,\vec{\delta}_j),\sigma} e^{ie\int_0^1 \vec{\delta}_j\cdot\vec{A}(\vec{x}+s\vec{\delta}_j,0)\,ds} + c.c\big)\rangle^{\phi}.$$

We find that, for any $j_0 \in \{1,2,3\}$,

$$\phi^{(0)}_{\vec{x},j} = \phi_0 + \Delta_0 \cos\left(\vec{p}^{+}_F(\vec{\delta}_j - \vec{\delta}_{j_0} - \vec{x})\right)$$

is a local minimum of the total energy, provided that $\phi_0 = c_0 g^2/\kappa + \cdots$ for a suitable constant c_0 and that Δ_0 satisfies a non-BCS gap equation. If Δ_0 is a non-trivial solution to the gap equation, then the system tends to spontaneously develop a Kekulé distortion pattern, see Fig.4.

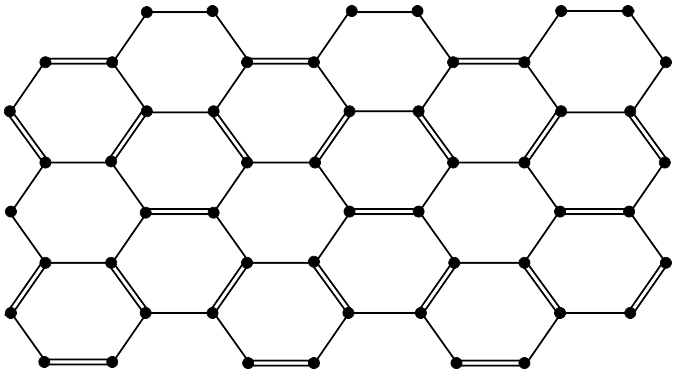

Fig. 3. The Kekulé distortion pattern. The hopping parameter is $t + \Delta_0$ and $t - \Delta_0/2$ on the double and single bonds respectively.

The non-BCS gap equation reads

$$\Delta_0 \simeq \frac{g^2}{\kappa} \int\limits_{\Delta \lesssim |\mathbf{k}'| \lesssim 1} d\mathbf{k}' \frac{Z^{-1}(\mathbf{k}')\Delta(\mathbf{k}')|\Omega(\vec{k}')|^2}{k_0^2 + v^2(\mathbf{k}')|\Omega(\vec{k}' + \vec{p}_F^+)|^2 + |\Delta(\mathbf{k}')|^2} ,$$

where $\Delta(\mathbf{k}') \sim \Delta_0 |\mathbf{k}'|^{-\eta_K}$ and $\eta_K = \frac{2e^2}{3\pi^2} + \cdots$ It admits a non-trivial solution for $g \geq g_c(e, v)$. At $e = 0$, $g_c(0, v) \sim \sqrt{v}$, in agreement with results in [32]. As e increases, g_c decreases. Second order perturbation theory suggests that for $e \geq e_c$ the critical phonon coupling is $g_c = 0$ (spontaneous Peierls-Kekulé distortion).

5. Conclusions

(1) We considered the 2D Hubbard model on the honeycomb lattice. At half-filling and weak coupling, the ground state thermodynamic functions and correlations can be constructed in the form of convergent (analytic) series in U.
(2) Its interacting correlations decay with the same exponents as the free ones, modulo a finite renormalization of some physical parameters (quasi-particles weight and Fermi velocity).
(3) Next, we considered a lattice gauge model for graphene with electromagnetic repulsion among electrons and we derived an order by order convergent resummed expansion.
(4) In the absence of lattice distortions, we predict that the long distance behavior of the interacting correlations are characterized by anomalous critical exponents: the system is a sort of "2D Luttinger liquid".
(5) In the presence of a small Kekulé distortion, we predict that the electron repulsion dramatically amplifies, with a non universal power law, the corresponding mass gap.
(6) The Kekulé-Peierls mass satisfies a non-BCS gap equation, which provides evidence of the fact that the electromagnetic interactions facilitate the spontaneous distortion of the lattice and the opening of a gap.
(7) The results are based on constructive fermionic Renormalization Group methods. In the short range case they are completely rigorous and they allowed us to provide the first construction of the ground state of a realistic 2D interacting electron system.
(8) In the case of electromagnetic interactions among electrons, these methods "only" allowed us to prove order by order convergence of a renormalized perturbation series. There is hope to prove convergence by combining "bosonic" and "fermionic" multiscale cluster expansion.

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RENORMALIZATION OF DIRAC'S POLARIZED VACUUM

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We review recent results on a mean-field model for relativistic electrons in atoms and molecules, which allows to describe at the same time the self-consistent behavior of the polarized Dirac sea. We quickly derive this model from Quantum Electrodynamics and state the existence of solutions, imposing an ultraviolet cut-off Λ. We then discuss the limit $\Lambda \to \infty$ in detail, by resorting to charge renormalization.

Keywords: Dirac's vacuum; vacuum polarization; Dirac-Hartree-Fock theory; relativistic Density Functional Theory; renormalization; Landau pole; Uehling potential.

For heavy atoms, it is necessary to take relativistic effects into account. However there is no equivalent of the well-known N-body (non-relativistic) Schrödinger theory involving the Dirac operator, because of its negative spectrum. The correct theory is Quantum Electrodynamics (QED). This theory has a remarkable predictive power but its description in terms of perturbation theory restricts its range of applicability. In fact a mathematically consistent formulation of the nonperturbative theory is still unknown. On the other hand, effective models deduced from nonrelativistic theories (like the Dirac-Hartree-Fock model [1, 2]) suffer from inconsistencies: for instance a ground state never minimizes the physical energy which is always unbounded from below.

Here we present an effective model based on a physical energy which can be minimized to obtain the ground state in a chosen charge sector. Our model describes the behavior of a finite number of particles (electrons), coupled to that of the Dirac sea which can become polarized. Our existence results are fully non-perturbative. Like in QED, the model contains divergences which have to be removed by renormalization.

We review several results obtained in collaboration with Christian Hainzl, Philippe Gravejat, Éric Séré and Jan Philip Solovej. These works have already been summarized in [3] and in the fourth chapter of [4], to which the interested reader is refered for more details.

1. A nonlinear Dirac equation

We present a mean-field model describing the self-consistent behavior of a finite number of 'real' electrons in an atom or a molecule, and, simultaneously, of the infinitely many 'virtual' electrons of the Dirac sea. The state of the system is described by a *one-body density matrix* P which is a self-adjoint operator acting on the Hilbert space $\mathfrak{H} := L^2(\mathbb{R}^2, \mathbb{C}^4)$, and satisfying the constraint $0 \leq P \leq 1$ (1 denotes the identity operator on $\mathfrak{H}$). The operator P describes the whole system consisting of the real and virtual electrons. We are interested in the following stationary equation [3, 5]:

$$\boxed{\begin{cases} P = \chi_{(-\infty,\mu)}\,(D) + \delta \\ D = D^0 + \alpha(\rho_{P-1/2} - \nu) * |x|^{-1} + X_P. \end{cases}} \tag{1}$$

In this section we explain the meaning of this equation at a formal level, before turning to rigorous results.

The operator D is a *mean-field* Hamiltonian which is seen by all the particles. The first term

$$D^0 := \boldsymbol{\alpha} \cdot (-i\nabla) + \beta$$

is the usual free Dirac operator [6] (with $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ where α_j are the usual Dirac matrices). For the sake of simplicity we have chosen units in which the speed of light is $c = 1$ and the mass of the electron is $m = 1$. The operator D^0 satisfies $(D^0)^2 = -\Delta + 1$ and its spectrum is $\sigma(D^0) = (-\infty, -1] \cup [1, \infty)$. The second term in the formula of D is the Coulomb potential induced by both a fixed external density of charge ν (typically $\nu = Z\delta_0$ for a pointwise nucleus of charge Z located at the origin), and the self-consistent density $\rho_{P-1/2}$ of the electrons (defined below). The number $\alpha = e^2$ which is the square of the (bare) charge e of the electron, is called the *bare coupling constant*. It will be renormalized later.

The third term X_P in the definition of D is an *exchange* operator whose form depends on the chosen model. In *Hartree-Fock (HF) theory* [3, 5], we have

$$X_P(x, y) = -\alpha \frac{(P - 1/2)(x, y)}{|x - y|} \tag{2}$$

which is called the *exchange term*. In *Relativistic Density Functional Theory* [7, 8],

$$X_P = \frac{\partial F_{\mathrm{xc}}}{\partial \rho}(\rho_{P-1/2}) \tag{3}$$

is the derivative of a chosen effective exchange-correlation functional, which depends only on the density $\rho_{P-1/2}$. In *reduced Hartree-Fock (rHF) theory*, we simply take

$$\boxed{X_P = 0.}$$

For the sake of clarity, we will mainly present the mathematical results that have been obtained in the simplest case of $X_P = 0$ and we will only make comments

on the Hartree-Fock case (2). The exchange-correlation approximation (3) has not been considered rigorously so far.

We use the notation $\chi_{(-\infty,\mu)}(D)$ to denote the spectral projector of D associated with the interval $(-\infty,\mu)$. Hence Equation (1) means that the electrons of the system fill all the energies of the mean-field Hamiltonian D, up to the Fermi level $\mu \in (-1,1)$. In practice we choose the chemical potential μ to fix the total charge of the system.[a] We have added in (1) the possibility of having a density matrix $0 \leq \delta \leq \chi_{\{\mu\}}(D)$ at the Fermi level, as is usually done in reduced Hartree-Fock theory [9]. So the operator P is not necessarily a projector but we still use the letter P for convenience. Later we will restrict ourselves to the case of P being an orthogonal projector.

Equation (1) is well-known in the physical literature. A model of the same form (with an exchange term X_P different from (2)) was proposed by Chaix and Iracane in [5]. Relativistic Density Functional Theory aims at solving the same Equation (1) with X_P given by (3) and additional classical electromagnetic terms accounting for the interactions with photons, see, e.g., [7, Eq. (6.2)] and [8, Eq. (62)]. Dirac already considered in [10] the first order term obtained from (1) in an expansion in powers of α, assuming $X_P = 0$.

Let us now elaborate on the exact meaning of $\rho_{P-1/2}$. The charge density of an operator $A : \mathfrak{H} \to \mathfrak{H}$ with integral kernel $A(x,y)_{\sigma,\sigma'}$ is formally defined as $\rho_A(x) = \sum_{\sigma=1}^4 A(x,x)_{\sigma,\sigma} = \mathrm{Tr}_{\mathbb{C}^4}(A(x,x))$. In usual Hartree-Fock theory, the charge density is $\rho_P(x)$. However, as there are infinitely many particles, this does not make sense here. In (1), the subtraction of half the identity is a convenient way to give a meaning to the density, independently of any reference, as we will explain later. One has formally, when P is a projector,

$$\rho_{P-1/2}(x) = \rho_{\frac{P-P^\perp}{2}}(x) = \frac{1}{2}\sum_{i\geq 1} |\varphi_i^-(x)|^2 - |\varphi_i^+(x)|^2$$

where $\{\varphi_i^-\}_{i\geq 1}$ is an orthonormal basis of $P\mathfrak{H}$ and $\{\varphi_i^+\}_{i\geq 1}$ is an orthonormal basis of $(1-P)\mathfrak{H}$. As was explained in [11] (see also Section 2), subtracting $1/2$ to the density matrix P renders the model invariant under charge conjugation.

The free vacuum

When there is no external field ($\nu \equiv 0$) and when $X_P = 0$, Equation (1) has an obvious solution for any $\mu \in (-1,1)$, the state made of all electrons with negative energy[b]

$$P = P_-^0 := \chi_{(-\infty,0)}(D^0),$$

[a] If the external field is not too strong, fixing the charge is the same as fixing the number of electrons. However in strong fields, electron-positron pairs can be created and fixing the charge might not lead to the expected number of electrons.

[b] In the Hartree-Fock case (2), the free Dirac sea $P = P_-^0$ is no more a solution of (1) when $\nu \equiv 0$. The Hartree-Fock free vacuum solving the nonlinear equation (1) was constructed in [11, 12], assuming an ultraviolet cut-off.

in accordance with Dirac's ideas [13–15]. Indeed $\rho_{P^0_- - 1/2} \equiv 0$, as is seen by writing in the Fourier representation

$$(P^0_- - 1/2)(p) = -\frac{\boldsymbol{\alpha} \cdot p + \beta}{2\sqrt{1+|p|^2}}$$

and using that the Dirac matrices are trace-less. This shows the usefulness of the subtraction of half the identity to P, since the free vacuum P^0_- now has a vanishing density.

For a general state P, we can use this to write (formally):

$$\rho_{P-1/2} = \rho_{P-1/2} - \rho_{P^0_- - 1/2} = \rho_{P-P^0_-}. \tag{4}$$

When P belongs to a suitable class of perturbations of P^0_- (for instance when $P - P^0_-$ is locally trace-class), the density $\rho_{P-P^0_-}$ is a well-defined mathematical object. We will give below natural conditions which garantee that $P - P^0_-$ has a well-defined density in our context.

Electrons interacting with the polarized vacuum

With external field ($\nu \neq 0$), Equation (1) models a system of electrons in the presence of a nucleus and with a self-consistent polarized Dirac sea. The number of 'real' electrons in the system will depend on the value of μ. Typically (for not too strong fields) when $\mu = 0$, one obtains the ground state of the polarized vacuum in the presence of ν, without any real electron. On the other hand $\mu > 0$ in general leads to systems with a finite number of real electrons (Fig. 1).

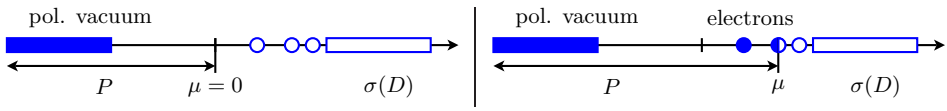

Fig. 1. State of the system depending on the value of the chemical potential μ.

Note that for a generic operator $0 \leq P \leq 1$ there is no natural distinction between real and virtual electrons. It is only for a solution of Equation (1) that we can interpret the eigenfunctions corresponding to the positive eigenvalues of D as describing 'real' electrons, and the rest of the spectrum as being the Dirac sea.

When $\mu > 0$ (and $\delta = 0$), the N filled eigenfunctions of D corresponding to the eigenvalues in $[0, \mu)$ solve the following system of nonlinear equations:

$$\left(D^0 + \alpha \left(\sum_{i=1}^{N} |\varphi_i|^2 - \nu \right) * \frac{1}{|x|} + \alpha\, \rho_{P_{\mathrm{vac}} - 1/2} * \frac{1}{|x|} \right) \varphi_i = \epsilon_i\, \varphi_i$$

for $i = 1, ..., N$. This equation has the same form as the well-known Dirac-Hartree-Fock equations [1, 2], without exchange term, and with an additional vacuum polarization potential induced by the vacuum state $P_{\mathrm{vac}} := \chi_{(-\infty,0)}(D)$. This remark

was used by Chaix and Iracane in [5] as a justification to the Dirac-Hartree-Fock model.

Most of the material of this section is purely formal and many objects (like $\rho_{P-1/2}$) do not really make sense as such. In Section 3 we will introduce an ultraviolet cut-off Λ and present rigorous results. We however first explain how the formal Equation (1) can be derived from Quantum Electrodynamics (QED).

2. Derivation from Quantum Electrodynamics

In this section we derive Equation (1) from first principles. We start with the *formal* QED Hamiltonian written in Coulomb gauge, in the presence of an external density of charge ν and an external magnetic potential a, see [16–20]:

$$\mathbb{H}^{\nu,a} = \int \Psi^*(x)\Big(\boldsymbol{\alpha}\cdot\big\{-i\nabla-\sqrt{\alpha}(\boldsymbol{A}(x)+a(x)\big\}+m\beta\Big)\Psi(x)\,dx \\ -\alpha\iint\frac{\rho(x)\nu(y)}{|x-y|}dx\,dy+\frac{\alpha}{2}\iint\frac{\rho(x)\rho(y)}{|x-y|}dx\,dy+H_f. \quad (5)$$

Here $\Psi(x)$ is the second quantized field operator which annihilates an electron at x and satisfies the anticommutation relation

$$\Psi^*(x)_\sigma\Psi(y)_\nu+\Psi(y)_\nu\Psi^*(x)_\sigma=2\delta_{\sigma,\nu}\delta(x-y). \quad (6)$$

In the formula of $\mathbb{H}^{\nu,a}$, $\rho(x)$ is the *density operator* defined by

$$\rho(x)=\sum_{\sigma=1}^{4}\frac{[\Psi^*_\sigma(x),\Psi_\sigma(x)]}{2} \quad (7)$$

where $[a,b]=ab-ba$. The operator H_f describes the kinetic energy of the photons:

$$H_f=\frac{1}{8\pi}\int\left(|\nabla\times\boldsymbol{A}(x)|^2+|\boldsymbol{E}_t(x)|^2\right)dx=\sum_{\lambda=1,2}\int_{\mathbb{R}^3}dk\,|k|a^*_\lambda(k)a_\lambda(k)+\mathrm{Cst}$$

(Cst indicates a constant which diverges in infinite volume). The operators $\boldsymbol{A}(x)$ and $\boldsymbol{E}_t(x)$ are the electromagnetic field operators for the photons and $a^*_\lambda(k)$ is the creation operator of a photon with momentum k and polarization λ. The Hamiltonian $\mathbb{H}^{\nu,a}$ formally acts on the Fock space $\mathcal{F}=\mathcal{F}_{\mathrm{e}}\otimes\mathcal{F}_{\mathrm{ph}}$ where $\mathcal{F}_{\mathrm{e}}$ is the fermionic Fock space for the electrons and $\mathcal{F}_{\mathrm{ph}}$ is the bosonic Fock space for the photons.

We emphasize that (5) does not contain any normal-ordering or notion of (bare) electrons and positrons: $\Psi(x)$ can annihilate electrons of negative kinetic energy. The distinction between electrons and positrons should be a result of the theory and not an input. The commutator used in the formula (7) of $\rho(x)$ is a kind of renormalization, independent of any reference. It is due to Heisenberg [16] (see also [21, Eq. (96)]) and it is necessary for a covariant formulation of QED, see [19, Eq. (1.14)] and [22, Eq. (38)]. More precisely, the Hamiltonian $\mathbb{H}^{\nu,a}$ possesses the interesting property of being invariant under charge conjugation since the following relations hold formally

$$\mathcal{C}\rho(x)\mathcal{C}^{-1}=-\rho(x),\qquad \mathcal{C}\mathbb{H}^{\nu,a}\mathcal{C}^{-1}=\mathbb{H}^{-\nu,a},$$

where $\mathcal{C}$ is the charge conjugation operator acting on the Fock space.

We now make two approximations: (i) we neglect photons and assume there is no external magnetic field, $a \equiv 0$; (ii) we work in a mean-field theory, i.e. we restrict the Hamiltonian $\mathbb{H}^{\nu,a}$ to (generalized) Hartree-Fock states.

Let us recall that the electronic *one-body density matrix* (two point function) of any electronic state $|\Omega\rangle \in \mathcal{F}_{\rm e}$ is defined as

$$P(x,y)_{\sigma,\sigma'} = \langle \Omega | \Psi^*(x)_\sigma \Psi(y)_{\sigma'} | \Omega \rangle$$

and it satisfies $0 \leq P \leq 1$. Generalized Hartree-Fock states form a subset of (mixed) states which are completely determined by their density matrix P, see [23]. The value of any product of creation and annihilation operators is computed by means of Wick's formula. The energy of a Hartree-Fock state $|{\rm HF}\rangle \otimes |0\rangle$ (with $|0\rangle \in \mathcal{F}_{\rm ph}$ being the photonic vacuum) is [11]

$$\langle \mathbb{H}^{\nu,0} \rangle = \mathcal{E}^\nu_{\rm HF}(P - 1/2) + {\rm Cst}$$

where Cst is a constant (diverging in the infinite volume limit) and

$$\begin{aligned} \mathcal{E}^\nu_{\rm HF}(P-1/2) = {\rm Tr}\,(D^0(P-1/2)) - \alpha \iint \frac{\rho_{P-1/2}(x)\nu(y)}{|x-y|}\,dx\,dy \\ + \frac{\alpha}{2}\iint \frac{\rho_{P-1/2}(x)\rho_{P-1/2}(y)}{|x-y|}dx\,dy - \frac{\alpha}{2}\iint \frac{|(P-1/2)(x,y)|^2}{|x-y|}dx\,dy. \quad (8) \end{aligned}$$

The reader can recognize in (8) the well-known Hartree-Fock energy [23, 24], but applied to the "renormalized" density matrix $P - 1/2$ instead of the usual density matrix P. The last two terms of the first line are respectively the kinetic energy and the interaction energy of the electrons with the external potential induced by the charge distribution ν. In the second line appear respectively the so-called *direct* and *exchange* terms. In Relativistic Density Functional Theory (RDFT) [7, 8], the exchange term is approximated by an exchange-correlation functional $F_{\rm xc}(\rho_{P-1/2})$ whereas in reduced Hartree-Fock theory, the exchange term is simply dropped.

Writing the first and second order stationarity conditions with respect to the density matrix P leads to the nonlinear equation (1) with $\mu = 0$. The equation with $\mu \neq 0$ is obtained by replacing D^0 by $D^0 - \mu$. Again our derivation is formal but (in the Hartree-Fock case) this was made rigorous by means of a thermodynamic limit in [11].

Remark 2.1. Instead of the vacuum, one can take a coherent state for the photons. This leads to a classical unknown magnetic field $A(x)$ interacting with the particles. So far, there are no mathematical results on such a model.

3. Existence and non existence of solutions

In the presence of an external field ($\nu \neq 0$), Equation (1) has *no solution* in any 'reasonable' Banach space [25] and it is necessary to introduce an ultraviolet reg-

ularization parameter Λ. The simplest method (although probably not optimal regarding regularity issues [26]) is to impose a cut-off at the level of the Hilbert space, that is to replace $\mathfrak{H} = L^2(\mathbb{R}^3; \mathbb{C}^4)$ by

$$\mathfrak{H}_\Lambda := \{f \in L^2(\mathbb{R}^3; \mathbb{C}^4),\ \mathrm{supp}(\widehat{f}) \subset B(0; \Lambda)\}$$

and to solve, instead of (1), the regularized equation in $\mathfrak{H}_\Lambda$:

$$\boxed{\begin{cases} P = \chi_{(-\infty,\mu)}\,(D) + \delta \\ D = \Pi_\Lambda \left(D^0 + \alpha(\rho_{P-P^0_-} - \nu) * |x|^{-1} \right) \Pi_\Lambda \end{cases}} \tag{9}$$

where Π_Λ is the orthogonal projector onto $\mathfrak{H}_\Lambda$ in $\mathfrak{H}$. We take $X_P = 0$ in the rest of the paper, that is we work in the reduced Hartree-Fock approximation. Note that we have used (4) to replace $\rho_{P-1/2}$ by $\rho_{P-P^0_-}$.

Existence of solutions

Existence of solutions to (9) was proved in [25] for $\mu = 0$ and in [26] for $\mu \in (-1, 1)$, for all values of the coupling constant $\alpha \geq 0$. The precise statement of this nonperturbative result is the following:

Theorem 3.1 (Nonperturbative existence of solutions to (9)**, [25, 26]).** *Assume that $\alpha \geq 0$, $\Lambda > 0$ and $\mu \in (-1, 1)$ are given. Let ν be in the so-called* Coulomb space*:*

$$\mathcal{C} := \left\{ f \ :\ \int_{\mathbb{R}^3} |k|^{-2} |\widehat{f}(k)|^2 dk < \infty \right\}.$$

Then, Equation (9) *has at least one solution P such that*

$$P - P^0_- \in \mathfrak{S}_2(\mathfrak{H}_\Lambda), \quad P^0_+(P - P^0_-)P^0_+ \in \mathfrak{S}_1(\mathfrak{H}_\Lambda), \quad \rho_{P-P^0_-} \in \mathcal{C} \cap L^2(\mathbb{R}^3). \tag{10}$$

All such solutions share the same density $\rho_{P-P^0_-}$.

In (10), $\mathfrak{S}_1(\mathfrak{H}_\Lambda)$ and $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$ are respectively the spaces of trace-class and Hilbert-Schmidt operators [27] on $\mathfrak{H}_\Lambda$, and $P^0_+ = 1 - P^0_-$. Note that thanks to the uniqueness of $\rho_{P-P^0_-}$, the mean-field operator D is also unique and only δ can differ between two solutions of (9).

Let us mention that it is natural to look for a solution of (9) such that $P - P^0_-$ is a Hilbert-Schmidt operator on $\mathfrak{H}_\Lambda$. If P is a projector, the Shale-Stinespring theorem [28] tells us that P yields a Fock representation equivalent to that of P^0_-. Even when P is not a projector, it will be associated with a unique Bogoliubov mixed state in the Fock space representation of P^0_-. This is a mathematical formulation of the statement that P should not be too far from P^0_-.

The method used in [25, 26] to prove Theorem 3.1, was to identify solutions of (9) with minimizers of the so-called *reduced Bogoliubov-Dirac-Fock energy* which is

nothing but the formal difference between the reduced Hartree-Fock energy of P and that of the reference state P_-^0. A formal calculation yields with $Q = P - P_-^0$

$$\begin{aligned}
&\text{“}\mathcal{E}^\nu_{\rm HF}(P-1/2) - \mathcal{E}^0_{\rm HF}(P_-^0 - 1/2)\text{”} \\
&\quad = \mathrm{Tr}\,\left(D^0 Q\right) - \alpha \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_Q(x)\nu(y)}{|x-y|}dx\,dy + \frac{\alpha}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\rho_Q(x)\rho_Q(y)}{|x-y|}dx\,dy \\
&\quad := \mathcal{E}^\nu_{\rm BDF}(P-P_-^0). \qquad (11)
\end{aligned}$$

The energy $\mathcal{E}^\nu_{\rm BDF}$ was introduced and studied with an exchange term by Chaix and Iracane in [5] (see also [29]). An adequate mathematical formalism was then provided by Bach, Barbaroux, Helffer and Siedentop [30] in the free case $\nu = 0$, and by Hainzl, Séré and the author in [25, 31] when $\nu \neq 0$.

The proof then reduces to finding the appropriate functional setting in which the minimization of the energy $\mathcal{E}^\nu_{\rm BDF}$ makes sense, providing a solution to (9). We quickly sketch the proof for the convenience of the reader.

Proof. We want to give a clear mathematical meaning to the energy (11) and minimize it. Let us first consider the kinetic energy term. Noticing [30] that

$$Q = P - P_-^0 \text{ with } 0 \le P \le 1 \quad \Longleftrightarrow \quad Q^2 \le Q^{++} - Q^{--}$$

where we have used the notation $Q^{\epsilon\epsilon'} := P_\epsilon^0 Q P_{\epsilon'}^0$ with $\epsilon, \epsilon' \in \{\pm\}$, we have (assuming all terms are well-defined),

$$\mathrm{Tr}\,(D^0 Q) = \mathrm{Tr}\,|D^0|(Q^{++} - Q^{--}) \ge \mathrm{Tr}\,|D^0|Q^2.$$

Hence the kinetic energy is nonnegative. Recalling $1 \le |D^0| \le \sqrt{1+\Lambda^2}$ on $\mathfrak{H}_\Lambda$, we also see that it is finite if and only if $Q^{\pm\pm} \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)$ and $Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$. This suggests to work in the following convex subset

$$\mathcal{K} := \left\{Q \in \mathcal{X} \ : \ Q^2 \le Q^{++} - Q^{--}\right\}$$

where $\mathcal{X}$ is the Banach space

$$\mathcal{X} := \left\{Q = Q^* \in \mathfrak{S}_2(\mathfrak{H}_\Lambda) \ : \ Q^{\pm\pm} \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)\right\},$$

and to use the following generalized kinetic energy [31]:

$$\mathrm{Tr}_{\,P_-^0}\,(D^0 Q) := \mathrm{Tr}\,|D^0|(Q^{++} - Q^{--}).$$

Using the ultraviolet cut-off Λ, it was proved in [32, Lemma 1] that the map $Q \in \mathcal{X} \mapsto \rho_Q \in L^2(\mathbb{R}^3) \cap \mathcal{C}$ is continuous. Hence the energy $\mathcal{E}^\nu_{\rm BDF}$ is well-defined for any state $Q \in \mathcal{K}$.

Now, when $\nu \in \mathcal{C}$, we can complete the square and obtain the lower bound

$$\begin{aligned}
\mathcal{E}^\nu_{\rm BDF}(Q) &= \mathrm{Tr}_{\,P_-^0}\,(D^0 Q) + \frac{\alpha}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{(\rho_Q-\nu)(x)(\rho_Q-\nu)(y)}{|x-y|}dx\,dy \\
&\qquad - \frac{\alpha}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\nu(x)\nu(y)}{|x-y|}dx\,dy \\
&\ge -\frac{\alpha}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\nu(x)\nu(y)}{|x-y|}dx\,dy. \qquad (12)
\end{aligned}$$

This proves that $\mathcal{E}^\nu_{\rm BDF}$ is bounded from below.

It is then an exercise to verify that $\mathcal{E}^\nu_{\rm BDF}$ is convex and lower semi-continuous on the convex set $\mathcal{K}$, hence that it possesses at least one minimizer $Q = P - P^0_-$. It is a solution of (9) with $\mu = 0$. Uniqueness of the density follows from the strict convexity of $\mathcal{E}^\nu_{\rm BDF}$ with respect to ρ_Q. To deal with the case $\mu \neq 0$, one replaces D^0 by $D^0 - \mu$. □

The variational argument provides solutions which *a priori* only satisfy (10) but one could think that they indeed have much better properties. As we will see in Section 4, this intuition is partially wrong: solutions are actually quite singular. In particular Q is in general *not* trace-class, which is related to renormalization.

The property $Q^{++}, Q^{--} \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)$ in (10) suggests to define the total 'charge' of the system by

$$q = \mathrm{Tr}\ (Q^{++} + Q^{--}) := \mathrm{Tr}_{P^0_-}(Q).$$

If Q is trace-class then we have $\mathrm{Tr}\,(Q) = \mathrm{Tr}_{P^0_-}(Q)$ but in general $\mathrm{Tr}\,(Q)$ is not well-defined. Properties of the generalized trace $\mathrm{Tr}_{P^0_-}$ have been provided in [31]. When $P = Q + P^0_-$ is a projector, $\mathrm{Tr}_{P^0_-}(Q)$ is always an integer which is indeed nothing but the relative index of the pair (P, P^0_-), see [31, 33].

Varying μ allows to pick the desired total charge, as we now explain. Let us introduce the following constrained minimization problem

$$E^\nu(q) := \inf_{\substack{Q\in\mathcal{K} \\ \mathrm{Tr}_{P^0_-}(Q)=q}} \mathcal{E}^\nu_{\rm BDF}(Q).$$

The function $q \mapsto E^\nu(q)$ is convex. Assume that $Q = P - P^0_-$ is a ground state for $E^\nu_{\rm BDF}(q)$. Then simple convexity arguments show that Q is also a *global* minimizer of the free energy $\mathcal{E}^\nu_{\rm BDF} - \mu \mathrm{Tr}_{P^0_-}$, with $\mu = \partial E^\nu(q)/\partial q$. Indeed it was shown in [26] that $E^\nu_{\rm BDF}$ is strictly convex on some interval (q_m, q_M) (corresponding to $\mu \in (-1, 1)$), which is also the largest interval on which $E^\nu(q)$ has ground states, see Fig. 2. Therefore varying μ in $(-1, 1)$ is exactly the same as solving the minimization problem $E^\nu(q)$ for $q \in (q_m, q_M)$.

Maximum ionization

The numbers q_m and q_M can be interpreted as the minimal and maximal possible ionization of the system in the presence of the external field ν. It is important to derive bounds on these quantities, in order to determine for which values of the charge q the system is stable. The following was proved in [26]:

Theorem 3.2 (Maximum ionization [26]). *We assume that* $\nu \in \mathcal{C} \cap L^1(\mathbb{R}^3)$, *with* $Z := \int \nu \geq 0$.

• (Existence of neutral atoms) *One has* $Z \in [q_m, q_M]$.

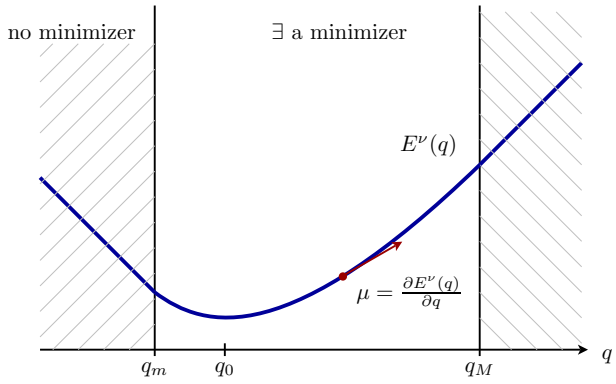

Fig. 2. Varying the chemical potential μ is, by convexity, equivalent to varying the total charge $q = \mathrm{Tr}_{P^0_-}(Q)$ of the system.

• (Ionization bounds for weak external fields) *For a regular ultraviolet cut-off, there exists constants $C, C' > 0$ such that the following holds: For $\alpha\|\nu\|_{\mathcal{C}} + \alpha(1 + \log\Lambda) \leq C'$ and $Z \geq 0$, one has*

$$-C\frac{\alpha\log\Lambda + 1/\Lambda + \alpha\|\nu\|_{\mathcal{C}}}{1 - C\alpha\log\Lambda} \leq q_m \leq 0 \leq Z \leq q_M \leq \frac{2Z + C\left(\alpha\log\Lambda + 1/\Lambda + \alpha\|\nu\|_{\mathcal{C}}\right)}{1 - C\alpha\log\Lambda}. \tag{13}$$

The bound (13) is a generalization to the BDF model of an estimate due to Lieb [34]. In the nonrelativistic limit (13) reduces to Lieb's result $Z \leq q_M \leq 2Z$.

In [26], the bound (13) is shown by using a more regular ultraviolet cut-off. To be more precise, the free Dirac operator D^0 was replaced by an operator which grows faster at infinity

$$\tilde{D}^0 = D^0\left(1 - \frac{\Delta}{\Lambda^2}\right)$$

and the model was settled in the whole space $\mathfrak{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$.

4. Renormalization

We have described results dealing with existence (and non existence for $q \notin [q_m, q_M]$) of solutions to Equation (9). All these solutions depend on the ultraviolet cut-off Λ and it is a natural question to investigate how. Indeed, the limit $\Lambda \to \infty$ for α fixed was shown to be very singular in [25, Theorem 2] and the correct way to tackle this issue is to resort to charge renormalization.

Let us start by recalling the spirit of renormalization. A physical theory usually aims at predicting physical observables in terms of the parameters in the model. Sometimes, interesting quantities are divergent and it is necessary to introduce cut-offs. In our case the parameters are the coupling constant $\alpha = e^2$, the cut-off Λ, the chemical potential μ and the external density ν. For simplicity we will take $\mu = 0$

and we will not emphasize the dependence in ν in our notation. In our system of units the mass of the electron is $m = 1$. Predicted physical quantities are functions $F(\alpha, \Lambda)$. The charge e (or equivalently its square, the coupling constant α) is also a physical observable and renormalization occurs when the value predicted by the theory is different from its 'bare' value:

$$\alpha_{\rm ph} = \alpha_{\rm ph}(\alpha, \Lambda) \neq \alpha. \tag{14}$$

In this case the parameter α is not observable in contrast with $\alpha_{\rm ph} = \alpha_{\rm ph}(m, \alpha, \Lambda)$ which has to be set equal to its experimental value. The relation (14) has to be inverted, in order to express the bare parameter in terms of the physical one:

$$\alpha = \alpha(\alpha_{\rm ph}, \Lambda). \tag{15}$$

This allows to express any observable quantity F as a function $\tilde{F}$ of the physical parameters and the cut-off Λ:

$$\tilde{F}(\alpha_{\rm ph}, \Lambda) = F\big(\alpha(\alpha_{\rm ph}, \Lambda)\,,\, \Lambda\big). \tag{16}$$

A possible definition of renormalizability is that *all such observable quantities have a limit when* $\Lambda \to \infty$*, for fixed* $\alpha_{\rm ph}$.

Important difficulties can be encountered when trying to complete this program. For instance the physical quantity $\alpha_{\rm ph}$ might be a *nonexplicit function of* α. The corresponding formulas can then only be inverted perturbatively to any order, as is the case in QED [20, 35, 36].

Nonperturbative charge renormalization formula

For the model presented in this article it is fortunate that there is an explicit and nonperturbative relation between $\alpha_{\rm ph}$ and α, as expressed in the following result:

Theorem 4.1 (Nonperturbative charge renormalization formula [26]). *Assume that* $\alpha \geq 0$, $\Lambda > 0$ *and* $\mu \in (-1, 1)$ *are given and let* P *be a solution of* (9) *as given by Theorem 3.1. If* $\nu \in \mathcal{C} \cap L^1(\mathbb{R}^3)$*, then* $\rho_{P - P^0_-} \in L^1(\mathbb{R}^3)$ *and it holds*

$$\boxed{\int_{\mathbb{R}^3} \nu - \int_{\mathbb{R}^3} \rho_{P-P^0_-} = \frac{\displaystyle\int_{\mathbb{R}^3} \nu - \operatorname{Tr}_{P^0_-}(P - P^0_-)}{1 + \alpha B_\Lambda}} \tag{17}$$

where

$$B_\Lambda = \frac{1}{\pi} \int_0^{\frac{\Lambda}{\sqrt{1+\Lambda^2}}} \frac{z^2 - z^4/3}{1 - z^2} dz = \frac{2}{3\pi} \log \Lambda - \frac{5}{9\pi} + \frac{2 \log 2}{3\pi} + O(1/\Lambda^2). \tag{18}$$

Note that, except in the neutral case $\operatorname{Tr}_{P^0_-}(P - P^0_-) = Z$, (17) implies that the solution $Q = P - P^0_-$ found in Theorem 3.1 cannot be trace-class. If Q were trace-class, we would have $\operatorname{Tr}_{P^0_-}(Q) = \operatorname{Tr}(Q) = \int_{\mathbb{R}^3} \rho_Q$ which contradicts (17).

The previous result is interpreted as follows. Assume that we put a nucleus of charge Z in the vacuum, and let P be the corresponding Dirac's polarized vacuum (that is we take $\mu = 0$ in (9)). When $\alpha\|\nu\|_{\mathcal{C}}$ is small enough,[c] it was proved in [25] that it holds $\|P - P^0_-\| < 1$. This itself implies that the relative index vanishes, $\mathrm{Tr}_{P^0_-}(P - P^0_-) = 0$, hence

$$Z - \int_{\mathbb{R}^3} \rho_{P-P^0_-} = \frac{Z}{1+\alpha B_\Lambda}.$$

In reality we never measure the charge of the nucleus alone, but we always also observe the corresponding vacuum polarization. Hence the physical coupling constant is given by the renormalization formula

$$\boxed{\alpha_{\mathrm{ph}} = \frac{\alpha}{1+\alpha B_\Lambda} \iff \alpha = \frac{\alpha_{\mathrm{ph}}}{1-\alpha_{\mathrm{ph}} B_\Lambda}.} \tag{19}$$

In our theory we must fix α_{ph} and not α. Using (19) we can express any physical quantity in terms of α_{ph} and Λ only.

Unfortunately it holds $\alpha_{\mathrm{ph}} B_\Lambda < 1$ hence it makes no sense to take $\Lambda \to \infty$ while keeping α_{ph} fixed (this is the so-called Landau pole [37]) and one has to look for a weaker definition of renormalizability. The cut-off Λ which was first introduced as a mathematical trick to regularize the model has actually a physical meaning. A natural scale occurs beyond which the model does not make sense. Fortunately, this corresponds to momenta of the order $e^{3\pi/2\alpha_{\mathrm{ph}}}$, a huge number for $\alpha_{\mathrm{ph}} \simeq 1/137$.

Asymptotic renormalization

It is convenient to define a renormalized density ρ_{ph} by the relation [25]

$$\alpha_{\mathrm{ph}}\rho_{\mathrm{ph}} = \alpha\big(\nu - \rho_{P-P^0_-}\big) \tag{20}$$

in such a way that $D = D^0 - \alpha_{\mathrm{ph}}\rho_{\mathrm{ph}} * |x|^{-1}$. This procedure is similar to wavefunction renormalization. By uniqueness of $\rho_{P-P^0_-}$ we can see ρ_{ph} as a function of α_{ph}, ν, μ and Λ (or κ). For the sake of clarity we do not emphasize the dependence in ν and we take $\mu = 0$ (this means that we consider the vacuum polarization in the presence of the nucleus, without any real electron). The self-consistent equation for ρ_{ph} was derived in [25].

It is explained in [38] that one can expand $\rho_{\mathrm{ph}} = \rho_{\mathrm{ph}}(\alpha_{\mathrm{ph}}, \Lambda)$ as follows:

$$\rho_{\mathrm{ph}}(\alpha_{\mathrm{ph}}, \Lambda) = \sum_{n=0}^{\infty} (\alpha_{\mathrm{ph}})^n \nu_{n,\Lambda} \tag{21}$$

where $\{\nu_{n,\Lambda}\}_n \subset L^2(\mathbb{R}^3) \cap \mathcal{C}$ is a sequence depending only on the external density ν and the cut-off Λ. This sequence is defined by an explicit induction formula which is detailed in [38] and that we do not write here for shortness. The series (21) has

[c] By scaling we can keep $\int_{\mathbb{R}^3} \nu$ fixed and choose $\alpha\|\nu\|_{\mathcal{C}}$ as small as we want.

a positive radius of convergence, which is however believed to shrink to zero when $\Lambda \to \infty$.

Assuming $\widehat{\nu}$ decays fast enough (see condition (22)), it is proved in [38] that for any fixed n, the limit $\nu_{n,\Lambda} \to \nu_n$ exists in $L^2(\mathbb{R}^3) \cap \mathcal{C}$. This is what is usually meant by renormalizability in QED: each term of the perturbation series in powers of the physical $\alpha_{\rm ph}$ has a limit when the cut-off is removed. The sequence $\{\nu_n\}_n$ is the one which is calculated in practice [7, 8, 20, 39]. One has for instance $\nu_0 = \nu$ and

$$\nu_1 * |x|^{-1} = \frac{1}{3\pi} \int_1^\infty dt\, (t^2-1)^{1/2} \left[\frac{2}{t^2} + \frac{1}{t^4}\right] \int_{\mathbb{R}^3} e^{-2|x-y|t} \frac{\nu(y)}{|x-y|}\, dy,$$

the *Uehling potential* [40, 41]. All the others ν_n can be calculated by induction in terms of $\nu_0, ..., \nu_{n-1}$. An explicit recursion relation is provided in [38].

The next natural question is to understand the link between the well-defined, cut-off dependent, series (21) and the *formal series* $\sum_{n=0}^\infty (\alpha_{\rm ph})^n \nu_n$. Recall that $\alpha_{\rm ph} B_\Lambda < 1$ by construction, so it is in principle not allowed to take the limit $\Lambda \to \infty$ while keeping $\alpha_{\rm ph}$ fixed.

It is more convenient to change variables and take as new parameters $\alpha_{\rm ph}$ and $\kappa = \alpha_{\rm ph} B_\Lambda$, with the additional constraint that $0 < \kappa < 1$. The new parameter κ is now independent of $\alpha_{\rm ph}$ and we ask ourselves whether predicted physical quantities will depend very much on the chosen value of $0 < \kappa < 1$. The purpose of [38] was precisely to prove that the asymptotics of any physical quantity in the regime $\alpha_{\rm ph} \ll 1$ is actually *independent of* κ to any order in $\alpha_{\rm ph}$, which is what was called *asymptotic renormalizability*. Note that fixing $\kappa \in (0,1)$ amounts to take an $\alpha_{\rm ph}$-dependent cut-off $\Lambda \simeq C e^{3\pi\kappa/2\alpha_{\rm ph}} \gg 1$.

Theorem 4.2 (Asymptotic renormalization of the nuclear density [38]). *Consider a function $\nu \in L^2(\mathbb{R}^3) \cap \mathcal{C}$ such that*

$$\int_{\mathbb{R}^3} \log(1+|k|)^{2N+2} |\widehat{\nu}(k)|^2 dk < \infty \tag{22}$$

for some integer N. Let $\rho_{\rm ph}(\alpha_{\rm ph}, \kappa)$ be the unique physical density defined by (20) *with $\mu = 0$, $\alpha_{\rm ph} > 0$ and $0 < \kappa < 1$, corresponding to the bare coupling constant $\alpha = (1-\kappa)^{-1}\alpha_{\rm ph}$ and the ultraviolet cut-off Λ such that $B_\Lambda = \kappa/\alpha_{\rm ph}$.*

Then, for every $0 < \epsilon < 1$, there exist two constants $C(N, \epsilon, \nu)$ and $a(N, \epsilon, \nu)$, depending only on N, ϵ and ν, such that one has

$$\boxed{\left\| \rho_{\rm ph}(\alpha_{\rm ph}, \kappa) - \sum_{n=0}^N \nu_n (\alpha_{\rm ph})^n \right\|_{L^2(\mathbb{R}^3)\cap\mathcal{C}} \leq C(N,\epsilon,\nu)\ {\alpha_{\rm ph}}^{N+1}} \tag{23}$$

for all $0 \leq \alpha_{\rm ph} \leq a(N,\epsilon,\nu)$ and all $\epsilon \leq \kappa \leq 1-\epsilon$.

The interpretation of Theorem 4.2 is that the renormalized density $\rho_{\rm ph}(\alpha_{\rm ph}, \kappa)$ is *asymptotically* given by the formal series $\sum_{n\geq 0} (\alpha_{\rm ph})^n \nu_n$, *uniformly in the renormalization parameter* κ in the range $\epsilon \leq \kappa \leq 1-\epsilon$. For a very large range of

cut-offs,

$$C_1 e^{3\epsilon\pi/2\alpha_{\rm ph}} \leq \Lambda \leq C_2 e^{3(1-\epsilon)\pi/2\alpha_{\rm ph}}$$

the result is independent of Λ for small $\alpha_{\rm ph}$. This formulation of renormalizability is more precise than the requirement that each $\nu_{n,\Lambda}$ converges. It also leads to the formal perturbation series in a very natural way.

It was argued by Dyson in [42] that the perturbation series $\sum_{n\geq 0}(\alpha_{\rm ph})^n \nu_n$ it is probably *divergent*, but there is no mathematical proof so far. In [38], some properties of the sequence $\{\nu_n\}$ were derived.

5. Conclusion

We have presented a mean-field theory for electrons in atoms and molecules, which describes at the same time the self-consistent behavior of Dirac's polarized vacuum. The model can be deduced from Quantum Electrodynamics by restricting to Hartree-Fock states and neglecting photons in the Coulomb gauge.

Existence of ground states could be established, with or without a charge constraint. The so-obtained states are rather singular, in particular they yield a perturbation Q of the free vacuum P^0_- which is in general not trace-class but still has $\rho_Q \in L^1(\mathbb{R}^3)$. This technical issue is at the origin of charge renormalization.

The formula linking the physical coupling constant $\alpha_{\rm ph}$ and the bare α is explicit and exhibits a Landau pole, rendering impossible to remove the ultraviolet cut-off Λ while keeping $\alpha_{\rm ph}$ fixed. Nevertheless in a regime where $\alpha_{\rm ph} \ll 1$ and $\Lambda \gg 1$ such that $\kappa = (2/3\pi)\alpha_{\rm ph} \log \Lambda$ stays bounded, the asymptotics is found to be independent of the value of κ, to any order in the physical coupling constant $\alpha_{\rm ph}$. The terms of the asymptotic expansion are the ones which are computed in practice. The first order term induces the famous Uehling potential.

The model which we have presented in this paper is probably not quantitative but it already possesses several of the qualitative properties of full Quantum Electrodynamics, with the advantage that they can be studied in a fully rigorous manner. A more quantitative model would include photons, for instance via an additional self-consistent classical magnetic field, as is done in Relativistic Density Functional Theory.

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CONVERGENCE RESULT FOR THICK GRAPHS

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Many physical systems have branching structures of thin transversal diameter. One can name for instance quantum wire circuits, thin branching waveguides, or carbon nano-structures. In applications, such systems are often approximated by the underlying one-dimensional graph structure, a so-called "quantum graph". In this way, many properties of the system like conductance can be calculated easier (sometimes even explicitly). We give an overview of convergence results obtained so far, such as convergence of Schrödinger operators, Laplacians and their spectra.

Keywords: Thick graphs; graph-like manifolds; spectral convergence; quantum graphs.

1. Introduction

In this note, we give an overview on convergence results of Laplace-like operators on shrinking tubular neighbourhoods of a metric graph. We start with defining the notion "graph-like manifold" and "thick graph", as well as the associated Laplace-like operators on these spaces. We also review some applications in Physics and Mathematics in Sec. 2. The current state of art of quantum graph models is described in the recent proceedings volume [11] to which we refer for an extensive bibliography. Section 3 is devoted to convergence results for the Neumann Laplacian as well as a general convergence scheme for operators acting in different Hilbert spaces. Section 4 contains results for the Dirichlet Laplacian on thick graphs, as well as operators on thick graphs converging to delta-couplings on the underlying metric graph. Finally, in Sec. 5 we comment on some work in progress and open problems.

2. Thick graphs

Roughly speaking, a *thick graph* is a family of neighbourhoods $\{X_\varepsilon\}_{\varepsilon>0}$ of a metric graph X_0 embedded in $\mathbb{R}^d$, which shrinks to X_0 if $\varepsilon \to 0$. Sometimes, we also refer to a single member X_ε of the family $\{X_\varepsilon\}_\varepsilon$ for a suitably small $\varepsilon > 0$ as a thick graph. We give a more formal definition below.

Thick graphs have a lot of different names in the literature, basically due to the intended application. Thick graphs are also called *fat graphs* (cf. [9]), *mesoscopic systems collapsing onto a graph* (cf. [23]), *graph neighbourhoods* (cf. [18]), *graph-like*

(thin) manifolds (cf. [12]), *quasi-one-dimensional spaces* (cf. [31]), *thin branched (quantum) waveguides* (cf. [13]) or *quantum networks modelled by graphs* (cf. [15]).

2.1. *Definition of a thick graph*

2.1.1. *Metric and quantum graphs*

We give here a brief outline of the concept of metric and quantum graphs. We refer to [22] for more details and further references.

Assume that X_0 is a *metric graph*, i.e., a topological graph X_0 with vertices V and edges E such that each edge $e \in E$ is associated a *length* $\ell_e > 0$. In this way, we can identify an edge e with the interval $I_e := [0, \ell_e]$ and the adjacent initial and terminal vertices $\partial_- e \in V$ and $\partial_+ e \in V$ with $0 \in I_e$ and $\ell_e \in I_e$. Note that we can view $s \in I_e$ as a *coordinate* on the edge e, which introduces an orientation on the graph X_0. Moreover, the coordinate allows to *integrate* and *differentiate* a function on the edge. We also allow edges of infinite length (so-called *infinite leads*), this edge is assumed to have only one adjacent initial vertex $\partial_- e \in I_e = [0, \infty)$.

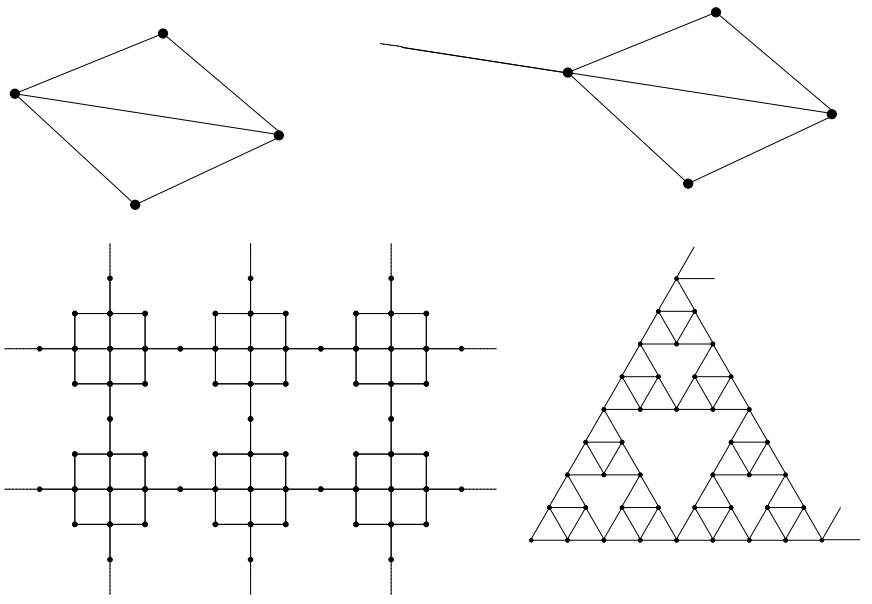

Fig. 1. Four examples of metric graphs: a *compact* one, a *non-compact* one with compact interior part and one infinite lead, a non-compact $\mathbb{Z}^2$-periodic metric graph and a self-similar non-compact example, the *Sierpiński* graph.

Thus, the topological graph X_0 can be turned into a *metric measure* space, by defining the distance of two points $x, y \in X_0$ to be the shortest distance of all Lipschitz continuous paths joining x and y, where the length of a path is defined in the obvious way. The measure on X_0 is determined by the Lebesque measure on each edge I_e.

Associated to a metric graph, we have a natural Hilbert space, namely

$$\mathscr{H}_0 := \mathsf{L}_2(X_0) := \bigoplus_e \mathsf{L}_2(I_e). \tag{1}$$

Moreover, we can naturally define differential operators, like e.g. a Laplace-type operator $(\Delta f)_e = -f_e''$ for a function $f = \{f_e\}_e \in \mathsf{H}^2_{\max}(X_0)$, where $\mathsf{H}^k_{\max}(X_0) := \bigoplus_e \mathsf{H}^k(I_e)$ and where $\mathsf{H}^k(I_e)$ denotes the Sobolev space with square-integrable derivatives up to order k on the interval I_e. In order to turn Δ into a self-adjoint operator, we have to fix vertex conditions on the boundary values

$$f_e(v) := \begin{cases} f_e(0), & v = \partial_- e \\ f_e(\ell_e), & v = \partial_+ e \end{cases} \quad \text{and} \quad f_e'(v) := \begin{cases} -f_e'(0), & v = \partial_- e \\ f_e'(\ell_e), & v = \partial_+ e \end{cases} \tag{2}$$

of the function at a vertex v and its adjacent edges $e \in E_v$, the *neighbouring edges of* v. A prominent example is given by the so-called *free* or *Kirchhoff* vertex conditions

$$f_{e_1}(v) = f_{e_2}(v) \quad \forall e_1, e_2 \in E_v \quad \text{and} \quad \sum_{e \in E_v} f_e'(v) = 0. \tag{3}$$

The first condition in (3) is referred to as *continuity* of the function f viewed as function on the topological space X_0, the second is a flux condition on the derivative viewed as vector field on X_0. The *free* or *Kirchhoff Laplacian* Δ_{X_0} on the metric graph X_0 is now the operator acting as $(\Delta f)_e = -f_e''$ for functions $f \in \mathsf{H}^2_{\max}(X_0)$ fulfilling (3). We will see in a moment that if we have a uniform lower *positive* bound on the edge length, i.e.,

$$\inf_{e \in E} \ell_e > 0, \tag{4}$$

then Δ_{X_0} is self-adjoint. We will give further examples of self-adjoint vertex conditions in Sec. 4.3.

Let us remark that the Kirchhoff Laplacian Δ_{X_0} is associated with the quadratic form

$$\mathfrak{d}_{X_0}(f) := \sum_e \int_0^{\ell_e} |f_e'|^2 \mathrm{d}s, \quad \operatorname{dom} \mathfrak{d}_{X_0} := \mathsf{H}^1(X_0), \tag{5}$$

where $\mathsf{H}^1(X_0)$ is the subspace of those functions $f \in \mathsf{H}^1_{\max}(X_0)$ such that f is continuous at each vertex. It follows from (4) that $\mathsf{H}^1(X_0)$ is a *closed* subspace in $\mathsf{H}^1_{\max}(X_0)$, and that $\mathfrak{d}_{X_0}$ is a *closed* non-negative quadratic form. Moreover, the associated operator is precisely Δ_{X_0}, which shows in particular that Δ_{X_0} is self-adjoint (see [22] for details and further references).

A *quantum graph* is a metric graph X_0 together with a self-adjoint differential operator H_0 acting on X_0. The most prominent example is a metric graph X_0 together with its Kirchhoff Laplacian Δ_{X_0} just defined.

2.1.2. *Graph-like manifolds and thick graphs*

Let us now give an abstract definition of — what we call in this review — a *graph-like manifold*. Let $\varepsilon > 0$ and let X_0 be a metric graph.

A *graph-like manifold* (associated to X_0) is a family of d-dimensional manifolds X_ε ($d \geq 2$) which can be decomposed into

$$X_\varepsilon = \bigcup_{e \in E} X_{\varepsilon,e} \cup \bigcup_{v \in V} X_{\varepsilon,v} \tag{6}$$

such that the closed sets $X_{\varepsilon,e}$ and $X_{\varepsilon,v}$ are disjoint or intersect only in submanifolds of dimension $d-1$. The so-called *edge* and *vertex neighbourhoods* $X_{\varepsilon,e}$ and $X_{\varepsilon,v}$ are supposed to have the following structure (cf. Fig. 2):

- The edge neighbourhood $X_{\varepsilon,e}$ is a cylinder, i.e., $X_{\varepsilon,e} := I_e \times \varepsilon Y_e$, where Y_e is a compact Riemannian manifold (with or without boundary) with metric h_e, called *transversal manifold*, and where εY_e denotes the *ε-homothetically scaled* Riemannian manifold, i.e., the manifold Y_e with metric $h_{\varepsilon,e} := \varepsilon^2 h_e$. In particular, X_ε carries the metric $g_e = ds^2 + \varepsilon^2 h_e$.
- The vertex neighbourhood $X_{\varepsilon,v}$ is ε-homothetic to a fixed Riemannian manifold X_v with metric g_v, i.e., $X_{\varepsilon,v}$ carries the metric $g_{\varepsilon,v} = \varepsilon^2 g_v$. Moreover, we assume that the boundary ∂X_v of X_v contains a subset $\mathring{\partial} X_v$ which is isometric to the disjoint union of Y_e, e adjacent to v.

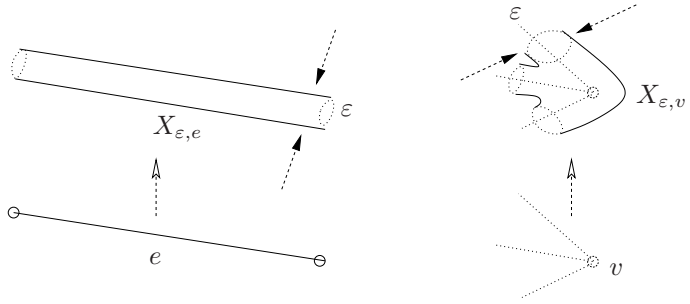

Fig. 2. An edge and an vertex neighbourhood associated to an edge e and a vertex v with three adjacent edges.

Let us give now an important example, which is a graph-like manifold in the sense above only in an *approximate* sense: Let $\widetilde{X}_\varepsilon$ denote the (closed) ε-neighbourhood of a metric graph X_0 embedded in $\mathbb{R}^d$ (such that the edges in a vertex meet non-tangentially), then a decomposition similar to (6) yields edge neighbourhoods $\widetilde{X}_{\varepsilon,e}$ with are only *approximate* cylinders of length ℓ_e, and vertex neighbourhoods $\widetilde{X}_{\varepsilon,v}$, which are only *approximately* ε-homothetic to a fixed manifold X_v.

First, this is due to the fact that the vertex neighbourhood needs some space, so that the length of the cylinder is only $\ell_e - 2\varepsilon$. Second, the embedded edge need

not to be straight. In both cases, one can show that the error made by introducing the coordinates $(s, y) \in I_e \times Y_e$ on the approximate cylinder $\widetilde{X}_{\varepsilon,e}$ yields a metric $\widetilde{g}_{\varepsilon,e}$ which is *close* to $g_{\varepsilon,e}$ up to some ε-depending errors. We call a space $\widetilde{X}_\varepsilon$ which is a graph-like manifold only up to small ε-depending errors a *thick graph*. A more detailed discussion of these errors can be found e.g. in [34, Secs. 5.3–5.6 and 6.7]. For simplicity, we call graph-like manifolds also *thick graphs*.

At first sight, the definition of a graph-like manifold looks pretty abstract in comparison with the concrete definition of a thick graph. The main reason for using the spaces $X_{\varepsilon,e}$ and $X_{\varepsilon,v}$ is to have ε-*independent* coordinates $(s, y) \in X_e = I_e \times Y_e$ and $x \in X_v$, and to put the ε-dependence only in the *metric* of the Riemannian manifold. This is a significant simplification in the reduction to a graph model; the particular error estimates coming from a concrete embedding of the metric graph X_0 into some ambient space do not enter into this reduction step.

For other shrinking behaviour at the vertices, we refer to [12, 24, 34].

2.1.3. *Operators on thick graphs*

On a thick graph, we typically consider a Laplace-like operator, e.g., the Neumann-Laplacian (if X_ε has boundary) or the Laplacian on X_ε (if X_ε has no boundary) defined via its quadratic form

$$\mathfrak{d}_{X_\varepsilon}(u) := \int_{X_\varepsilon} |du|^2_{g_\varepsilon}, \quad \mathscr{H}_\varepsilon := \mathsf{H}^1(X_\varepsilon), \tag{7}$$

in the Hilbert space $\mathscr{H} := \mathsf{L}_2(X_\varepsilon)$. Note that the Neumann boundary condition $\partial_{\mathrm{n}} u = 0$ on ∂X_ε only enters in the corresponding *operator* domain via a partial integration formula.

We will see below that the Neumann case and the Laplacian on a manifold without boundary can be treated in the same way. The main reason for this fact is that on the transversal manifolds Y_e, the lowest eigenfunction is *constant* in both cases with corresponding eigenvalue 0.

If $\partial X_\varepsilon \neq \emptyset$, then we also consider the Dirichlet-Laplacian $\Delta^{\mathrm{D}}_{X_\varepsilon}$ on X_ε defined via the quadratic form $\mathring{\mathfrak{d}}_{X_\varepsilon}$ defined as above, but with domain $\operatorname{dom} \mathring{\mathfrak{d}}_{X_\varepsilon} := \mathring{\mathsf{H}}^1(X_\varepsilon)$, the closure of $\mathsf{C}^\infty_{\mathrm{c}}(X_\varepsilon)$ of the space of smooth functions with compact support *away* from ∂X_ε in $\mathsf{H}^1(X_\varepsilon)$.

2.2. *Examples of thick graphs*

The thick graph X_ε may have boundary or not, depending on whether the transversal manifolds Y_e have boundary or not.

2.2.1. *An abstract example*

We can construct a graph-like manifold X_ε according to a given metric graph X_0 by associating appropriate manifolds Y_e and X_v to each edge e and vertex v as in

Sec. 2.1.2. It is not difficult to see that one can define a globally smooth metric g_ε on the underlying manifold such that the decomposition (6) holds with $X_{\varepsilon,e} = I_e \times \varepsilon Y_e$ and $X_{\varepsilon,v} = \varepsilon X_v$ (see also Fig. 2).

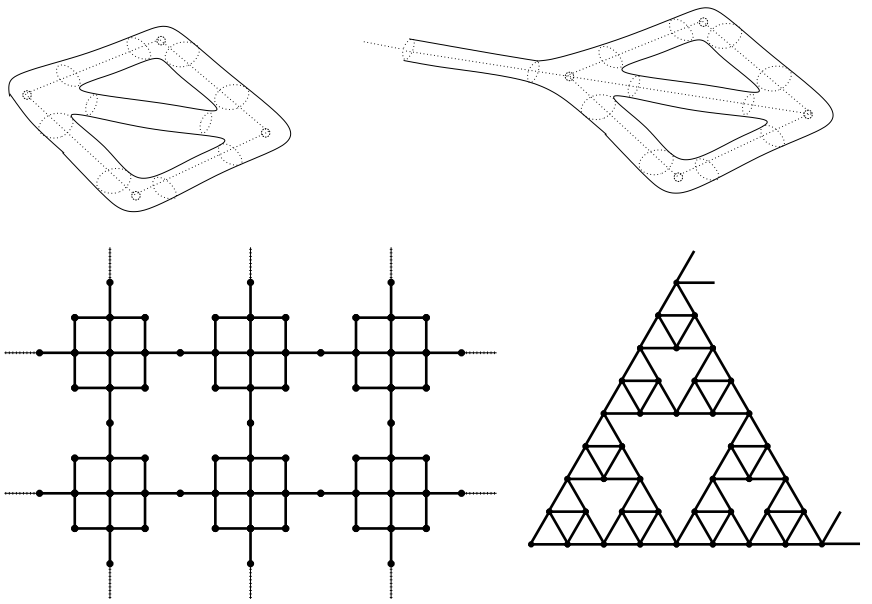

Fig. 3. Four examples of thick graphs: the first two are examples of thick graphs, viewed either as 2-dimensional manifold without boundary (the surface of the pipeline network) or as 3-dimensional manifold with boundary. The examples in the second row correspond to the periodic and self-similar metric graphs of Fig. 1.

2.2.2. *Examples with boundary from embedded graphs*

Let X_0 be a metric graph embedded in $\mathbb{R}^d$ such that the angle between two edges meet in a vertex always with a non-zero angle. Let $\widetilde{X}_\varepsilon$ be the ε-neighbourhood, then $\widetilde{X}_\varepsilon$ is close to a thick graph X_ε as discussed above. This example has boundary, and corresponds to the case with transversal manifold Y_e being a ball in $\mathbb{R}^d$. In this situation, the boundary ∂X_ε may have corners (but with non-zero angle). This does not bother us, inasmuch as we can define a Neumann Laplacian with compact resolvent (if X_ε is compact).

2.2.3. *Examples without boundary*

If we choose $\widetilde{X}_\varepsilon$ to be (a smoothed version of) the boundary of the ε-neighbourhood of an embedded graph in $\mathbb{R}^{d+1}$ as above, then we obtain an example which is close to a thick graph X_ε (a d-dimensional manifold without boundary), with transversal manifold being a $(d-1)$-dimensional in $\mathbb{R}^d$ (see also Fig. 3).

2.3. *Appearance of thick graphs in Physics and Mathematics*

2.3.1. *Physical models*

Possibly the first time thick graphs appeared is in [36], where Ruedenberg and Scherr used thick graphs as justification of quantum graph models for the spectra of aromatic hydrocarbons. Although the justification is mathematically not correct (the limit of a shifted Dirichlet Laplacian on a thick graph is generally *not* the Kirchhoff Laplacian, see Sec. 4), the quantum graph models lead to a good approximation of the spectra.

Since quantum graphs are generally believed to provide good models for electronic and optical nano-structures, a natural question arises:

Is the quantum graph model a good approximation of a physically more realistic system with finite, but non-vanishing thickness $\varepsilon > 0$*?*

Moreover, one is interested in modelling devices with certain properties like a quantum switch modelled by a certain vertex condition in a quantum graph.

Is it possible to find a thick graph model converging to a prescribed quantum graph vertex coupling?

On a quantum graph, many physical properties like the conductance or existence of bound states can be calculated explicitly. Such models are called *solvable models*, since mathematically, the calculation on a quantum graph mostly reduces to a system of coupled ODEs. Note that the conductance of a periodic medium (a periodic semi-conductor or a photonic crystal transmitting light) is guaranteed if the spectrum of the corresponding operator has *band structure* and is absolutely continuous. If the energy of a particle lies in such a band, then it can "travel" through the medium; if the energy lies outside the bands (i.e., in a *spectral gap*, then no transport is possible.

Thick graph models are also used in other areas; e.g. thick graphs as models for proteins have been analysed recently in [29].

2.3.2. *Thick graphs in Mathematics: Spectral geometry*

In Spectral Geometry, one investigates relations of the spectrum of the Laplacian (or related operators) on a Riemannian manifold to its geometry. Graph-like manifolds may serve as toy models in order to show certain properties, or to disprove a conjecture. Maybe the first mathematical treatment of convergence results for thick graphs is provided by Colin de Verdière [7]:

Theorem 2.1. *Given a compact oriented manifold* M *of dimension* $d \geq 3$ *without boundary and a natural number* $n \geq 1$*, then there exists a metric* g_n *such that the first non-zero eigenvalue of the associated Laplacian has multiplicity* n*.*

In dimension 2, the multiplicity of the non-zero eigenvalues is bounded from above by the genus of the surface (see [4]). If $d \geq 3$, Colin de Verdière embeds a complete metric graph X_0 with $n+1$ vertices in M. Such an embedding is possible, since

$\dim M \geq 3$. Then he deforms a given metric g on M into a family of metrics $\{g_\varepsilon\}$ such that g_ε equals g on a small ε–neighbourhood X_ε of X_0 and which is small outside. He then shows that the eigenvalues of $\Delta_{(M,g_\varepsilon)}$ are close to the eigenvalues of the Neumann Laplacian on $(X_\varepsilon, g_\varepsilon)$. In a second step, it can be seen that these Neumann eigenvalues converge to the eigenvalues of the Kirchhoff Laplacian on X_0, using methods discussed below (cf. Theorem 3.1). If all lengths of the metric graph are the same, then the first non-zero eigenvalue of the Kirchhoff Laplacian has the desired multiplicity n. The use of enough parameters (the lengths of the edges in the metric graph X_0) allows to find a path in this parameter space such that the multiplicity is preserved. A similar construction is used in [8] in order to show the following more general result: Let $d \geq 3$, and let $\lambda_1 = 0 < \lambda_2 \leq \cdots \leq \lambda_n$ be a sequence of n numbers. Then there exists a metric g such that the corresponding Laplacian has $\lambda_1, \ldots, \lambda_n$ as its first n eigenvalues.

2.3.3. *Thick graphs in Mathematics: Global analysis*

The heat kernel of a Riemannian manifold X is the smallest positive fundamental solution to the heat equation $-\partial_t u = \Delta_X u$ (recall that $\Delta_X \geq 0$).

On a complete Riemannian manifold X with non-negative Ricci curvature, Li and Yau [25] showed that the heat kernel $p_t(x, y)$ has the asymptotic behaviour (8) with $\beta = 2$ for all times t, i.e., the heat kernel behaves very similar as the heat kernel of the Laplacian on $X = \mathbb{R}^d$, namely

$$p_t(x, y) = \frac{1}{(4\pi t)^{d/2}} \exp\Big(-\frac{|x-y|^2}{4t}\Big)$$

for $t > 0$ and $x, y \in \mathbb{R}^d$. In contrast, on self-similar graphs X_0 (like the Sierpiński graph, see Fig. 1), in general, a different asymptotic behaviour occurs, e.g.,

$$p_t(x, y) \sim \frac{1}{\operatorname{vol} B_x(\sqrt{t})} \exp\Big(-\frac{d(x, y)^\beta}{ct}\Big) \tag{8}$$

for some $c > 0$ and $\beta = \log 5/\log 2 > 2$ for the Sierpiński graph, where $d(x, y)$ denotes the geodesic distance between the points $x, y \in X$ and $\operatorname{vol} B_x(r)$ denotes the volume of a geodesic ball $B_x(r)$.

Up to recent time it was believed that Gaussian estimates with $\beta > 2$ are typical only for such self-similar spaces Surprisingly, one can construct a fractal-like Riemannian manifold X according to the metric graph X_0 having the Gaussian estimate with $\beta = \log 5/\log 2 > 2$ for *large* times t, and the classical Gaussian estimate $\beta = 2$ for *short* times (see [1, 2] and references therein).

From a probabilistic point of view, this behaviour can be understand as follows: $p_t(x, y)$ is the probability density that a particle starting at the point x is at the point y in time t. A particle moving on a fractal-like manifold sees the smooth structure for short times, but for large times, the fractal nature becomes apparent.

3. Neumann Laplacians on thick graphs

Let X_ε be a thick graph constructed from the building blocks $X_{\varepsilon,v} = \varepsilon X_v$ and $X_{\varepsilon,e} = I_e \times \varepsilon Y_e$ with transversal manifolds εY_e. Let H_ε be the Laplacian on X_ε (in our notation, $H_\varepsilon \geq 0$) associated to the quadratic form $\mathfrak{d}_{X_\varepsilon}$, cf. (7). If $\partial X_\varepsilon \neq \emptyset$ we assume Neumann boundary conditions.

On the limit space, the metric graph, we consider a *weighted* Kirchhoff Laplacian, namely, $(H_0 f)_e = -f_e''$ for $f \in \mathsf{H}^2_{\max}(X_0)$ fulfilling

$$f \text{ continuous}, \qquad \sum_{e \in E_v} (\mathrm{vol}_{d-1} Y_e) f_e'(v) = 0. \tag{9}$$

3.1. *Convergence results for Neumann Laplacians*

Let us first assume that the thick graph and the metric graph are compact. In this case, H_ε and H_0 have purely discrete spectrum, denoted by $\lambda_k(H_\varepsilon)$ and $\lambda_k(H_0)$, written in increasing order and repeated according to their multiplicity.

The following convergence result on the discrete spectrum shows that the Kirchhoff Laplacian on the metric graph is natural in the sense that it occurs as a limit of an ε-neighbourhood of the graph. It was proven for the first time by Colin de Verdière, where he showed Theorem 2.1 above. Since this convergence result is used as a technical step only and presented in a brief way, the paper seemed to be overlooked in much of the mathematical physics community until recently. Later on, Rubinstein-Schatzman [35] proved it in a concrete embedded situation, and Kuchment-Zeng [23] simplified some arguments. In [12] we introduced *graph-like manifolds* and stressed the geometric point of view of the analysis.

Theorem 3.1. *Let X_ε be a compact thick graph with underlying compact metric graph X_0, and let H_ε be the (Neumann-)Laplacian on X_ε, and let H_0 be the weighted Kirchhoff Laplacian on X_0, then*

$$\lambda_k(H_\varepsilon) - \lambda_k(H_0) = \mathscr{O}(\varepsilon^{1/2}) \qquad \text{as } \varepsilon \to 0.$$

Idea of the proof: The proof uses a variational characterisation of eigenvalues (the *Min-max principle*) and identification operators for quadratic form domains $J^1 \colon \mathsf{H}^1(X_0) \to \mathsf{H}^1(X_\varepsilon)$ and $J'^1 \colon \mathsf{H}^1(X_\varepsilon) \to \mathsf{H}^1(X_0)$. The main step in the proof is then to compare the Rayleigh quotients

$$\frac{\|f'\|^2_{\mathsf{L}_2(X_0)}}{\|f\|^2_{\mathsf{L}_2(X_0)}} \qquad \text{and} \qquad \frac{\|du\|^2_{\mathsf{L}_2(X_\varepsilon)}}{\|u\|^2_{\mathsf{L}_2(X_\varepsilon)}}. \qquad \square$$

In all of the above-cited papers, the underlying spaces are assumed to be compact, and therefore, only the discrete spectrum was considered, and the spectral convergence does not (directly) imply the convergence of eigenfunctions. We introduce the following notion of *convergence of operators acting in different Hilbert spaces*, developed (to our knowledge) for the first time in [31]; implying in particular

the convergence of the discrete and essential spectrum for non-compact graph-like spaces (in the fast decaying case).

Definition 3.1. For each $\varepsilon \geq 0$, let H_ε be a non-negative operator acting in a Hilbert space $\mathscr{H}_\varepsilon$. We say that $H_\varepsilon \xrightarrow{\text{gnr}} H_0$ *in the generalised norm resolvent sense* of order $\mathscr{O}(\varepsilon^{1/2})$ iff there is a bounded operator $J\colon \mathscr{H}_0 \to \mathscr{H}_\varepsilon$ such that

$$J^*J = \mathrm{id}_0, \quad \|(\mathrm{id}_\varepsilon - JJ^*)R_\varepsilon\| = \mathscr{O}(\varepsilon^{1/2}) \quad \text{and} \quad \|JR_0 - R_\varepsilon J\| = \mathscr{O}(\varepsilon^{1/2}),$$

where $R_\varepsilon := (H_\varepsilon + 1)^{-1}$ denotes the resolvent for $\varepsilon \geq 0$.

This is not the most general condition, more details can be found in [34].

For the following result, we need some uniformity conditions on the metric and thick graph: We say that a metric graph X_0 is *uniform* iff there is a positive lower bound on the edge lengths, cf. (4).[a] We say that a graph-like manifold X_ε is *uniform* iff

$$\inf_{e\in E} \lambda_2^{\mathrm{N}}(Y_e) > 0, \quad \inf_{v\in V} \lambda_2^{\mathrm{N}}(X_v) > 0 \quad \text{and} \quad \sup_{v\in V} \frac{\mathrm{vol}_d X_v}{\mathrm{vol}_{d-1} \mathring{\partial} X_v} < \infty. \tag{10}$$

Here, $\lambda_2^{\mathrm{N}}(M)$ denotes the second (first non-zero) eigenvalue of the Neumann Laplacian on the manifold M. Recall that $\mathring{\partial} X_v$ is the part of the boundary of X_v where the edge neighbourhoods are attached.

For a thick graph (in our notation, a graph-like manifold up to some error terms), one needs in general more assumptions on the embedding, e.g., one needs a lower bound on the angles of two adjacent edges at a vertex, and upper bounds on the curvature of an edge embedded in $\mathbb{R}^d$, cf. [31] and [34, Sec. 6.7].

The following result was first proven in [31], see also [34]:

Theorem 3.2. *Let X_ε be a uniform thick graph with underlying uniform metric graph X_0, and let H_ε be the (Neumann-)Laplacian on X_ε, and let H_0 be the weighted Kirchhoff Laplacian on X_0 defined in* (9)*, then $H_\varepsilon \xrightarrow{\text{gnr}} H_0$ of order $\mathscr{O}(\varepsilon^{1/2})$. Moreover, the error depends only on the bounds in* (4) *and* (10)*.*

Idea of the proof. Let us motivate why a condition like $\|(\mathrm{id}_\varepsilon - JJ^*)R_\varepsilon\| = \mathscr{O}(\varepsilon^{1/2})$ should be true:

- JJ^* is the projection onto *transversally constant* functions, and functions vanishing on vertex neighbourhoods $X_{\varepsilon,v}$;
- functions in $(\operatorname{ran} JJ^*)^\perp$ have high energy (spectral parameter of H_ε);
- the resolvent "cuts off" high energies.

In other words: eigenfunctions u_ε of H_ε with bounded eigenvalues $\lambda_\varepsilon \leq \mathrm{const}$ *do not concentrate* on $X_{\varepsilon,v}$ and are almost *transversally constant*. Actually, the arguments for a rigorous proof of $H_\varepsilon \xrightarrow{\text{gnr}} H_0$ are very similar to the arguments for the proof of Theorem 3.1. □

[a] In [31], we assumed additionally that the graph has uniformly bounded vertex degrees. Actually, this is not needed, cf. [34].

Freidlin and Wentzell consider the problem from a probabilistic point of view in [16]. They show that a suitable Markov process on a thin graph neighbourhood converges to a Markov process on the metric graph. In essence, they prove strong resolvent convergence of the Laplacian with Neumann boundary conditions on the graph neighbourhood to a Laplace-type operator on the metric graph. A similar result for tree graphs is proven by Saito in [37].

Results for certain classes of *compact* manifolds converging in the Gromov-Hausdorff distance are given in the works of Kasue [20, 21] (see also the references therein and [3, 17] for related results); in particular, the convergence of the discrete spectrum and *strong* convergence of resolvents is shown. Typically, these results need some uniform curvature bounds, which are in general not fulfilled for a family $\{X_\varepsilon\}_\varepsilon$ of graph-like manifolds, and imply only *strong* resolvent convergence.

For the convergence of resonances, we refer to [13] and the survey article [14].

3.2. *Convergence of operators in different Hilbert spaces*

Let us comment on the generalised norm resolvent convergence, cf. [31] and [34, Ch. 4] for more results):

Theorem 3.3. *Assume that* $H_\varepsilon \xrightarrow{\text{gnr}} H_0$*, then the following assertions hold:*

(i) Convergence of operator functions: *We have*

$$\|\varphi(H_\varepsilon)J - J\varphi(H_0)\| \to 0 \quad \textit{and} \quad \|\varphi(H_\varepsilon) - J\varphi(H_0)J^*\| \to 0$$

for suitable functions φ *(in particular,* $\lim_{\lambda\to\infty}\varphi(\lambda)$ *exists), e.g.* $\varphi(\lambda) = \mathrm{e}^{-t\lambda}$ *or* $\varphi = \mathbb{1}_I$*,* $I \subset \mathbb{R}$ *with* $\partial I \cap \sigma(H_0) = \emptyset$*.*

(ii) Convergence of discrete spectrum: *Let* λ_0 *be a (for simplicity) simple discrete eigenvalue of* H_0 *with corresponding normalised eigenfunction* φ_0*, then there exist simple discrete eigenvalues* λ_ε *of* H_ε *with corresponding eigenfunctions* φ_ε *such that* $\lambda_\varepsilon \to \lambda_0$ *and* $\|J\varphi_0 - \varphi_\varepsilon\| \to 0$*.*

(iii) Convergence of essential spectrum: $\sigma_{\text{ess}}(H_\varepsilon) \to \sigma_{\text{ess}}(H_0)$ *converges uniformly in* $[0, \Lambda]$ *for all* $\Lambda > 0$*. In particular,* H_ε *has a spectral gap if* H_0 *has (provided* $\varepsilon > 0$ *is small enough).*

In particular, the convergence of all discrete eigenvalues Theorem 3.1 follows. Under certain additional assumptions (*positivity* and *contractivity*, fulfilled for the above example of the Neumann Laplacian on a thick graph, we also have convergence of $\varphi(H_\varepsilon) - J\varphi(H_0)J^* \to 0$ in the operator norm on $\mathscr{B}(\mathsf{L}_p(X_\varepsilon))$ (cf. [28]).

As a consequence for thick graphs, we know that a thick graph has spectral gaps once the corresponding metric graph has spectral gaps. A typical example of an operator having spectral gaps is given by a *periodic* operator; in [26], we showed, that the Kirchhoff Laplacian on the periodic graph of Fig. 1 (lower left) has spectral gaps; so the same is true for a corresponding thick graph.

Another interesting example is given by the self-similar *Sierpiński graph*: Teplyaev showed in [38] that the spectrum of the discrete Laplacian on this graph

is fractal, a simple argument shows that the same is true for a corresponding (equilateral) metric graph (cf. e.g. [32]). In particular, $\sigma(H_0)$ has *infinitely* many components in any *compact* spectral interval $I \subset [0,\infty)$. Therefore, Theorem 3.3 implies that the number of components of $\sigma(H_\varepsilon) \cap I$ tends to ∞ as $\varepsilon \to 0$. Note that our analysis is too weak in order to show that the number of components is actually infinite for a positive $\varepsilon > 0$.

4. Dirichlet and other Laplacians on thick graphs

4.1. *Dirichlet Laplacians on thick graphs*

Let us now review some results concerning the *Dirichlet* Laplacian on a thick graph. For a more detailed review especially on the Dirichlet case we refer to [19]. Related results are proven in [10, 27].

Let us assume (for simplicity) that X_ε is a *compact* graph-like manifold associated to a metric graph X_0. Moreover, we assume that X_ε has "straight" edge neighbourhoods $X_{\varepsilon,e} = I_e \times \varepsilon Y_e$ (the non-compact case and the case of curved embedded edges can be found in [33, Sec. 6.11].

We assume that each transversal manifold has non-empty boundary $\partial Y_e \neq \emptyset$. On a single tubular neighbourhood $X_{\varepsilon,e} = [0,1] \times \varepsilon Y_e$ with Dirichlet conditions on $[0,\ell_e] \times \varepsilon \partial Y_e$ and Neumann conditions on $\{0,\ell_e\} \times \varepsilon Y_e$, the spectrum is given by

$$\sigma(\Delta^{\mathrm{DN}}_{X_{\varepsilon,e}}) = \Big\{ \frac{p^2\pi^2}{\ell_e^2} + \frac{\lambda_q(\Delta^{\mathrm{D}}_{Y_e})}{\varepsilon^2} \,\Big|\, p = 0,1,\dots, q = 1,2,\dots \Big\}, \tag{11}$$

where $\lambda_q(\Delta^{\mathrm{D}}_{Y_e})$ denotes the q-th Dirichlet eigenvalue of Y_e. Since the first Dirichlet eigenvalue is non-negative, we have to consider a *shifted* operator in order to expect a convergence limit. Let $\lambda_1 := \min_e \lambda_1(\Delta^{\mathrm{D}}_{Y_e})$ and set

$$H_\varepsilon := \Delta^{\mathrm{D}}_{X_\varepsilon} - \frac{\lambda_1}{\varepsilon^2}.$$

Note that only the "thickest" edges (i.e., the edges with $\lambda_1 = \lambda_1(\Delta^{\mathrm{D}}_{Y_e})$) count. Let us assume for simplicity that $\lambda_1 = \lambda_1(\Delta^{\mathrm{D}}_{Y_e})$ for all edges $e \in E$.

A first result for the Dirichlet Laplacian is the following (cf. [30]):

Theorem 4.1. *Let* $H_\varepsilon = \Delta^{\mathrm{D}}_\varepsilon - \lambda_1/\varepsilon^2$. *If* $\min_v \lambda_1(\Delta^{\mathrm{DN}}_{X_v}) > \lambda_1$ *then*

$$\lambda_k(H_\varepsilon) \to \lambda_k(H_0),$$

where $H_0 = \bigoplus_e \Delta^{\mathrm{D}}_{I_e}$ *is the* decoupled *Dirichlet Laplacian on the metric graph* X_0.

A vertex neighbourhood X_v fulfilling the condition $\lambda_1(\Delta^{\mathrm{DN}}_{X_v}) > \lambda_1(Y_e)$ may look like in Fig. 4. Here, $\Delta^{\mathrm{DN}}_{X_v}$ is the Laplacian on X_v with Neumann boundary conditions at the "inner" boundary $\mathring{\partial} X_v$ (where the edge neighbourhoods are attached) and with Dirichlet conditions on the remaining part. We call such manifolds X_v *spectrally small*. Note that this condition implies that $H_\varepsilon \geq 0$: Introducing additional Neumann boundary conditions at the junctions of $X_{\varepsilon,e}$ and $X_{\varepsilon,v}$ gives a lower bound

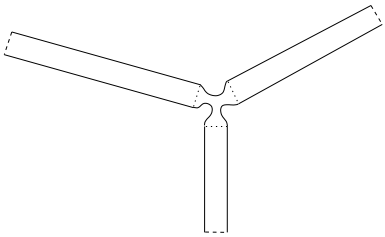

Fig. 4. A vertex neighbourhood X_v in the centre which is *spectrally small*. For the graph-like manifold, the whole space is scaled by ε.

on the shifted Dirichlet Laplacian, i.e.,

$$H_\varepsilon \geq \bigoplus_e \Big(\Delta^{\mathrm{DN}}_{X_{\varepsilon,e}} - \frac{\lambda_1}{\varepsilon^2}\Big) \oplus \bigoplus_v \Big(\Delta^{\mathrm{DN}}_{X_{\varepsilon,v}} - \frac{\lambda_1}{\varepsilon^2}\Big).$$

Now the shifted Laplacians on $X_{\varepsilon,e}$ are non-negative since λ_1 is the lowest transversal mode, see (11), and the shifted Laplacians on $X_{\varepsilon,v}$ are non-negative since X_v is spectrally small and since $\Delta^{\mathrm{DN}}_{X_{\varepsilon,v}} - \lambda_1/\varepsilon^2 = \varepsilon^{-2}(\Delta^{\mathrm{DN}}_{X_v} - \lambda_1)$.

Note that the usual ε-neighbourhood is *not* spectrally small, as one can easily see by inserting test functions in the Rayleigh quotient of the quadratic form associated to H_ε. One obtains that there are eigenvalues $\tau_k(\varepsilon)$ of H_ε with associated eigenfunctions localised near $X_{\varepsilon,v}$ such that $\tau_k(\varepsilon) \to -\infty$ as $\varepsilon \to 0$ (from Theorem 4.2 below we actually conclude $\tau_k(\varepsilon) = (\tau_k - \lambda_1)/\varepsilon^2 < 0$).

A full description of the asymptotic behaviour of the Dirichlet spectrum (and other boundary conditions) was first given in [18, 27]. The main observation is to consider the rescaled space

$$\varepsilon^{-1} X_\varepsilon \to \bigcup\nolimits_v^{\cdot} X_v^\infty =: X^\infty \qquad \text{as } \varepsilon \to 0,$$

i.e., to turn the rescaled compact space $\varepsilon^{-1}X_\varepsilon$ into a disjoint union of the star graph neighbourhoods X_v^∞ with infinite edges attached.

Denote by $\tau_1, \dots, \tau_{k_0}$ the L_2-eigenvalues of the Dirichlet Laplacian $\Delta^{\mathrm{D}}_{X^\infty}$ on X^∞ *below* the threshold λ_1. The first result is the following (see [18, 27]):

Theorem 4.2. *The eigenvalues of the Dirichlet Laplacian on the graph-like manifold X_ε below the threshold λ_1 have the asymptotic expansion $\lambda_k(\Delta^{\mathrm{D}}_{X_\varepsilon}) = \dfrac{\tau_k}{\varepsilon^2} + \mathscr{O}(\mathrm{e}^{-c/\varepsilon})$ for $k = 1, \dots, k_0$ as $\varepsilon \to 0$.*

Note that the spectral smallness assumption $\lambda_1(\Delta^{\mathrm{DN}}_{X_v}) > \lambda_1$ implies that there are no such eigenvalues (i.e., $k_0 = 0$).

Let us now treat the spectrum without these low-lying eigenvalues located at the vertex neighbourhoods. Denote by $H_\varepsilon := (\Delta^{\mathrm{D}}_{X_\varepsilon} - \lambda_1/\varepsilon^2)_+$ the non-negative part of the shifted Laplacian, where $A_+ := \mathbb{1}_{[0,\infty)}(A)A$.

It turns out that the asymptotic behaviour of the Dirichlet eigenvalues is determined by a *scattering problem* on the star graph neighbourhood X_v^∞. Denote by

$S_v(\lambda)$ the *scattering matrix* of $\Delta^{\mathrm{D}}_{X_v^\infty}$ at the energy $\lambda \geq \lambda_1$, which is a $(\deg v \times \deg v)$-matrix.

Let $\mathscr{V}_v := \ker(S_v(\lambda_1) - 1)$, and let H_0 be the Laplacian on the underlying metric graph X_0 with vertex conditions

$$\{f_e(v)\}_{e\in E_v} \in \mathscr{V}_v \quad \text{and} \quad \{f'_e(v)\}_{e\in E_v} \in \mathscr{V}_v^\perp \subset \mathbb{C}^{E_v}. \tag{12}$$

Note that this vertex condition turns out to be the (unweighted) Kirchhoff condition if $\mathscr{V}_v = \mathbb{C}(1, \dots, 1)$.

Grieser [18] proved the following result (see also the results of Molchanov and Vainberg [27]):

Theorem 4.3. *Let $H_\varepsilon := (\Delta^{\mathrm{D}}_{X_\varepsilon} - \lambda_1/\varepsilon^2)_+$ be the non-negative part of the shifted Dirichlet Laplacian on a compact graph-like manifold X_ε, and let H_0 be the metric graph Laplacian with vertex condition as in* (12)*, then the k-th eigenvalue has the asymptotics $\lambda_k(H_\varepsilon) - \lambda_k(H_0) = \mathscr{O}(\varepsilon)$ as $\varepsilon \to 0$.*

Note that Grieser's also gives an asymptotic expansion of the eigenvalues. This method also applies to other boundary conditions. In the Neumann case, this method gives the right error term of order ε instead of $\varepsilon^{1/2}$ as obtained by the simpler eigenvalue comparison techniques of Theorem 3.1.

4.2. *Difference between Neumann and Dirichlet case*

Let us make some comments why the case of Neumann boundary conditions on a thick graph is much easier to treat than the case of Dirichlet (or other) boundary conditions:

Let us first give an interpretation of the scattering matrix $S_v(\lambda)$ of the Dirichlet Laplacian on the star graph neighbourhood X_v^∞. One observes that the *vertex space* $\mathscr{V}_v$ (the range of the function values $\{f_e(v)\}_{e\in E_v}$ in a vertex condition), defined by $\mathscr{V}_v := \ker(S_v(\lambda_1) - 1)$ is *non-trivial* iff there exist *generalised (bounded) eigenfunctions* ψ_v such that $\psi_{v,e}(x, y) \sim \varphi_e(y)$ as $x \to \infty$ on the edge neighbourhood X_e ($e \in E_v$), where φ_e is the eigenfunction on Y_e associated to λ_1: Such functions ψ_v are called *energy resonance at* λ_1.

As a consequence, a *non-trivial* coupling at the vertex v, i.e., a vertex space $\mathscr{V}_v \neq 0$, is a "rare" event: generically, one only has a decoupling *Dirichlet* vertex condition as in Theorem 4.1. Actually, the spectral smallness condition ensures that there is no energy resonance at λ_1.

In the Neumann (or boundaryless) case, the threshold is $\lambda_1 = 0$, and the energy resonance at 0 is just given by the constant function $\psi_v = \mathbb{1}$, and the corresponding vertex space is $\mathscr{V}_v = \mathbb{C}(1, \dots, 1)$. Note that in this case, the energy resonance function $\psi_v = \mathbb{1}$ *exactly* matches with the lowest transversal eigenfunctions φ_e (appropriately scaled), which are also constant, i.e., we have $\psi_e(x, y) = \varphi_e(y)$ for *all* $(x, y) \in X_e$.

Since this energy resonance function at 0 does not see the geometry of X_v, it is not seen in the limit operator, the Kirchhoff Laplacian, either. Moreover, the

embedding of the metric graph X_0 into an ambient space like $\mathbb{R}^2$ does not enter in the limit either. In contrast, in the Dirichlet case, a curved edge leads to an additional potential on the metric graph determined by the curvature of the edge, see [30], [34, Sec. 6.11] and references therein.

4.3. *Other vertex conditions in the limit*

We first give a non-existence result for certain vertex couplings. We claim that it is impossible to approximate a delta-coupling by a pure Laplacian, using a topological argument.

Let H_0 be the the Laplacian on a compact metric graph X_0 with delta-coupling of strength $q(v) > 0$ at each vertex v, i.e., $(H_0 f)_e = -f_e''$, and

$$f \text{ is continuous and } \quad \sum_{e \in E_v} f_e'(v) = q(v) f(v). \tag{13}$$

Note that $H_0 \geq 0$ iff $q(v) \geq 0$ for all $v \in V$. We formally write $H_0 = \Delta_{X_0} + \sum_v q(v)\delta_v$ for this vertex condition.

We now want to factorise H_0 as $H_0 = d_0^* d_0$. An easy calculation shows that this can be done by choosing $d_0 f := (f', (\sqrt{q(v)})_v) \in \mathsf{L}_2(X_0) \oplus \mathbb{C}^V =: \mathscr{H}_0$ with $\operatorname{dom} d_0 = \mathsf{H}^1(X_0)$, the Sobolev space of order 1 with *continuous* functions at the vertices. Similarly, we can factorise the Laplacian on a graph-like manifold as $H_\varepsilon = d_\varepsilon^* d_\varepsilon$ with $d_\varepsilon u \in \mathsf{L}_2^{\text{exact}}(T^* X_\varepsilon) =: \hat{\mathscr{H}}_\varepsilon$, the space of *exact* 1-forms.

A simple example is given as follows: Let $X_0 = \mathbb{S}^1$ be a loop graph with only one vertex v, and let $X_\varepsilon = \mathbb{S}^1 \times_{r_\varepsilon} Y$ be a *warped product*, i.e., the product manifold with metric $g_\varepsilon = \mathrm{d}x^2 + r_\varepsilon(x)^2 h$, where (Y, h) is a closed manifold. Note that the warped product here corresponds to a manifold $\mathbb{S}^1 \times Y$ with variable radius given by the function $r_\varepsilon(x)$. It is an easy calculation that the index $\operatorname{ind} d_0$ (defined as $\operatorname{ind} d_0 := \dim \ker d_0 - \dim \ker d_0^*$) equals 0 on the loop graph, but $\operatorname{ind} d_\varepsilon = 1$ on the warped product.

As a consequence of the different indices we claim (work in progress with Claudio Cacciapuoti):

Conjecture 4.1. *It is impossible to approximate a (non-trivial) delta-coupling H_0 via a pure Laplacian $H_\varepsilon = \Delta_{X_\varepsilon}$ with $X_\varepsilon = \mathbb{S}^1 \times_{r_\varepsilon} Y$ such that $H_\varepsilon \xrightarrow{\text{gnr}} H_0$.*

The arguments leading to this conjecture are rather simple: Since $H_\varepsilon \geq 0$ the limit operator also has to be non-negative, i.e., i.e., $q(v) \geq 0$. Moreover, H_ε is unitarily equivalent to the family of one-dimensional Schrödinger operators

$$\{H_{0,k}\}_k = \Big(-\frac{d^2}{\mathrm{d}x^2} + K_\varepsilon + \frac{\lambda_k(Y)}{r_\varepsilon^2} \Big)_k, \quad \text{where} \quad K_\varepsilon = P_\varepsilon^2 + P_\varepsilon', \quad P_\varepsilon := \frac{m}{2} \cdot \frac{r_\varepsilon'}{r_\varepsilon}$$

and $m = \dim Y$. If one tries to approximate a delta-coupling by the lowest member of the family $H_{0,0} f = -f'' + K_\varepsilon f$ for appropriate radius functions r_ε, one *always* ends up with a trivial coupling strength $q(v) = 0$. Moreover, the above conjecture should

also hold for more general spaces, since the approximation is *local*, i.e., depends only on the behaviour of r_ε near the vertex.

In order to obtain a delta-coupling we need to change either the operator or the topology of the approximating space. One result in this direction is to use *scaled Schrödinger operators* on the vertex neighbourhoods: Let X_ε be a thick graph associated to a metric graph X_0 (for simplicity with all transversal volumes being the same, e.g., $\mathrm{vol}_{d-1} Y_e = 1$). Set $H_\varepsilon := \Delta^{\mathrm{N}}_{X_\varepsilon} + Q_\varepsilon$ with Neumann boundary conditions (if $\partial X_\varepsilon \neq \emptyset$), where $Q_\varepsilon = \sum_v \varepsilon^{-1} Q_v$ is a potential supported on the vertex neighbourhood $X_{\varepsilon,v}$ only.

In the limit, we have the Laplacian with delta-couplings as in (13), i.e., $H_0 = \Delta_{X_0} + \sum_v q(v)\delta_v$, with coupling strengths $q(v) = \int_{X_v} Q_v$.

Under the same uniformity assumptions as in Theorem 3.2, we proved in [15]:

Theorem 4.4. *Let X_ε be a uniform thick graph with underlying uniform metric graph X_0, let $H_\varepsilon := \Delta^{\mathrm{N}}_{X_\varepsilon} + \sum_v \varepsilon^{-1} Q_v$ be the scaled Schrödinger operator, and let $H_0 := \Delta_{X_0} + \sum_v q(v)\delta_v$ be the Laplacian with delta-coupling with strengths $q(v) = \int_{X_v} Q_v$, then $H_\varepsilon \xrightarrow{\mathrm{gnr}} H_0$ of order $\mathscr{O}(\varepsilon^{1/2})$.*

The proof is very similar to the proof of Theorem 3.2, only the estimate of $\|(H_\varepsilon + 1)^{-1} J - J(H_0+1)^{-1}\|$ is slightly different (actually, in Theorem 3.2 and Theorem 4.4, we used the corresponding *quadratic forms* instead of the operators, making the verification of the estimates simpler, but the presentation a bit more technical).

Using arguments of [5, 6], one can now approximate a *general vertex condition* of a Laplacian H_0 on X_0 at a vertex v by the operator H^a on a metric graph X_0^a, where H^a and X_0^a are constructed from H_0 and X_0 using *properly scaled delta interactions* and *additional edges*, such that $X_0^a \to X_0$ as $a \to 0$.

If we now approximate H^a by H_ε with appropriate $a = a_\varepsilon$ and delta strengths, we can find a family of thick graphs X_ε and operators H_ε such that $H_\varepsilon \xrightarrow{\mathrm{gnr}} H_0$. The example of a delta-coupling is presented in [15].

Another possibility of obtaining a delta-coupling is to use *scaled Robin boundary conditions*: Let $H_\varepsilon := \Delta_{X_\varepsilon}$ with Robin boundary conditions

$$\partial_{\mathrm{n}_\varepsilon} u + \beta_\varepsilon u = 0 \quad \text{on} \quad \partial X_\varepsilon = \bigcup_v \Gamma_{\varepsilon,v} \cup \bigcup_e \Gamma_{\varepsilon,e},$$

i.e., we decompose the boundary of the thick graph ∂X_ε into the parts of the vertex neighbourhoods $\Gamma_{\varepsilon,v} = \varepsilon \partial X_v \cap \partial X_\varepsilon$ and the edge neighbourhoods $\Gamma_{\varepsilon,e} = I_e \times \varepsilon \partial Y_e$. Denote the corresponding restriction of β_ε by $\beta_{\varepsilon,v}$ and $\beta_{\varepsilon,e}$. Let $H_0 = \Delta_{X_0} + \sum_v q(v)\delta_v$ be the Laplacian on X_0 with delta interactions of strength $q(v)$. In [28], we proved the following:

Theorem 4.5. *Assume that $\beta_{\varepsilon,e} = \mathscr{O}(\varepsilon^{1+1/2})$, $\beta_{\varepsilon,v} = \beta_v$ and $q(v) = \int_{\Gamma_v} \beta_v$, then $H_\varepsilon \xrightarrow{\mathrm{gnr}} H_0$ of order $\mathscr{O}(\varepsilon^{1/2})$.*

Idea of proof. The lowest eigenvalue $\lambda_{1,e}(x,\varepsilon)$ on the scaled transversal manifold $\{x\} \times \varepsilon Y_e$ with Robin condition $\varepsilon^{-1}\partial_{\mathrm{n}} u(x,\cdot) + \beta_\varepsilon u(x,\cdot) = 0$ on $\{x\} \times \partial Y_e$ is of order

$\lambda_{1,e}(x,\varepsilon) = \mathcal{O}(\varepsilon^{1/2}) \to 0$, i.e., this eigenvalue problem is *close* to the Neumann case. Therefore, we can use similar arguments as in the proof of Theorem 3.2. Moreover, the scaling behaviour of β_ε at the vertex neighbourhood is just the right one for a delta-coupling as $\varepsilon \to 0$. □

If we used scale invariant conditions, i.e., $\beta_\varepsilon = \beta/\varepsilon$, then the lowest transversal Robin eigenvalue would be of order $\lambda_{1,e}(\varepsilon) = \mathcal{O}(\varepsilon^{-2})$, and the arguments of Theorem 4.3 have to be applied.

5. Outlook and open problems

5.1. *Work in progress and open problems*

In a current project together with Jussi Behrndt, we show the convergence of the *Dirichlet-to-Neumann* operator on a graph-like manifold X_ε with cylindrical finite ends (which determine the boundary for the Dirichlet-to-Neumann operator) to a corresponding object on the underlying metric graph X_0. The main point here is to introduce Dirichlet-to-Neumann operators via *boundary triples* associated to quadratic forms.

There are still no conrete examples of vertex neighbourhoods known, such that the shifted and cut Dirichlet Laplacian $H_\varepsilon = (\Delta^{\mathrm{D}}_{X_\varepsilon} - \lambda_1/\varepsilon^2)_+$ converges to a Laplacian with *non-trivial* vertex couplings at the vertices. Moreover, the convergence in the generalised norm resolvent convergence in the Dirichlet case is not yet shown, although some work has been done in [10] in this direction.

5.2. *Conclusion*

Thick graphs (or fat graphs, graph-like manifolds . . .) provide an interesting class of *almost* solvable models and a *"construction kit"* for examples with special spectral behaviour. Neumann (and related) operators on thick graphs have a rather "simple" limit behaviour (Kirchhoff and related vertex conditions in the limit) independent of the vertex neighbourhoods, and can be treated with general (weak) methods. In contrast, Dirichlet and other operators with *non-zero* (large) first eigenvalue of order ε^{-2} are more complicated; the limit behaviour depends on the scattering matrix at the threshold, and the limit operator is *generically* decoupled. Finally, The generalised resolvent convergence is a *very general* scheme: it can be applied to many cases; a stronger version using quadratic forms allows results with *minimal* smoothness assumptions; a similar convergence scheme is also available for sectorial operators (see [28]).

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SPECTRAL PROPERTIES OF WIGNER MATRICES

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In these notes we review recent progress (and, in Section 5, we announce a new result) concerning the statistical properties of the spectrum of Wigner random matrices.

1. Introduction

The general goal of random matrix theory consists in determining the statistical properties of the eigenvalues (and the eigenvectors) of $N \times N$ matrices whose entries are random variables with given laws in the limit $N \to \infty$.

In these notes, we restrict our attention to ensembles of hermitian Wigner matrices, whose entries are, up to the constraints due to hermiticity, independent and identically distributed random variables. This assumption guarantees that all eigenvalues are real. Most of the results that I am going to present can also be extended to ensembles of Wigner matrices with different symmetries (real symmetric and quaternion hermitian ensembles).

Wigner matrices have been first introduced by Wigner in 1955 to describe the excitation spectra of heavy nuclei. For complex systems like heavy nuclei, it is practically impossible to write down the precise Hamilton operator. For this reason, Wigner assumed the matrix elements of the Hamiltonian to be random variables, and he tried to establish properties of the spectrum holding for almost every realization of the randomness. Remarkably, Wigner's intuition was confirmed by the experimental data. More generally, the study of the spectrum of Wigner matrices can be considered as a starting point for the analysis of the spectrum of systems with disorder. It is believed, in fact, that the spectrum of Wigner matrices shares many similarity with the spectrum of more complicated systems, such as random Schrödinger operators in the metallic (delocalization) phase.

Definition 1.1. An ensemble of hermitian Wigner matrices consists of $N \times N$ matrices $H = (h_{j\ell})_{1 \leq j,\ell \leq N}$. The entries have the form

$$h_{j\ell} = \frac{1}{\sqrt{N}}(x_{j\ell} + iy_{j\ell}) \qquad \text{for } 1 \leq j < \ell \leq N$$

$$h_{jj} = \frac{1}{\sqrt{N}}\, x_{jj} \qquad \text{for } 1 \leq j \leq N$$

where $\{x_{jj}, x_{j\ell}, y_{j\ell}\}$, $1 \le j \le N$, $j < \ell \le N$, is a collection of N^2 independent real random variables. We will assume that the variables $\{x_{j\ell}, y_{j,\ell}\}_{1\le j<\ell\le N}$ have a common law, with $\mathbb{E}\, x_{j\ell} = 0$, and $\mathbb{E}\, x_{j\ell}^2 = 1/2$. We will also assume that the variables $\{x_{jj}\}_{j=1}^N$ are identically distributed, with $\mathbb{E}\, x_{jj} = 0$, and $\mathbb{E}\, x_{jj}^2 = 1$. Throughout these notes, we are going to assume sub-Gaussian decay of the entries at infinity, in the sense that there exists $\nu > 0$ such that

$$\mathbb{E} e^{\nu |x_{j\ell}|^2} < \infty, \qquad \mathbb{E}\, e^{\nu |x_{jj}|^2} < \infty$$

for some (and thus all) $1 \le j < \ell \le N$.

The assumption of sub-Gaussian decay can be relaxed to subexponential decay, but then some of the statements have to be modified slightly. From the definition above, we observe that entries of Wigner matrices scale as $N^{-1/2}$ with the dimension N. This choice guarantees that, as $N \to \infty$, the spectrum of Wigner matrices remains bounded (in fact, as we will see below, with this choice the spectrum is contained, almost surely in the limit $N \to \infty$, in the interval $[-2, 2]$).

Observe that Definition 1.1 does not specify the precise distribution for the entries of the matrix. In fact, one of the main point of the results that will be presented below is exactly the fact that they apply to a large class of Wigner matrices, and that they are independent of the particular choice for the probability law of the entries. The analysis becomes much easier if one assumes the entries of the matrix to be Gaussian random variables. The Gaussian Unitary Ensemble (GUE) is the ensemble of hermitian Wigner matrices (as defined in Definition 1.1) where all entries are Gaussian. In this case, it is possible to write the probability density for the matrix H as

$$dP(H) = \text{const} \cdot e^{-\frac{N}{2} \operatorname{tr} H^2} dH \quad \text{where} \qquad dH = \prod_{1\le \ell < m \le N} dh_{\ell m} dh_{\ell m}^* \prod_{j=1}^N dh_{jj}$$

is the product of the Lebesgue measure of the entries of H. What makes GUE particularly simple to analyze is its invariance with respect to unitary conjugation. If H is a GUE matrix, and U is an arbitrary (fixed) unitary matrix, then also UHU^* is a GUE matrix. It is possible to show that GUE is the only ensemble of hermitian Wigner matrices which enjoys unitary invariance. Because of the unitary invariance, for GUE it is possible to find an explicit expression for the probability density function p_N of the N eigenvalues:

$$p_N(\mu_1, \dots, \mu_N) = \text{const} \cdot \prod_{i<j}^N (\mu_i - \mu_j)^2\, e^{-\frac{N}{2} \sum_{j=1}^N \mu_j^2}. \tag{1}$$

The Gaussian factor reflects the Gaussian distribution of the entries. The correla-

tions among the eigenvalues are described by the Vandermond determinant squared

$$\prod_{i<j}^{N}(\mu_i-\mu_j)^2=\Delta(\mu_1,\ldots,\mu_N)^2=\left[\det\begin{pmatrix}1 & \ldots 1\\ \mu_1 & \ldots \mu_N\\ & \ldots\\ \mu_1^{N-1} & \ldots \mu_N^{N-1}\end{pmatrix}\right]^2. \tag{2}$$

Using this explicit expression for the joint probability density function of the N eigenvalues of GUE matrices, one can compute the local eigenvalue statistics. For fixed $k=1,\ldots,N$, we define the k point correlation function

$$p_N^{(k)}(\mu_1,\ldots,\mu_k)=\int d\mu_{k+1}\ldots d\mu_N\, p_N(\mu_1,\ldots\mu_N)$$

It turns out that, as $N\to\infty$, the local correlation functions of GUE converge, after appropriate rescaling, to the Wigner-Dyson distribution. For any fixed $k\in\mathbb{N}$,

$$\frac{1}{\rho_{\rm sc}^k(E)}\,p_N^{(k)}\left(E+\frac{x_1}{N\rho_{\rm sc}(E)},\ldots,E+\frac{x_k}{N\rho_{\rm sc}(E)}\right)\to\det\left(\frac{\sin(\pi(x_i-x_j))}{(\pi(x_i-x_j))}\right)_{1\le i,j\le k} \tag{3}$$

as $N\to\infty$. Here

$$\rho_{\rm sc}(E)=\begin{cases}\frac{1}{2\pi}\sqrt{1-\frac{E^2}{4}} & \text{if } |E|\le 2\\ 0 & \text{otherwise}\end{cases} \tag{4}$$

is the *semicircle law*, which describes the density of the eigenvalues around E (we will discuss the semicircle law in more details in Section 2). The convergence in (3) is pointwise in E and holds weakly in the variables $x_1,\ldots,x_k$. One refers to the left hand side of (3) as *local* correlations because the arguments of $p_N^{(k)}$ vary in an interval of size $1/N$. As we discussed above, the choice of the N dependence of the matrix entries implies that all eigenvalues are contained in a finite interval; this means that the typical distance between neighboring eigenvalues is of the order N^{-1}. Hence, to observe non trivial correlations, the relevant length scale is exactly of the order N^{-1}. Eq. (3) was first proven for GUE by Dyson in [2] using the explicit expression (1) and the asymptotics of Hermite polynomials. Although (1) only holds true for GUE, and there is no explicit expression for the joint probability density function of the eigenvalues of any other ensembles of Wigner matrices, the convergence (3) is expected to hold true independently of the law of the matrix entries. One expects, in other words, the local eigenvalue correlations to be *universal*; we will present a proof of universality in Section 4. In fact, universality should hold even more generally; the Wigner-Dyson statistics is expected to describe the local eigenvalue correlations in a large class of systems with disorder (for example, random Schrödinger operators in the metallic phase).

2. Density of States and the Semicircle Law

The first rigorous result in random matrix theory has been obtained in [22], where Wigner proved the convergence of the density of states to the semicircle law for

arbitrary ensembles of Wigner matrices (hermitian, real symmetric, or quaternion hermitian). For $a < b$, let $\mathscr{N}[a;b]$ denote the number of eigenvalues in the interval $[a;b]$. The density of the eigenvalues, or density of states, in the interval $[a;b]$ is defined as

$$\rho_{[a;b]} = \frac{\mathscr{N}[a;b]}{N|b-a|}\,,$$

where the factor of N in the denominator makes sure that, typically, $\rho_{[a;b]}$ is a quantity of order one. The density of states $\rho_{[a;b]}$ is a random variable whose precise value depend on the realization of the randomness. Nevertheless, Wigner proved that, as $N \to \infty$, $\rho_{[a;b]}$ approaches a deterministic limit. More precisely, he showed that, for any $\delta > 0$,

$$\lim_{N\to\infty} \mathbb{P}\left(\left|\frac{\mathscr{N}[a;b]}{N|b-a|} - \frac{1}{|b-a|}\int_a^b ds\,\rho_{\mathrm{sc}}(s)\right| \geq \delta\right) = 0$$

where $\rho_{\mathrm{sc}}(s)$ denotes the semicircle law defined in (4). After considering the limit $N \to \infty$, we can also let $\eta = |b-a| \to 0$; in this limit the density of state converges to the semicircle law at $E = (a+b)/2$. Hence, Wigner's result can be formulated as

$$\lim_{\eta\to 0}\lim_{N\to\infty} \mathbb{P}\left(\left|\frac{\mathscr{N}\left[E-\frac{\eta}{2};E+\frac{\eta}{2}\right]}{N\eta} - \rho_{\mathrm{sc}}(E)\right| \geq \delta\right) = 0\,.$$

It is worth noticing that the semicircle law, and therefore the limiting density of states, is independent of the choice of the probability law for the entries of the Wigner matrix. It is also important to observe that Wigner's result concerns the density of states on *macroscopic* intervals, that is intervals which typically contain order N eigenvalues (for fixed $\eta > 0$, the interval $[E-(\eta/2);E+(\eta/2)]$ contains order N eigenvalues). What happens if we consider the density of states in smaller intervals, namely in intervals whose size shrinks to zero as $N \to \infty$? These intervals will not contain order N eigenvalues. However, as long as the number of eigenvalues is large as $N \to \infty$, we may expect the fluctuations of the density of states to be negligible in the limit. This is the content of the next theorem, which was proven in [9] (extending previous results from [7, 8]).

Theorem 2.1. *Consider an ensemble of hermitian Wigner matrices as in Def. 1.1. Let $|E| < 2$. Then, for any $K > 0$,*

$$\mathbb{P}\left(\left|\frac{\mathscr{N}\left[E-\frac{K}{2N};E+\frac{K}{2N}\right]}{K} - \rho_{sc}(E)\right| \geq \delta\right) \lesssim e^{-c\delta^2\sqrt{K}}$$

uniformly in N, for all N large enough. This quantitative bound implies, in particular, that

$$\lim_{K\to\infty}\lim_{N\to\infty} \mathbb{P}\left(\left|\frac{\mathscr{N}\left[E-\frac{K}{2N};E+\frac{K}{2N}\right]}{K} - \rho_{sc}(E)\right| \geq \delta\right) = 0\,. \tag{5}$$

This theorem establishes convergence of the density of states to the semicircle law on *microscopic* intervals, that is on intervals containing, typically, a constant (N independent) number of eigenvalues. From convergence on the microscopic scale, we also obtain convergence to the semicircle law on intermediate scales; for any sequence $\eta(N) > 0$ such that $\eta(N) \to 0$ and $N\eta(N) \to \infty$ as $N \to \infty$ we have

$$\lim_{N\to\infty} \mathbb{P}\left(\left| \frac{\mathscr{N}\left[E - \frac{\eta(N)}{2}; E + \frac{\eta(N)}{2}\right]}{N\eta(N)} - \rho_{\mathrm{sc}}(E) \right| \geq \delta \right) = 0\,.$$

Note that, if $\eta(N) \lesssim 1/N$, the fluctuations of the density of states are certainly important, and one cannot expect convergence in probability; in this sense, (5) establishes convergence to the semicircle law on the optimal scale.

The proof of Theorem 2.1 relies on two main ingredients, an upper bound on the density of states and a fixed point equation for the Stieltjes transform of the empirical eigenvalue distribution.

Upper bound. Consider a sequence $\eta(N) \geq (\log N)^2/N$. Then there are constants K_0, C, c such that

$$\mathbb{P}\left(\frac{\mathscr{N}\left[E - \frac{\eta(N)}{2}; E + \frac{\eta(N)}{2}\right]}{N\eta(N)} \geq K \right) \lesssim e^{-c\sqrt{KN\eta(N)}} \tag{6}$$

for all $K > K_0$ and N large enough.

A similar statement is valid also for smaller intervals, of size $2/N \leq \eta(N) \leq (\log N)^2/N$, but its proof is more involved (see Theorem 5.1 in [9]).

To show (6), we observe that (using $\eta \equiv \eta(N)$)

$$\mathscr{N}\left[E - \frac{\eta}{2}; E + \frac{\eta}{2}\right] = \sum_{\alpha=1}^{N} \mathbf{1}(|\mu_\alpha - E| \leq \eta/2) \lesssim \eta \,\mathrm{Im} \sum_{\alpha=1}^{N} \frac{1}{\mu_\alpha - E - i\eta}$$

where $\{\mu_\alpha\}_{\alpha=1}^N$ are the eigenvalues of H. Hence

$$\frac{\mathscr{N}\left[E - \frac{\eta}{2}; E + \frac{\eta}{2}\right]}{N\eta} \lesssim \frac{1}{N}\mathrm{Im}\ \mathrm{tr}\, \frac{1}{H - E - i\eta} = \frac{1}{N}\mathrm{Im} \sum_{j=1}^{N} \frac{1}{H - E - i\eta}(j,j)\,. \tag{7}$$

To bound the diagonal entries of the resolvent, we use (for the case $j = 1$):

$$\frac{1}{H - E - i\eta}(1,1) = \frac{1}{h_{11} - E - i\eta - \langle \mathbf{a}, (B - E - i\eta)^{-1}\mathbf{a}\rangle} \tag{8}$$

where $\mathbf{a} = (h_{21}, h_{31}, \ldots, h_{N1}) \in \mathbb{C}^{N-1}$ is the first row of H after removing the $(1,1)$-entry, and B is the $(N-1) \times (N-1)$ minor of H obtained by removing the first row and the first column. Using the spectral decomposition of the minor B, we find,

$$\frac{1}{H - E - i\eta}(1,1) = \frac{1}{h_{11} - E - i\eta - \frac{1}{N}\sum_{\alpha=1}^{N-1} \frac{\xi_\alpha}{\lambda_\alpha - E - i\eta}} \tag{9}$$

where $\xi_\alpha = N|\mathbf{a}\cdot\mathbf{u}_\alpha|^2$ and where $\{\lambda_\alpha\}_{\alpha=1}^{N-1}$ and $\{\mathbf{u}_\alpha\}_{\alpha=1}^{N-1}$ are the eigenvalues and, respectively, the eigenvectors of the minor B. We conclude that

$$\mathrm{Im}\,\frac{1}{H-E-i\eta}(1,1) \le \frac{1}{\eta + \mathrm{Im}\frac{1}{N}\sum_{\alpha=1}^{N}\frac{\xi_\alpha}{\lambda_\alpha - E - i\eta}} \le \frac{1}{\mathrm{Im}\frac{1}{N}\sum_{\alpha=1}^{N}\frac{\xi_\alpha}{\lambda_\alpha - E - i\eta}}\,. \quad (10)$$

Since $\mathbf{a}$ is independent of the minor B (and therefore of its eigenvectors), we have

$$\mathbb{E}\,\xi_\alpha = N\mathbb{E}\sum_{i,j} a_i\overline{a}_j\overline{u}_\alpha(j)u_\alpha(i) = N\mathbb{E}\sum_{i,j}\frac{\delta_{ij}}{N}\,\overline{u}_\alpha(j)u_\alpha(i) = 1\,.$$

Moreover, it turns out that ξ_α is well concentrated around its expectation. Therefore, up to a set with small probability, we find from (10) that

$$\mathrm{Im}\,\frac{1}{H-E-i\eta}(1,1) \lesssim \frac{K^2}{\mathrm{Im}\frac{1}{N}\sum_{\alpha=1}^{N}\frac{1}{\lambda_\alpha - E - i\eta}} = \frac{K^2}{\mathrm{Im}\frac{1}{N}\mathrm{tr}\frac{1}{B-E-i\eta}} \quad (11)$$

for a sufficiently large constant $K > 0$. A more precise analysis shows that the measure of the excluded set (on which the bound (11) may fail) is at most $\exp(-c\sqrt{KN\eta})$; see Lemma 4.7 in [9]. Using (7), but for B instead of H, we obtain

$$\mathrm{Im}\,\frac{1}{H-E-i\eta}(1,1) \lesssim \frac{K^2}{\frac{\mathscr{N}_B\left[E-\frac{\eta}{2};E+\frac{\eta}{2}\right]}{N\eta}} \lesssim \frac{K^2}{\frac{\mathscr{N}\left[E-\frac{\eta}{2};E+\frac{\eta}{2}\right]}{N\eta}}$$

where $\mathscr{N}_B[a;b]$ denotes the number of eigenvalues of B in the interval $[a;b]$ and where, in the second inequality, we used the fact that the eigenvalues of B are interlaced between the eigenvalues of H.

Analogously, for any $j = 2,\dots,N$, we find that

$$\mathrm{Im}\,\frac{1}{H-E-i\eta}(j,j) \lesssim \frac{K^2}{\frac{\mathscr{N}\left[E-\frac{\eta}{2};E+\frac{\eta}{2}\right]}{N\eta}} \quad (12)$$

up to a set with probability smaller than $\exp(-c\sqrt{KN\eta})$. Since, by assumption, $N\eta \ge (\log N)^2$, the total measure of the union of these N "bad" sets is bounded by $\exp(-(c/2)\sqrt{KN\eta(N)})$. On the complementary set, (12) is correct for all $j = 1,\dots,N$, and thus, from (7), we find

$$\frac{\mathscr{N}\left[E-\frac{\eta}{2};E+\frac{\eta}{2}\right]}{N\eta} \lesssim \frac{K^2}{\frac{\mathscr{N}\left[E-\frac{\eta}{2};E+\frac{\eta}{2}\right]}{N\eta}} \qquad \Rightarrow \qquad \frac{\mathscr{N}\left[E-\frac{\eta}{2};E+\frac{\eta}{2}\right]}{N\eta} \lesssim K$$

which shows the upper bound (6).

Stieltjes transform. We define the Stieltjes transform of the empirical eigenvalue measure by

$$m_N(z) = \frac{1}{N}\mathrm{tr}\,\frac{1}{H-z} = \frac{1}{N}\sum_{\alpha=1}^{N}\frac{1}{\mu_\alpha - z}\,.$$

We are going to compare $m_N(z)$ with the Stieltjes transform of the semicircle law, given by

$$m_{sc}(z) = \int \frac{ds\rho_{sc}(s)}{s-z} = -\frac{z}{2} + \sqrt{\frac{z^2}{4} - 1}\,.$$

It turns out that Theorem 2.1 follows, if we can show that the difference $m_N(z) - m_{sc}(z)$ converges to zero as $N \to \infty$, for all $z = E + i\eta$ with $|E| < 2$ and $\eta \geq K/N$ (see the proof of Corollary 4.2 in [7]). It is worth noticing that $m_{sc}(z)$ satisfies the fixed point equation

$$m_{sc}(z) + \frac{1}{z + m_{sc}(z)} = 0\,. \tag{13}$$

It turns out that this equation is stable away from the spectral edges $E = \pm 2$. Hence to show that $|m_N(z) - m_{sc}(z)| \leq C\delta$ with high probability, it is enough to prove that $m_N(z)$ is an approximate solution of (13), that is that

$$\left| m_N(z) + \frac{1}{z + m_N(z)} \right| \leq \delta \tag{14}$$

with high probability.

To establish (14), we use again the expression (9):

$$m_N(z) = \frac{1}{N}\sum_{j=1}^{N} \frac{1}{H-z}(j,j) = \frac{1}{N}\sum_{j=1}^{N} \frac{1}{h_{jj} - z - \frac{1}{N}\sum_{\alpha=1}^{N-1} \frac{\xi_\alpha^{(j)}}{\lambda_\alpha^{(j)} - z}} \tag{15}$$

where $\xi^{(j)} = N|\mathbf{a}^{(j)} \cdot \mathbf{u}_\alpha^{(j)}|^2$, $\mathbf{a}^{(j)} = (h_{j1}, \ldots, h_{j,j-1}, h_{j,j+1}, h_{jN}) \in \mathbb{C}^{N-1}$ is the j-th row of H without diagonal element, and where $\lambda_\alpha^{(j)}$ and $\mathbf{u}_\alpha^{(j)}$ are the eigenvalues and the eigenvectors of the minor $B^{(j)}$ obtained from H by removing the j-th row and the j-th column. From (15), we obtain

$$\begin{aligned} m_N(z) &= \frac{1}{N}\sum_{j=1}^{N} \frac{1}{-z - m_N(z) - X^{(j)}(z)} \\ &= \frac{-1}{z + m_N(z)} + \frac{1}{N}\sum_{j=1}^{N} \frac{X^{(j)}(z)}{(z + m_N(z))(z + m_N(z) + X^{(j)}(z))}\,. \end{aligned} \tag{16}$$

Here we defined

$$X^{(j)}(z) = -h_{jj} + \left(\frac{N-1}{N} m_{N-1}^{(j)}(z) - m_N(z) \right) + \frac{1}{N}\sum_{\alpha=1}^{N-1} \frac{\xi_\alpha - 1}{\lambda_\alpha - z}$$

where

$$m_N^{(j)}(z) = \frac{1}{N-1}\mathrm{tr}\,\frac{1}{B^{(j)} - z} = \frac{1}{N-1}\sum_{\alpha=1}^{N-1} \frac{1}{\lambda_\alpha^{(j)} - z}$$

is the Stieltjes transform of the minor $B^{(j)}$.

From (16) we obtain (14) if we can show that $X^{(j)}(z)$ is small with high probability. The first summand in $X^{(j)}(z)$, $-h_{jj}$, is of the order $N^{-1/2}$ and therefore small. The second summand in $X^{(j)}(z)$, the difference $(\frac{N-1}{N} m^{(j)}_{N-1}(z) - m_N(z))$, is small (with probability one); this is a consequence of the interlacing between the eigenvalues of $B^{(j)}$ and H. The main difficulty consists therefore in showing the smallness of the random variable

$$Y^{(j)}(z) = \frac{1}{N} \sum_{\alpha=1}^{N-1} \frac{\xi_\alpha - 1}{\lambda_\alpha - z} \,. \tag{17}$$

To show that $Y^{(j)}(z)$ is small, with high probability, we use the upper bound (6), which guarantees that the denominator in (17) can only be large for a small number of α's; details can be found in Section 6 of [9].

3. Delocalization of Eigenvectors of Wigner Matrices

As a first application of Theorem 2.1, we show delocalization of the eigenvectors of Wigner matrices. Given a vector $\mathbf{v} \in \mathbb{C}^N$ with ℓ^2 norm equal to one, we say that it is completely *localized* if one of its component has size one, and all other vanish. $\mathbf{v}$ is called completely *delocalized*, if all its components have the same size (namely $N^{-1/2}$). To distinguish between localized and delocalized vectors, we can compute the ℓ^p norm of $\mathbf{v}$, for $p > 2$. If $\mathbf{v}$ is completely localized, its ℓ^p norm equals to one, for all $2 < p \leq \infty$, and for all N. On the other hand, if $\mathbf{v}$ is completely delocalized,

$$\|\mathbf{v}\|_p = N^{-\frac{1}{2}+\frac{1}{p}}$$

and therefore converges to zero, as $N \to \infty$ (for all $p > 2$). The next theorem was proved in [9], extending results from [7, 8].

Theorem 3.1. *Consider an ensemble of hermitian Wigner matrices as in Def. 1.1. Let $|E| < 2$, $K > 0$, $2 < p < \infty$. Then there exists $c, C > 0$ such that*

$$\mathbb{P}\left(\exists \mathbf{v} : H\mathbf{v} = \mu \mathbf{v}, |\mu - E| \leq \frac{K}{2N}, \|\mathbf{v}\|_2 = 1, \|\mathbf{v}\|_p \geq M N^{-\frac{1}{2}+\frac{1}{p}} \right) \leq C e^{-c\sqrt{M}} \tag{18}$$

for all $M > 0$, and N large enough.

If we take $M > (\log N)^2$, the statement can be modified as follows. For every $\kappa > 0$, and $2 < p \leq \infty$, there exist $c, C > 0$ such that

$$\mathbb{P}\left(\exists \mathbf{v} : H\mathbf{v} = \mu \mathbf{v}, |\mu| \leq 2 - \kappa, \|\mathbf{v}\|_2 = 1, \|\mathbf{v}\|_p \geq M N^{-\frac{1}{2}+\frac{1}{p}} \right) \leq C e^{-c\sqrt{M}} \tag{19}$$

for all $M > (\log N)^2$, and all N large enough.

The interpretation of (18) and (19) is straightforward; eigenvectors of Wigner matrices are completely delocalized. Up to the parameter $M > 0$, which tunes the probability, all components of the eigenvectors have the same size.

The proof of (19) is a simple application of Theorem 2.1 ((18) requires a little bit more work, but the main ideas are the same). For $p = \infty$, we need an upper bound

on the components of an eigenvector $\mathbf{v} = (v_1, v_2, \ldots, v_N)$. To bound, for example, v_1, we write $\mathbf{v} = (v_1, \mathbf{w})$, with $\mathbf{w} = (v_2, \ldots, v_N)$. From $H\mathbf{v} = \mu\mathbf{v}$, we find

$$\mathbf{w} = -v_1(B-\mu)^{-1}\mathbf{a}$$

where $\mathbf{a} = (h_{21}, \ldots, h_{N1})$ is the first column of H, after removing the first component, and where B is the $(N-1)\times(N-1)$ minor of H obtained by removing the first row and column. The normalization condition $v_1^2 + \mathbf{w}^2 = 1$ implies that

$$v_1^2 = \frac{1}{1+\langle \mathbf{a}, (B-\mu)^{-2}\mathbf{a}\rangle} = \frac{1}{1+\frac{1}{N}\sum_{\alpha=1}^{N}\frac{\xi_\alpha}{(\lambda_\alpha-\mu)^2}} \leq \frac{1}{\frac{1}{N}\sum_{\alpha=1}^{N}\frac{\xi_\alpha}{(\lambda_\alpha-\mu)^2}}$$

where, as in Section 2, $\xi_\alpha = N|\mathbf{u}_\alpha \cdot \mathbf{a}|^2$, and λ_α and $\mathbf{u}_\alpha$ are the eigenvalues and the eigenvectors of the minor B. Restricting the sum to those α for which $|\lambda_\alpha - \mu| \leq K/N$, and using the fact that ξ_α concentrates around one, we obtain that, with high probability,

$$v_1^2 \lesssim \frac{K^2}{N}\frac{1}{|\{\alpha : |\lambda_\alpha - \mu| \leq K/N\}|} \lesssim \frac{K}{N}$$

where, in the last inequality, we use the fact that, by Theorem 2.1, the density of states on the interval $[\mu - (K/N); \mu + (K/N)]$ converges, with high probability, to $\rho_{sc}(\mu) > 0$. This shows (19).

4. Bulk Universality for Hermitian Wigner Matrices

Universality for hermitian Wigner matrices refers to the fact that the local eigenvalue statistics are independent of the particular choice for the probability law of the entries of the matrix. One should distinguish between local correlations close to the edges and in the bulk of the spectrum. The correlations at the edges are described by the Tracy-Widom distribution; for GUE this was first observed in [21]. In [18], Soshnikov established *edge universality* of the Tracy-Widom distribution (recently, Tao and Vu found a new proof of edge universality in [20]). In these notes, I will restrict my attention to universality in the bulk of the spectrum; to show *bulk universality*, we need to prove the convergence of the local eigenvalues correlations to the Wigner-Dyson distribution (3).

A first partial result towards bulk universality for hermitian Wigner matrices was obtained by Johansson, who proved, in [15], convergence to the Wigner-Dyson statistics for ensembles of Wigner matrices with a Guassian component. Johansson considered Wigner matrices of the form

$$H = H_0 + t^{1/2}V \tag{20}$$

where H_0 is an arbitrary Wigner matrix, V is a GUE matrix, independent of H_0, and $t > 0$ measures the strength of the Gaussian component. Strictly speaking, in order for H to obey Definition 1.1, we should renormalize it by a t dependent factor to make sure that the variance of the entries remains constant. However, this

rescaling only affects the eigenvalue statistics in a trivial way, and therefore in the following we will work with the matrix H, as defined in (20).

It turns out that H emerges from H_0 by letting every entry evolve through independent Brownian motions up to time t. This stochastic evolution of the matrix entries induces a stochastic dynamics for the eigenvalues, known as the *Dyson Brownian motion*. The Dyson Brownian motion can be described as a flow for the density of the eigenvalues. The joint probability density function of the N eigenvalues of $H = H_0 + t^{1/2}V$ can be written as

$$p_{N,t}(\mathbf{x}) = \int d\mathbf{y}\, q_t(\mathbf{x};\mathbf{y}) p_{N,0}(\mathbf{y}) \tag{21}$$

where $\mathbf{x} = (x_1, \ldots, x_N)$, $\mathbf{y} = (y_1, \ldots, y_N)$, $p_{N,0}$ is the joint probability density function of the eigenvalues of the initial matrix H_0, and q_t is the kernel describing the Dyson Brownian Motion (describing, in other words, the addition of a GUE matrix to H_0). The kernel q_t can be computed explicitly:

$$q_t(\mathbf{x};\mathbf{y}) = \frac{N^{N/2}}{(2\pi t)^{N/2}} \frac{\Delta(\mathbf{x})}{\Delta(\mathbf{y})} \det\left(e^{-N(x_j-y_k)^2/2t}\right)_{j,k=1}^{N}, \tag{22}$$

with the Vandermonde determinant $\Delta(\mathbf{x})$ defined in (2). From (21), we can express the k-point correlation function of $p_{N,t}$ as

$$p_{N,t}^{(k)}(x_1, \ldots, x_k) = \int d\mathbf{y}\, q_t^{(k)}(x_1, \ldots, x_k; \mathbf{y})\, p_{N,0}(\mathbf{y}) \tag{23}$$

where

$$\begin{aligned} q_t^{(k)}(x_1, \ldots, x_k; \mathbf{y}) &= \int q_t(\mathbf{x};\mathbf{y})\, dx_{k+1} \ldots dx_N \\ &= \frac{(N-k)!}{N!} \det\left(K_{t,N}(x_i, x_j; \mathbf{y})\right)_{1\le i,j\le k} \end{aligned} \tag{24}$$

with

$$\begin{aligned} K_{t,N}(u, v; \mathbf{y}) &= \frac{N}{(2\pi i)^2 (v-u) t} \\ &\times \int_\gamma dz \int_\Gamma dw\, (e^{-N(v-u)(w-r)/t} - 1) \prod_{j=1}^{N} \frac{w - y_j}{z - y_j} \\ &\times \frac{1}{w-r} \Big(w - r + z - u - \frac{t}{N} \sum_j \frac{y_j - r}{(w-y_j)(z-y_j)} \Big) e^{N(w^2 - 2vw - z^2 + 2uz)/2t}. \end{aligned}$$

Here γ is the union of two horizontal lines $\mathbb{R} \ni s \to s - i\delta$, $\mathbb{R} \ni s \to -s + i\delta$, for some $\delta > 0$, and Γ is a vertical line $\mathbb{R} \ni s \to \kappa + is$ and $r \in \mathbb{R}$ is arbitrary.

From (23), we observe that universality for matrices of the form (20) can be proven by showing that

$$\frac{1}{N\rho_t(E)} K_{t,N}\left(E + \frac{x_1}{N\rho_t(E)}, E + \frac{x_2}{N\rho_t(E)}; \mathbf{y}\right) \to \frac{\sin \pi(x_2 - x_1)}{\pi(x_2 - x_1)} \tag{25}$$

for all $\mathbf{y}$ in a subset of $\mathbb{R}^N$ whose $p_{N,0}$-measure tends to one, as $N \to \infty$. In (25),

$$\rho_t(E) = \frac{1}{2\pi(1+t)^2}\sqrt{1-\frac{E^2}{4(1+t)^2}}$$

is the rescaled semicircle law (the rescaling is needed because the variance of the entries of H grows with t).

To show (25), Johansson writes

$$\begin{aligned}\frac{1}{N\rho_t(E)}K_{t,N}\Big(E, E+\frac{\tau}{N\rho_t(E)};\mathbf{y}\Big) \\ = N\int_\gamma \frac{dz}{2\pi i}\int_\Gamma \frac{dw}{2\pi i}\, h_N(w)g_N(z,w)e^{N(f_N(w)-f_N(z))}\end{aligned} \tag{26}$$

with

$$\begin{aligned} f_N(z) &= \frac{1}{2t}(z^2-2uz)+\frac{1}{N}\sum_j \log(z-y_j) \\ g_N(z,w) &= \frac{1}{t(w-r)}[w-r+z-u]-\frac{1}{N(w-r)}\sum_j \frac{y_j-r}{(w-y_j)(z-y_j)} \\ h_N(w) &= \frac{1}{\tau}\Big(e^{-\tau(w-r)/t\varrho}-1\Big)\end{aligned}$$

and he performs a detailed asymptotic analysis of the integral (26). He finds the saddle points of the exponent $f_N(w)-f_N(z)$, he shifts the contours γ, Γ to go through the saddles, he shows that the contributions of the saddles gives exactly the sine-kernel, and that the contributions away from the saddles vanish as $N \to \infty$. Following this strategy, Johansson proved convergence to the sine-kernel for ensembles of the form (20), for arbitrary fixed $t > 0$.

To prove universality for general ensembles of hermitian Wigner matrices, we would like to take $t = 0$ in (20). As an intermediate step, we may ask what happens if one chooses $t = t(N)$ depending on N, so that $t(N) \to 0$ as $N \to \infty$. The algebraic identities discussed above are still valid, and universality follows again by showing that the r.h.s. of (26) converges to the sine-kernel as $N \to \infty$. The difference is that now the parameter t entering the definition of $f_N(z), g_N(z,w), h_N(w)$ depends on N and vanishes as $N \to \infty$; this makes the asymptotic analysis more delicate. It turns out, however, that, using Theorem 2.1, it is still possible to perform the asymptotic analysis of the integral in (26) and to show convergence to the sine-kernel, as long as $t(N) \geq N^{-1+\delta}$ for some $\delta > 0$.Theorem 2.1 is really the crucial ingredient of this analysis; the requirement $t(N) \geq N^{-1+\delta}$ is, in fact, a consequence of the fact that we only have convergence to the semicircle law on intervals of size K/N or larger. The next theorem was proven in [4].

Theorem 4.1. *Let H_0 be an ensemble of hermitian Wigner matrices as in Def. 1.1. Choose a sequence $t(N)$ such that $t(N) \to 0$ as $N \to \infty$ and $t(N) \geq N^{-1+\delta}$ for*

some $\delta > 0$. Let V be a GUE matrix, independent of H_0. Then, the local eigenvalue statistics of $H = H_0 + t(N)^{1/2}V$ are such that

$$\frac{1}{\rho_{sc}^k(E)} p_N^{(k)}\left(E + \frac{x_1}{N\rho_{sc}(E)}, \ldots, E + \frac{x_k}{N\rho_{sc}(E)}\right) \to \det\left(\frac{\sin(\pi(x_i - x_j))}{(\pi(x_i - x_j))}\right)_{1\le i,j\le k} \tag{27}$$

for all $|E| < 2$. The convergence here holds after integrating against a bounded and compactly supported observable in the variables $x_1, \ldots, x_k$.

One may hope to show that the small Gaussian perturbation cannot change the local eigenvalue correlations by comparing the laws of H and H_0. If the entries of H_0 have the probability density function h, then the probability density function h_t of the entries of $H_0 + t^{1/2}V$ is given by

$$h_t = e^{tL}h, \qquad \text{with } L = \frac{d^2}{dx^2}$$

At least formally, this implies that $|h_t - h| \simeq tLh$. Hence, for small $t(N) \simeq N^{-1+\delta}$, the laws of the entries of H and H_0 are very close. However, to compare the eigenvalue correlations of H and of H_0, we would need to compare N^2 entries; therefore, the total distance between the laws of H and of H_0 is not small in the limit $N \to \infty$. To overcome this problem, we use a time-reversal type idea.

Suppose that H is an ensemble of hermitian Wigner matrices, whose entries have the probability density function h. We can then introduce a new probability density function

$$\widetilde{h} = \left(1 - tL + \frac{t^2L^2}{2} - \cdots \pm \frac{t^nL^n}{n!}\right) h \tag{28}$$

and we can define a new Wigner matrix $\widetilde{H}$ whose entries have the law $\widetilde{h}$. The probability density function of the entries of $H_t = \widetilde{H} + t^{1/2}V$ is then given by

$$h_t = e^{tL}\widetilde{h} = e^{tL}\left(1 - tL + \frac{t^2L^2}{2} - \cdots \pm \frac{t^nL^n}{n!}\right) h$$

Universality for the matrix H_t follows from Theorem 4.1 if $t = t(N) \ge N^{-1+\delta}$. Moreover, the density h_t is now much closer to the initial h compared with $e^{tL}h$. Formally, we find

$$|h_t - h| \simeq \frac{t^{n+1}}{(n+1)!} L^{n+1}h\,. \tag{29}$$

Taking $t = t(N) \simeq N^{-1+\delta}$, the r.h.s. can be made smaller than any power of N by choosing $n \in \mathbb{N}$ sufficiently large. Hence, if we choose n large enough, we can compare the correlations of H with the ones of H_t, and conclude universality for H (from universality for H_t). From (29), it is clear that, to choose n large, we need to assume sufficient regularity of h; this explains the origin of the regularity conditions in the next theorem, which appeared in [4].

Theorem 4.2. *Let H be an ensemble of hermitian Wigner matrices, whose entries have the probability density function $h(x) = e^{-g(x)}$. Fix $k \geq 1$ and assume $g \in C^{2(n+1)}(\mathbb{R})$ for some integer $n > k/2$, with*

$$\sum_{j=1}^{2(n+1)} |g^{(j)}(x)| \leq C(1+x^2)^m$$

for some $m \in \mathbb{N}$. Then we have

$$\frac{1}{\rho_{sc}^k(E)} p_N^{(k)}\left(E + \frac{x_1}{N\rho_{sc}(E)}, \ldots, E + \frac{x_k}{N\rho_{sc}(E)}\right) \to \det\left(\frac{\sin(\pi(x_i - x_j))}{(\pi(x_i - x_j))}\right)_{1\leq i,j\leq k}$$

for all $|E| < 2$ (after integrating against a bounded and compactly supported function $O(x_1, \ldots, x_k)$).

Shortly after this result was posted, Tao and Vu obtained, in [19], another proof of universality for hermitian ensembles of Wigner matrices. Their proof uses different techniques, but is also based on the convergence to the semicircle law on microscopic scales (more precisely, it is based on the delocalization of the eigenvectors of Wigner matrices, established in Theorem 3.1). The result of Tao and Vu requires the third moment of the matrix entries to vanish, but, otherwise, almost no regularity. Comparing the two works, we realized that the two approaches could be combined to yield an even stronger result. The following theorem was proven in [5].

Theorem 4.3. *Let H be an ensemble of Wigner matrices. Then, for every $k \in \mathbb{N}$, $\delta > 0$, $E_0 \in (-2+\delta; 2-\delta)$, and for every compactly supported and bounded $O(x_1, \ldots, x_k)$, we have*

$$\lim_{N\to\infty} \int_{E_0-\delta}^{E_0+\delta} dE \int dx_1 \ldots dx_k \; O(x_1, \ldots, x_k) \\ \times \left[\frac{1}{\rho_{sc}^k(E)} p_N^{(k)}\left(E + \frac{x_1}{N\rho_{sc}(E)}, \ldots, E + \frac{x_k}{N\rho_{sc}(E)}\right) - \det\left(\frac{\sin(\pi(x_i - x_j))}{(\pi(x_i - x_j))}\right)\right] = 0 \tag{30}$$

If, moreover, $\mathbb{E}\, x_{ij}^3 = 0$ ($x_i j$ is the real part of the (i,j)-entry of H), we do not need to average over E. In other words, we have, for every fixed $|E| < 2$,

$$\lim_{N\to\infty} \int dx_1 \ldots dx_k \, O(x_1, \ldots, x_k) \, \frac{1}{\rho_{sc}^k(E)} p_N^{(k)}\left(E + \frac{x_1}{N\rho_{sc}(E)}, \ldots, E + \frac{x_k}{N\rho_{sc}(E)}\right) \\ = \int dx_1 \ldots dx_k \; O(x_1, \ldots, x_k) \, \det\left(\frac{\sin(\pi(x_i - x_j))}{(\pi(x_i - x_j))}\right)_{1\leq i,j\leq k} \tag{31}$$

It is interesting to note that the results on universality we just discussed do not generalized easily to ensemble of Wigner matrices with different symmetry (real symmetric and quaternion hermitian ensembles). The reason is that the expressions (22) and (24) are based on a formula due to Harish-Chandra to integrate over the

unitary group and, unfortunately, there is no analogous formula for integrating over the orthogonal (or the quaternion unitary) group. Also the result obtained in [19] by Tao and Vu can only be applied to ensembles of real symmetric or quaternion hermitian Wigner matrices if the first four moments of the matrix entries match exactly the corresponding Gaussian moments. To establish universality for real symmetric or quaternion hermitian ensembles of Wigner matrices, we developed new techniques, based on the introduction of a local relaxation flow, which approximates Dyson Brownian Motion, but is characterized by a faster relaxation time. In this case, we only prove universality after integrating the variable E over an (arbitrarily small) interval (as in (30)). Details can be found in [10].

5. Extensions and Applications of Universality

In [17], Péché shows universality (pointwise in E) for ensembles of complex *sample covariance matrices* extending the approach outlined in Section 4. In [11], we prove universality for ensembles of (real or complex) sample covariance matrices (but only after integration over E in a small interval).

In [12, 13], Erdős, Yau and Yin extend the results presented above to so called *generalized Wigner matrices*. Up to the symmetry constraints, the entries of generalized Wigner matrices are independent, but not necessarily identically distributed. Instead, one assumes that the variances $\sigma_{ij} = \mathbb{E}\, x_{ij}^2$, $1 \leq i, j \leq N$ are such that $c_1 \leq N\sigma_{ij} \leq c_2$.

In [14], the same authors show that the eigenvalues of generalized Wigner matrices are localized with very high probability within distances of order $(\log N)^\alpha/N$ from the position where the semicircle law predicts they should be.

More related results are also presented in the review paper [3].

To conclude these notes, we mention a new result concerning the *average density of states* for hermitian Wigner matrices. Theorem 2.1 establishes the convergence of the density of states to the semicircle law on the microscopic scale. On shorter scale we cannot expect the density of states to converge in probability, because its fluctuations are certainly important. Nevertheless, we may still ask whether on these extremely short scales the expectation of the density of states, known as the average density of states, converges. The next theorem (see [16]) gives a positive answer to this question.

Theorem 5.1. *Let H be an ensemble of hermitian Wigner matrices. Assume that the probability density of the matrix entries has the form $h(x) = e^{-g(x)}$ and satisfies the bounds*

$$\left|\widehat{h}(p)\right| \leq \frac{1}{(1+Cp^2)^{\sigma/2}}\,, \quad \left|\widehat{hg''}(p)\right| \leq \frac{1}{(1+Cp^2)^{\sigma/2}} \quad \text{for some } \sigma > 9.$$

Then, for any $|E| < 2$, we have

$$\frac{1}{\varepsilon}\,\mathbb{E}\,\mathcal{N}\left[E - \frac{\varepsilon}{2N}; E + \frac{\varepsilon}{2N}\right] \to \rho_{sc}(E) \tag{32}$$

as $N \to \infty$, uniformly in $\varepsilon > 0$. In other words, we have

$$\lim_{N\to\infty} \limsup_{\varepsilon\to 0} \mathbb{E}\, \frac{\mathscr{N}\left[E-\frac{\varepsilon}{2}; E+\frac{\varepsilon}{2}\right]}{N\varepsilon} = \lim_{N\to\infty} \liminf_{\varepsilon\to 0} \mathbb{E}\, \frac{\mathscr{N}\left[E-\frac{\varepsilon}{2}; E+\frac{\varepsilon}{2}\right]}{N\varepsilon} = \rho_{sc}(E).$$

Universality (in the form (31)) implies that

$$\mathbb{E}\, \frac{\mathscr{N}\left[E-\frac{\kappa}{2N}; E+\frac{\kappa}{2N}\right]}{\kappa} = \int \frac{\mathbf{1}(|x| \le \kappa/2)}{\kappa}\, p_N^{(1)}(E+\frac{x}{N}) \to \rho_{sc}(E) \tag{33}$$

for an arbitrary fixed (N independent) $\kappa > 0$. Hence, to prove Theorem 5.1, we need to understand how (33) can be extended to intervals of size ε/N with ε going to zero as $N \to \infty$ (or even $\varepsilon \to 0$ before $N \to \infty$). Eq. (32) follows, if we can show

$$\frac{1}{\pi}\, \mathbb{E}\, \mathrm{Im}\; m_N\left(E + i\frac{\varepsilon}{N}\right) \to \rho_{\mathrm{sc}}(E) \tag{34}$$

uniformly in $\varepsilon > 0$. To this end, we establish an upper bound of the form

$$\left|\frac{d}{dE}\, \mathbb{E}\, \mathrm{Im}\; m_N\left(E + i\frac{\varepsilon}{N}\right)\right| \le CN \tag{35}$$

uniformly in $\varepsilon > 0$. From (35), it follows that $\mathbb{E}\,\mathrm{Im}\; m_N(E + i(\varepsilon/N))$ remains essentially constant if E varies within an interval of size κ/N, for a small (but fixed) $\kappa > 0$. This means that

$$\begin{aligned}
&\frac{1}{\pi}\, \mathbb{E}\, \mathrm{Im}\; m_N\left(E + i\frac{\varepsilon}{N}\right) \\
&\qquad \simeq \mathbb{E}\, \frac{N}{\pi\kappa} \int_{E-\frac{\kappa}{2N}}^{E+\frac{\kappa}{2N}} dE'\, \mathrm{Im}\; m_N\left(E' + i\frac{\varepsilon}{N}\right) \\
&\qquad = \mathbb{E}\, \frac{1}{\pi\kappa} \sum_\alpha \left[\mathrm{arctg}\left(\frac{N\left(\mu_\alpha - E - \frac{\kappa}{2N}\right)}{\varepsilon}\right) - \mathrm{arctg}\left(\frac{N\left(\mu_\alpha - E + \frac{\kappa}{2N}\right)}{\varepsilon}\right)\right] \\
&\qquad \simeq \mathbb{E}\, \frac{1}{\kappa}\, \mathscr{N}\left[E - \frac{\kappa}{2N}; E + \frac{\kappa}{2N}\right] \to \rho_{sc}(E)
\end{aligned}$$

as $N \to \infty$, by (33). It remains to show the upper bound (35); here we use a Wegner estimate from [9], which implies that the average density of states remains uniformly bounded on arbitrarily small intervals. The same techniques used in [9] to show the Wegner estimate can be extended to obtain the bound (35). Details can be found in [16].

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LIEB-ROBINSON BOUNDS AND QUASI-LOCALITY FOR THE DYNAMICS OF MANY-BODY QUANTUM SYSTEMS

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We review a recently proven Lieb-Robinson bound for general, many-body quantum systems with bounded interactions. Several basic examples are discussed as well as the connection between commutator estimates and quasi-locality.

Keywords: Lieb-Robinson bounds; quasi-locality; quantum dynamics.

1. Introduction

Much physical intuition is based on locality properties of the system under consideration. Objects (or particles) are associated with regions (or points) in space and non-trivial interactions typically occur over short distances. For systems governed by a relativistic dynamics, the time evolution preserves this notion of locality.

In condensed matter physics, however, many interesting physically relevant phenomena are modeled by quantum many-body systems, e.g., super-conductivity and Bose-Einstein condensation. More abstractly, the models of quantum computation and discrete versions of field theory are described in terms of quantum lattice systems. For these non-relativistic systems, defined e.g. by a Hamiltonian with nearest neighbor interactions, the associated dynamics does not preserve locality in the sense that there is no strict equivalent to a finite speed of light.

Remarkably, Lieb and Robinson, see [1], proved that an approximate form of locality, which we refer to as *quasi-locality*, does hold for the dynamics associated to certain quantum spin systems. This important result establishes the existence and proves a bound for an approximate light cone which limits the rate at which disturbances, as evolved by the dynamics, can propagate through the system. More concretely, they proved that a local observable evolved for a time $t > 0$ remains essentially localized to a region of space whose diameter is proportional to t. They dubbed their estimate as a bound on the system's group velocity, but we prefer to describe the analysis as a Lieb-Robinson bound and the resulting estimate: the Lieb-Robinson velocity.

After the initial result by Lieb and Robinson in 1972 and some calculations for

specific models [2] a few years later, these locality estimates for quantum systems received relatively little attention. It was not until Hastings' impressive work of 2004, see [3], that a genuinely renewed interest in these bounds was established. Since then, a number of generalizations of the original result [4–11] and a wealth of interesting applications [3, 12–27] have demonstrated the importance of these bounds.

In this brief note, we introduce the general set-up for Lieb-Robinson bounds in the context of quantum systems with bounded interactions. We describe the correspondence between quasi-locality and the usual commutator estimates typically referred to as Lieb-Robinson bounds. The final section is a short list of further generalizations and a variety of applications.

Before we begin, we make the following useful observation. In quantum mechanics, one is often interested in a single quantum system, i.e., a specific Hilbert space $\mathscr{H}$ and a densely defined, self-adjoint operator H. For each normalized vector, or state $\psi \in \mathscr{H}$, the solution of the Schrödinger equation

$$\partial_t \psi = -iH\psi \tag{1}$$

governs the dynamics of this system. The solution, of course, is $\psi(t) = e^{-itH}\psi$. For particles in a domain $\Lambda \subset \mathbb{R}^\nu$, the typical Hilbert space is $\mathscr{H} = L^2(\Lambda)$ and it is common to have H a self-adjoint realization of the Laplacian. Corresponding to any normalized vector $\psi \in L^2(\Lambda)$ the solution $\psi(t)$ is called a wave function, and it is interesting to investigate the evolution of this function in space, i.e. Λ.

This is *not* the form of locality established by a Lieb-Robinson bound. Lieb-Robinson bounds are about collections of interacting quantum systems distributed in space. The bounds estimate the rate at which disturbances propagate through this collection.

2. The General Set-Up

As discussed above, Lieb-Robinson bounds estimate the rate at which disturbances propagate through a collection of quantum systems. The basic set-up is as follows.

2.1. *Collections of Quantum Systems*

Let Γ be a countable set, and consider a collection of quantum systems labeled by $x \in \Gamma$. By this, we mean that corresponding to each site $x \in \Gamma$ there is a Hilbert space $\mathscr{H}_x$ and a densely defined, self-adjoint operator H_x acting on $\mathscr{H}_x$. The operator H_x is typically referred to as the on-site Hamiltonian. For finite $\Lambda \subset \Gamma$, the Hilbert space of states corresponding to Λ is given by

$$\mathscr{H}_\Lambda = \bigotimes_{x\in\Lambda} \mathscr{H}_x \,, \tag{2}$$

and the algebra of observables is

$$\mathscr{A}_\Lambda = \bigotimes_{x\in\Lambda} \mathscr{B}(\mathscr{H}_x) = \mathscr{B}(\mathscr{H}_\Lambda) \,, \tag{3}$$

where $\mathscr{B}(\mathscr{H})$ is the set of bounded linear operators over the Hilbert space $\mathscr{H}$. Thus an observable $A \in \mathscr{A}_\Lambda$ depends only on those degrees of freedom in Λ. Of course, for any finite $X \subset \Lambda$, an observable $A \in \mathscr{A}_X$ can be uniquely identified with the observable $A \otimes \mathbb{1}_{\Lambda \setminus X} \in \mathscr{A}_\Lambda$, and therefore $\mathscr{A}_X \subset \mathscr{A}_\Lambda$.

In general, these collections of quantum systems are used to describe many interesting physical phenomena e.g., the moments associated with atoms in a magnetic material, a lattice of coupled oscillators, or an array of qubits in which quantum information is stored. Below we indicate two important types of examples.

Example 2.1. A *quantum spin system* over Γ is defined by associating a finite dimensional Hilbert space to each site $x \in \Gamma$, e.g., $\mathscr{H}_x = \mathbb{C}^{n_x}$ for some integer $n_x \geq 2$. The dimension of $\mathscr{H}_x$ is related to the spin at site x by $n_x = 2J_x + 1$, i.e. $n_x = 2$ corresponds to spin $J_x = 1/2$, $n_x = 3$ corresponds to spin $J_x = 1$, etc. As an on-site Hamiltonian, a common choice is to select a spin matrix in the n_x-dimensional irreducible representation of $su(2)$. When $n_x = 2$, these are just the Pauli spin matrices:

$$S^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \text{and} \quad S^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4}$$

Example 2.2. A *quantum oscillator system* over Γ corresponds to associating an L^2 space to each site of Γ, e.g. one can take $\mathscr{H}_x = L^2(\mathbb{R})$ for each $x \in \Gamma$. In contrast to the previous example, each single site Hilbert space is infinite dimensional, and moreover, the on-site Hamiltonians are typically functions of position q_x, the multiplication operator by q_x in $L^2(\mathbb{R}, dq_x)$, and momentum $p_x = -i\frac{d}{dq_x}$; both unbounded self-adjoint operators.

Despite the fact that these examples are quite different, the general techniques described below apply equally well to both cases.

2.2. *Interactions and Models*

The systems described above are of particular interest when they are allowed to interact. In general, a *bounded interaction* for such quantum systems is a mapping Φ from the set of finite subsets of Γ into the algebra of observables which satisfies

$$\Phi(X)^* = \Phi(X) \in \mathscr{A}_X \quad \text{for all finite } X \subset \Gamma. \tag{5}$$

A *model* is defined by the set Γ, the collection of quantum systems $\{(\mathscr{H}_x, H_x)\}_{x\in\Gamma}$, and an interaction Φ.

Associated to a given model there is a family of *local Hamiltonians*, $\{H_\Lambda\}$, parametrized by the finite subsets of Γ. In fact, to each finite $\Lambda \subset \Gamma$,

$$H_\Lambda = \sum_{x\in\Lambda} H_x + \sum_{X\subset\Lambda} \Phi(X) \tag{6}$$

is a densely defined, self-adjoint operator. Here the second sum is over all finite subsets of Λ, and is therefore finite. By Stone's theorem, the corresponding *Heisenberg*

dynamics, τ_t^Λ, given by

$$\tau_t^\Lambda(A) = e^{itH_\Lambda} A e^{-itH_\Lambda} \quad \text{for all } A \in \mathscr{A}_\Lambda \text{ and } t \in \mathbb{R}, \tag{7}$$

is a well-defined, one-parameter group of automorphisms on $\mathscr{A}_\Lambda$. Here are two typical models of interest.

Example 2.3. Fix an integer $\nu \geq 1$ and let $\Gamma = \mathbb{Z}^\nu$. Consider the quantum spin system obtained by setting $\mathscr{H}_x = \mathbb{C}^2$ for all $x \in \mathbb{Z}^\nu$. Take as on-site Hamiltonian $H_x = S^3$ using the notation from (4) above. Let Φ be the interaction defined by setting

$$\Phi(X) = \begin{cases} S_x^1 S_y^1 + S_x^2 S_y^2 + S_x^3 S_y^3 & \text{if } X = \{x, y\} \text{ and } |x - y| = 1, \\ 0 & \text{otherwise} \end{cases} \tag{8}$$

where for each $z \in \mathbb{Z}^\nu$, any $k \in \{1, 2, 3\}$, and each finite volume $\Lambda \subset \mathbb{Z}^\nu$, the quantity

$$S_z^k = \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes S^k \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} \tag{9}$$

where S^k, again from (4), appears in the z-th factor of $\mathscr{A}_\Lambda = \bigotimes_{x \in \Lambda} \mathscr{B}(\mathbb{C}^2)$.

A nearest neighbor, spin 1/2 Heisenberg model on $\mathbb{Z}^\nu$ corresponds to

$$\begin{aligned} H_\Lambda &= h \sum_{x \in \Lambda} H_x + J \sum_{X \subset \Lambda} \Phi(X) \\ &= \sum_{x \in \Lambda} h S_x^3 + \sum_{\substack{x, y \in \Lambda: \\ |x-y|=1}} J \left(S_x^1 S_y^1 + S_x^2 S_y^2 + S_x^3 S_y^3 \right) \end{aligned} \tag{10}$$

for all finite subsets $\Lambda \subset \mathbb{Z}^\nu$. Here h and J are real-valued parameters of the model.

Example 2.4. Fix an integer $\nu \geq 1$ and let $\Gamma = \mathbb{Z}^\nu$. Consider the quantum oscillator system obtained by setting $\mathscr{H}_x = L^2(\mathbb{R})$ for all $x \in \mathbb{Z}^\nu$. A nearest neighbor, anharmonic model on $\mathbb{Z}^\nu$ is defined analogously, e.g. with

$$H_\Lambda = \sum_{x \in \Lambda} p_x^2 + V(q_x) + \sum_{\substack{x, y \in \Lambda: \\ |x-y|=1}} \Phi(q_x - q_y) \tag{11}$$

for all finite subsets $\Lambda \subset \mathbb{Z}^\nu$. The parameters of this model are V and Φ. Of course, V must be chosen so that the on-site Hamiltonian $H_x = p_x^2 + V(q_x)$ is self-adjoint, and Φ is assumed to be in $L^\infty(\mathbb{R})$.

2.3. *Observables and Support*

The support of an observable plays a crucial role in Lieb-Robinson bounds. We introduce this notion here. Let Γ be a countable set and $\{(\mathscr{H}_x, H_x)\}_{x \in \Gamma}$ a collection of quantum systems. As we have seen above, for any two finite sets $\Lambda_0 \subset \Lambda \subset \Gamma$, each $A \in \mathscr{A}_{\Lambda_0}$ can be identified with a unique element $A \otimes \mathbb{1}_{\Lambda \setminus \Lambda_0} \in \mathscr{A}_\Lambda$. For this reason, $\mathscr{A}_{\Lambda_0} \subset \mathscr{A}_\Lambda$ for any $\Lambda_0 \subset \Lambda$.

Given an observable $A \in \mathscr{A}_\Lambda$, we say that A is *supported* in $X \subset \Lambda$ if A can be written as $A = \tilde{A} \otimes \mathbb{1}_{\Lambda \setminus X}$ with $\tilde{A} \in \mathscr{A}_X$. The *support* of an observable A is then

the minimal set X such that A is supported in X. We will denote the support of an observable A by $\mathrm{supp}(A)$.

Due to the fact that we are considering non-relativistic systems, i.e., models for which there is no strict equivalent to a finite speed of light, the following observation is generally true. Let $X \subset \Lambda \subset \Gamma$. Consider a local Hamiltonian H_Λ defined in terms of a non-trivial interaction; assume e.g. the interaction is nearest neighbor. Then, for general $A \in \mathscr{A}_X$, $\mathrm{supp}(\tau_0(A)) = \mathrm{supp}(A) \subset X$, however, $\mathrm{supp}(\tau_t^\Lambda(A)) = \Lambda$ for all $t \neq 0$. Hence, a strict notion of *locality*, implicitly defined here in terms of the support of an observable, is not generally preserved by the Heisenberg dynamics.

Lieb-Robinson bounds address the following simple question: Does the Heisenberg dynamics corresponding to, e.g. short range interactions, satisfy some weaker form of locality?

2.4. *From Locality to Commutators*

Lieb-Robinson bounds are often expressed in terms of commutator estimates. The relationship between these estimates and the support of local observables is due mainly to the tensor product structure of the observable algebras. We briefly discuss this fact in this section.

Let Γ be countable set and $\{(\mathscr{H}_x, H_x)\}_{x\in\Gamma}$ denote a collection of quantum systems. Consider two finite sets $X, Y \subset \Gamma$. If $A \in \mathscr{A}_X$, $B \in \mathscr{A}_Y$, and $X \cap Y = \emptyset$, then for any finite set $\Lambda \subset \Gamma$ for which $X \cup Y \subset \Lambda$ we can regard $A, B \in \mathscr{A}_\Lambda$ and as such $[A, B] = 0$ due to the structure of the tensor product. In words, observables with disjoint supports commute.

Conversely, Schur's lemma demonstrates the following. If $A \in \mathscr{A}_\Lambda$ and

$$[A, \mathbb{1}_{\Lambda\setminus Y} \otimes B] = 0 \quad \text{for all } B \in \mathscr{A}_Y\,, \tag{12}$$

then $\mathrm{supp}(A) \subset \Lambda \setminus Y$. In fact, a more general statement is true. If $A \in \mathscr{A}_\Lambda$ almost commutes with all $B \in \mathscr{A}_Y$, then A is approximately supported in $\Lambda \setminus Y$. The following lemma appears in [28].

Lemma 2.1. *Let $\mathscr{H}_1$ and $\mathscr{H}_2$ be Hilbert spaces and $A \in \mathscr{B}(\mathscr{H}_1 \otimes \mathscr{H}_2)$. Suppose there exists $\epsilon \geq 0$ for which*

$$\|[A, \mathbb{1}_1 \otimes B]\| \leq \epsilon \|B\| \quad \text{for all } B \in \mathscr{B}(\mathscr{H}_2). \tag{13}$$

Then, there exists $A' \in \mathscr{B}(\mathscr{H}_1)$, such that

$$\|A' \otimes \mathbb{1}_2 - A\| \leq \epsilon. \tag{14}$$

Equipped with this lemma, we see that uniform estimates on commutators provide approximate information on the support of observables. Thus, for any $A \in \mathscr{A}_X$, we can approximate $\mathrm{supp}(\tau_t^\Lambda(A))$ by bounding $\|[\tau_t^\Lambda(A), B]\|$ for all B with $\mathrm{supp}(B) \subset Y$. Here the estimates will, of course, depend on the distance between X and Y in Γ and the time t for which the observable has been evolved. This is the basic idea of a Lieb-Robinson bound.

3. Lieb-Robinson Bounds

In this section, we describe in detail assumptions on the set Γ and the interactions Φ under which one can prove a Lieb-Robinson bound. We also present a precise statement of the estimate and discuss several relevant consequences. For a proof in this setting, we refer the interested reader to [9].

3.1. *On the Geometry of* Γ

For many models, e.g both Examples 2.3 and 2.4, the set $\Gamma = \mathbb{Z}^\nu$. In general, though, the lattice structure of $\mathbb{Z}^\nu$ is not necessary to prove a Lieb-Robinson bound. The following assumptions are sufficient. Let Γ be a set equipped with a metric d. If Γ has infinite cardinality, we further assume that there is a non-increasing function $F : [0, \infty) \to (0, \infty)$ which satisfies two conditions. First, we assume that F is *uniformly integrable* over Γ, i.e.,

$$\|F\| = \sup_{x\in\Gamma} \sum_{y\in\Gamma} F(d(x, y)) < \infty\,. \tag{15}$$

Next, we assume there exists $C > 0$ such that the following *convolution condition* is satisfied: for all $x, y \in \Gamma$,

$$\sum_{z\in\Gamma} F(d(x, z))F(d(z, y)) \;\le\; C\,F(d(x, y)). \tag{16}$$

The inequality (16) is quite useful in the iteration scheme which is at the heart of proving a Lieb-Robinson bound.

Here is an important observation. Let Γ be a set with a metric and F satisfy the properties mentioned above with respect to Γ. In this case, the function F_a defined by setting $F_a(r) = e^{-ar}F(r)$ for any $a \ge 0$ also satisfies (15) and (16) above with $\|F_a\| \le \|F\|$ and $C_a \le C$. The choice of an exponential weight here is convenient, but not necessary. In fact, $G = wF$ satisfies (15) and (16) for any positive, non-increasing, *logarithmically super-additive* weight w, i.e. a function w for which $w(x + y) \ge w(x)w(y)$.

Example 3.1. Consider the case of $\Gamma = \mathbb{Z}^\nu$. For any $\epsilon > 0$, the function $F(r) = (1 + r)^{-(\nu+\epsilon)}$ is positive, non-increasing, and

$$\|F\| = \sum_{x\in\mathbb{Z}^\nu} \frac{1}{(1 + |x|)^{\nu+\epsilon}} < \infty. \tag{17}$$

A short calculation shows that the convolution constant for this F satisfies $C \le 2^{\nu+\epsilon+1}\|F\|$. Thus, such functions do exist. As a final remark, we note that the exponential function *does not* satisfy the convolution condition (16) on $\mathbb{Z}^\nu$, however, $F_a(r) = e^{-ar}/(1 + r)^{\nu+\epsilon}$ certainly does.

3.2. *Assumptions on the Interaction Φ*

Locality estimates are valid when the interactions are sufficiently short range. For general sets Γ, a sufficient decay assumption can be made precise in terms of the F function introduced in the previous sub-section.

Let Γ be a set with a metric d and a function F as in Section 3.1. For any $a \geq 0$, denote by $\mathscr{B}_a(\Gamma)$ the set of all those interactions Φ for which

$$\|\Phi\|_a = \sup_{x,y\in\Gamma} \frac{1}{F_a(d(x,y))} \sum_{\substack{X\subset\Gamma:\\ x,y\in X}} \|\Phi(X)\| < \infty. \tag{18}$$

Example 3.2. Many interesting models have finite range interactions, see e.g. Examples 2.3 and 2.4. An interaction Φ is said to be of finite range if there exists a number $R > 0$ for which $\Phi(X) = 0$ whenever the diameter of X exceeds R. In the case of $\Gamma = \mathbb{Z}^\nu$ and $F(r) = (1+r)^{-\nu-\epsilon}$, it is easy to see that all uniformly bounded, finite range interactions satisfy $\|\Phi\|_a < \infty$ for all $a \geq 0$.

Example 3.3. Another important class of models involve pair interactions. An interaction Φ is called a pair interaction if $\Phi(X) = 0$ unless $X = \{x, y\}$ for some points $x, y \in \Gamma$. In the case of $\Gamma = \mathbb{Z}^\nu$ and $F(r) = (1+r)^{-\nu-\epsilon}$, it is easy to see that all uniformly bounded, pair interactions that decay exponentially in $|x-y|$ satisfy $\|\Phi\|_a < \infty$ for some $a > 0$. In fact, if the pair interactions decay faster than an appropriate inverse polynomial, then $\|\Phi\|_0 < \infty$, and this is sufficient for a decay estimate on the relevant commutators.

3.3. *The Main Result*

We can now state a Lieb-Robinson bound, proven in [9], for the systems introduced above.

Theorem 3.1. *Let Γ be a set with a metric d and a function F as described in Section 3.1. Fix a collection of quantum systems $\{(\mathscr{H}_x, H_x)\}_{x\in\Gamma}$ over Γ, and for any $a \geq 0$, let $\Phi \in \mathscr{B}_a(\Gamma)$. Then, the model defined by Γ, $\{(\mathscr{H}_x, H_x)\}_{x\in\Gamma}$, and Φ satisfies a Lieb-Robinson bound. In fact, for each fixed finite subsets $X, Y \subset \Gamma$, and any finite $\Lambda \subset \Gamma$ with $X \cup Y \subset \Lambda$, the estimate*

$$\|[\tau_t^\Lambda(A), B]\| \leq 2\|A\|\|B\| \min\left[1, g_a(t) \sum_{x\in X, y\in Y} F_a\left(d(x,y)\right)\right] \tag{19}$$

holds for any $A \in \mathscr{A}_X$, $B \in \mathscr{A}_Y$, and $t \in \mathbb{R}$. Here the function g_a is given by

$$g_a(t) = \begin{cases} C_a^{-1}\left(e^{2\|\Phi\|_a C_a|t|} - 1\right) & \text{if } X \cap Y = \emptyset, \\ C_a^{-1} e^{2\|\Phi\|_a C_a|t|} & \text{otherwise.} \end{cases} \tag{20}$$

As a corollary, a more familiar form of the Lieb-Robinson bound can be expressed in terms of $d(X,Y) = \min_{x\in X, y\in Y} d(x,y)$, namely

Corollary 3.1. *Given the assumptions of Theorem 3.1 and $a > 0$, the estimate*

$$\|[\tau_t^\Lambda(A), B]\| \leq \frac{2\|A\|\|B\|\|F\|}{C_a} \min[|X|, |Y|] e^{-a(d(X,Y)-v_\Phi(a)|t|)} \tag{21}$$

is valid. Here $|X|$ denotes the cardinality of X and the quantity $v_\Phi(a)$ is given by

$$v_\Phi(a) = \frac{2\|\Phi\|_a C_a}{a}\,. \tag{22}$$

Let us make a few remarks to help interpret these bounds. As we indicated in Section 2.2, the Heisenberg dynamics, τ_t^Λ, forms a one-parameter group of automorphisms on $\mathscr{A}_\Lambda$ and so the estimate $\|[\tau_t^\Lambda(A), B]\| \leq 2\|A\|\|B\|$ is always true. What we see from (19), and more directly in (21), is that if A and B have disjoint supports X and Y respectively, then $[\tau_0(A), B] = [A, B] = 0$ and the estimate on $[\tau_t(A), B]$ is small in the distance $d(X, Y)$ for times

$$|t| \leq \frac{d(X,Y)}{v_\Phi(a)}\,. \tag{23}$$

For this reason, the quantity $v_\Phi(a)$ is called a Lieb-Robinson velocity for the model under consideration. In fact, using Lemma 2.1, we see that for each $A \in \mathscr{A}_X$ the time evolution $\tau_t^\Lambda(A)$ is approximately supported in a ball of radius $v_\Phi(a)|t|$ about X. Thus the dynamics of the system remain essentially confined to a light cone defined by this Lieb-Robinson velocity. Moreover, the velocity $v_\Phi(a)$, see (22), which governs the rate at which disturbances propagate through the system, depends only on the interaction Φ and the geometry of Γ; specifically, it is independent of the on-site Hamiltonians.

Another crucial fact about these Lieb-Robinson bounds is that the explicit estimates, in particular the velocity, do not depend on the finite volume Λ on which the dynamics is defined. This suggests, and can be proven in this setting see e.g. [27], that a thermodynamic limit for the dynamics exists. It too satisfies the same Lieb-Robinson bound.

As has been useful in a variety of applications, it is interesting to note the dependence of these bounds on the support of the corresponding observables. Since only the minimum cardinality appears, one of two the observables could be allowed to be volume, i.e. Λ, dependent without sacrificing the bound. In fact, a more detailed analysis shows that only the minimum cardinality of the boundary of the supports of the observables is relevant, see [9] for a precise statement.

When $\Phi \in \mathscr{B}_a(\Gamma)$ for some $a > 0$, the Lieb-Robinson bounds decay exponentially in the distance between the supports of the observables. The rate of this exponential decay, here the number $a > 0$, is usually of little consequence. For this reason, if $\Phi \in \mathscr{B}_a(\Gamma)$ for all $a \in (\alpha, \beta)$, the optimal Lieb-Robinson velocity is given by

$$\inf_{a\in(\alpha,\beta)} v_\Phi(a) = \inf_{a\in(\alpha,\beta)} \frac{2\|\Phi\|_a C_a}{a}\,. \tag{24}$$

We now estimate this optimum velocity for the previously mentioned examples.

Example 3.4. Let $\Gamma = \mathbb{Z}^\nu$, $F(r) = (1+r)^{-\nu-\epsilon}$, and consider the spin 1/2 Heisenberg model introduced in Example 2.3. Clearly, for any $a > 0$,

$$\|\Phi\|_a = e^a 2^{\nu+\epsilon} 3J < \infty\,, \tag{25}$$

and therefore, a bound on the optimal velocity of this model is given by

$$3Je2^{2(\nu+\epsilon+1)} \sum_{x\in\mathbb{Z}^\nu} \frac{1}{(1+|x|)^{\nu+\epsilon}}\,. \tag{26}$$

As we observed above, this estimate on the velocity is independent of the on-site parameter h.

Example 3.5. Let $\Gamma = \mathbb{Z}^\nu$, $F(r) = (1+r)^{-\nu-\epsilon}$, and consider the anharmonic Hamiltonian introduced in Example 2.4. A similar calculation gives a bound on the optimal velocity of

$$\|\Phi\|_\infty e2^{2(\nu+\epsilon+1)} \sum_{x\in\mathbb{Z}^\nu} \frac{1}{(1+|x|)^{\nu+\epsilon}}\,, \tag{27}$$

which is independent of the on-site function V, so long as the self-adjointness assumption is satisfied.

4. Some Words on Generalizations and Applications

Over the past few years applications have driven a number of interesting generalizations of the original Lieb-Robinson bounds. Several review articles have been devoted to many of these specific applications, see [8, 29], and some lecture notes from schools on topics concerning locality are now available [30, 31]. In this short note, we make no attempt to give an exhaustive list of generalizations and applications, but rather we list many relevant works to give the interested reader a reasonable starting point to further investigate this active area of research.

4.1. *On Generalizations*

The Lieb-Robinson bound stated in Theorem 3.1, and proven in [9], already includes several generalizations of the original result. Most importantly, it applies to quantum systems with infinite dimensional, single site Hilbert spaces. In addition, no assumption on the lattice structure of Γ is necessary, and the dependence of the bound on the support of the observables has been refined.

Recently, Lieb-Robinson bounds have been proven for time-dependent interactions, see [28]. Moreover, Poulin demonstrated in [11] that these estimates also hold for an irreversible, semi-group dynamics generated by Lindblad operators.

Quite some time ago, it was proven in [32] that the analogue of Lieb-Robinson bounds hold for the non-relativistic dynamics corresponding to classical Hamiltonian systems. In the past few years, further work in this direction has appeared in [33] and [34].

An important open question is: To what extent do Lieb-Robinson bounds apply in the case of unbounded interactions? For certain simple systems, there has been some progress on this issue. Lieb-Robinson bounds for general harmonic systems first appeared in [7]. It was proven in [9], see also [21, 27], that these estimates also hold for anharmonic systems if the perturbation is sufficiently weak. A recent result in [35] suggests that such bounds apply much more generally. Finally, a Lieb-Robinson estimate for commutator bounded operators appeared in [10].

4.2. *On Applications*

Many of the generalizations mentioned above came about by pursuing concrete applications. As discussed in the main text, the resurgence of interest in Lieb-Robinson bounds was mainly motivated by Hastings' 2004 paper [3] on a proof of the multi-dimensional Lieb-Schultz-Mattis theorem. In this incredibly influential paper, Hastings discussed generalized Lieb-Robinson bounds, an Exponential Clustering theorem, and pioneered his notion of a quasi-adiabatic evolution. This single work inspired a flurry of activity which continues to this day.

The Lieb-Schultz-Mattis theorem, see [36], concerns the spectral gap between the ground state energy and that of the first excited state for the nearest-neighbor, spin 1/2 Heisenberg model in one dimension. They proved that for a finite volume of size L, if the ground state is unique, then the gap is bounded by C/L, for some constant C. Further generalizations, to models with arbitrary half-integer spin and to a statement valid in the thermodynamic limit appeared in [37]. Hastings paper [3] developed a multi-dimensional analogue of this result. In fact, his argument yields a gap estimate applicable in a great deal of generality, see [15] for a precise statement. Recent reviews of these results appear in [8] and [30].

The Exponential Clustering theorem is a proof that the ground state expectations of gapped systems decay exponentially in space. Proofs of this result first appeared in [4] and [5]. A refinement of the dependence of the estimates on the support of the observables was proven in [8], and this fact was later used by Matsui in [26] to investigate a split property for quantum spin chains.

It is well known that, for quantum spin systems, a Lieb-Robinson bound may be used to establish the existence of a thermodynamic limit for the Heisenberg dynamics, see e.g. [38]. Improved estimates allowed for this result to be generalized, e.g., the case of polynomially decaying interactions was covered in [6] and the existence of the dynamics for the general systems considered here was proven in [27]. For perturbations of the harmonic system, the existence of the thermodynamic limit has been proven with two distinct methods, see [21] and [27].

An area law for gapped one-dimensional systems was proven by Hastings in [14]. In general, the area law conjecture states that the von Neumann entropy of the restriction of gapped ground states to a finite volume of size Λ grows no faster than a quantity proportional to the surface area of Λ. Certain aspects of Hastings' argument generalize to the multi-dimensional setting, e.g. a factorization property

of gapped ground states was proven in [19], but a proof of the area law for general gapped systems in arbitrary dimension remains an important open question. Some progress on a class of unfrustrated spin Hamiltonians appears in [22]. A review of these topics is contained in [29], see also [31].

Quantization of the Hall conductance for a general class of interacting fermions was recently proven in [20]. This intriguing result makes crucial use of improved Lieb-Robinson bounds and the methods associated with Hastings' quasi-adiabtic evolution. A detailed analysis of this technique, with specific regards to its implications for perturbation theory, is the main topic of [28].

Finally, stability of topological order was addressed in [23, 24]. There the authors consider a class of Hamiltonians that are the sum of commuting short-range terms, such as the toric code model developed by Kitaev in [39], and proved that the topological order of the ground states is stable under arbitrary, small short-range perturbations.

Developing a better understanding of quantum dynamics and its perturbation theory will be crucial in providing new insight into complex physical phenomena. As indicated by the number of recent generalizations and applications, the analysis of Lieb-Robinson bounds is a thriving area of active research which attempts to address this very issue.

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DISORDER-INDUCED DELOCALIZATION ON TREE GRAPHS*

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Highlighting a mechanism for the emergence of absolutely continuous spectrum through fluctuation-enabled resonance, we resolve an existing question concerning the mobility edge for Schrödinger operators with random (unbounded) potential on regular tree graphs. We find that the disorder driven resonance mechanism causes the somewhat surprising appearance of absolutely continuous spectrum well beyond the energy band of the operator's hopping term. For weak disorder this includes a Lifshits tail regime of very low density of states.

Keywords: Random operators; absolutely continuous spectrum; Lifshits tail regime.

Summary

Random Schrödinger operators, which combine a hopping term and random potential,

$$H_\lambda(\omega) \;=\; T + \lambda\, V(\omega)\,, \tag{1}$$

acting in the Hilbert space $\ell^2(\mathscr{T})$ of square summable functions over a regular tree graph ($\mathscr{T}$), are among the earlier studied models of Anderson localization [1–4]. The possible existence of extended (generalized) eigenstates for operators which incorporate disorder is important for the discussions of conduction within simple models of condensed matter physics. Yet, broadly speaking, mathematical understanding of this topic is still lagging.

More specifically, we refer here to a regular tree graph $\mathscr{T}$ of degree $(K+1)$ (i.e., each sites having that many neighbors), and T the generator of 'hopping' transitions between neighboring sites, i.e., $T_{x,y} = \delta_{|x-y|,1}$). The second term in (1) is a random potential $V(\omega)$ scaled by the disorder parameter $\lambda \geq 0$. It is defined in terms of independent and identically distributed random variables $V_x(\omega)$ associated with the vertices of the graph, $x \in \mathscr{T}$. We focus on the case that the support of the distribution coincides with the whole real line $\mathbb{R}$; examples are Gaussian or Cauchy random potentials. As a consequence, the almost-sure spectrum of the operator (1)

*Talk presented at QMath11 by Simone Warzel.

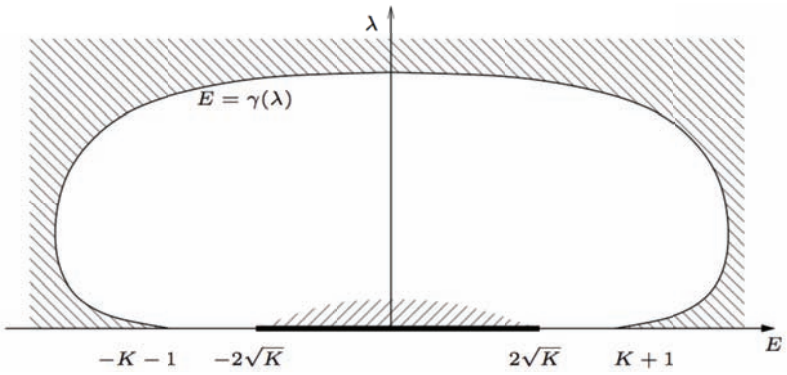

Fig. 1. A sketch of the previously known parts of the phase diagram. The outer region is of proven spectral and dynamical localization, the smaller hatched region is of proven delocalization and absolutely continuous spectrum. The latter is extended by the result mentioned here, into a region in which the density of states vanishes faster than any power. The intersection of the curve with the energy axis is stated exactly, while in other details the depiction is only schematic.

changes discontinuously from $\sigma(T) = [-2\sqrt{K}, 2\sqrt{T}]$ at zero disorder to $\sigma(H_\lambda) = \mathbb{R}$ for any $\lambda > 0$.

Rigorous results which were previously derived for such operators include proofs of the existence of both localization regimes, where the spectrum is pure-point type [5, 6], and delocalization, with absolutely continuous spectrum [7–9]. However, there has been a curious gap between the regimes for which the results were obtained: localization was proven under a fractional moment condition which holds in a regime whose rough outline is given in Figure 1, which for $\lambda \downarrow 0$ does not connect to $\sigma(T)$, whereas each of the different methods by which delocalization was established applies only in the close vicinity of $\sigma(T)$ (as depicted in Figure 1). As was stressed in [10], the gap between the results has included a regime where the disorder causes Lifshits tail phenomena: extremely low density of states, and the breakup of its spacial support into well separated clusters of low density. At various points, different views have been expressed as to the possible spectrum in this regime.

The talk presented at the QMath11 conference focused on a recent result which addresses the above question. It is shown there that, somewhat surprisingly, the spectrum in the regime described above is absolutely continuous. The analysis may be of additional interest (e.g. for the problems discussed in [11, 12]) , as it brought up a mechanism through which conduction may be enabled through disorder-enabled tunneling.

The exact statement of the result, and a heuristic explanation, can be found in [13]. The detailed mathematical derivation will be provided in [14].

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SEMICLASSICAL SPECTRAL BOUNDS AND BEYOND

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We summarize some of the improvements on Lieb-Thirring estimates during the past decade. In particular, we discuss logarithmic Lieb-Thirring estimates and Berezin-Li-Yau bounds with second order remainder terms.

Keywords: Eigenvalue estimates; Lieb-Thirring bounds.

1. Setting of the Problem. Lieb-Thirring bounds

Let

$$H(V) = (-\Delta)^l - V(x), \qquad l > 0,\ x \in \mathbb{R}^d,$$

be a Schrödinger type operator of order $2l$ on $L^2(\mathbb{R}^d)$. For suitable potential wells $-V(x) \le 0$[a] the spectrum of $H(V)$ consists of an essential part $\sigma_{ess}(H(V)) = [0, +\infty)$ and of negative eigenvalues $-\lambda_j(V)$. We number these eigenvalues in increasing order counting multiplicities and study the sums

$$S_{d,\gamma}(V) = \sum_j \lambda_j^\gamma = \mathrm{Tr}\ (H(V))_-^\gamma\,, \quad \gamma \ge 0\,.$$

For $\gamma = 0$ these spectral averages are understood as the counting function for the negative eigenvalues of $H(V)$. The Lieb-Thirring estimates

$$S_{d,\gamma}(V) \le R(d,\gamma,l) S^{\mathrm{cl}}_{d,\gamma}(V) \tag{1}$$

compare the spectral quantities $S_{d,\gamma}(V)$ with the classical phase space averages

$$S^{\mathrm{cl}}_{d,\gamma}(V) = \iint_{\mathbb{R}^d\times\mathbb{R}^d} (|\xi|^{2l} - V(x))_- \frac{dx d\xi}{(2\pi)^d} = L^{\mathrm{cl}}_{d,\gamma,l} \int_{\mathbb{R}^d} V^{\gamma+\varkappa}(x) dx\,,$$

where

$$L^{\mathrm{cl}}_{d,\gamma,l} = \frac{\gamma\Gamma(\gamma)\Gamma(\varkappa+1)}{2^d\pi^{\frac{d}{2}}\Gamma(\frac{d}{2}+1)\Gamma(\varkappa+\gamma+1)} \quad \text{and} \quad \varkappa = \varkappa(d,l) = \frac{d}{2l}\,.$$

[a] For simplicity we assume throughout the paper that $V(x) \ge 0$ unless explicitely stated otherwise.

Put $\gamma_{\rm cr} = 1 - \varkappa$. The bound (1) holds true for all $V \in L_{\gamma+\varkappa}(\mathbb{R}^d)$, if and only if

$$\gamma \geq \gamma_{\rm cr} \qquad \text{for dimensions} \qquad d < 2l\,, \tag{2}$$

$$\gamma > \gamma_{\rm cr} = 0 \qquad \text{for the dimension} \qquad d = 2l\,, \tag{3}$$

$$\gamma \geq 0 \qquad \text{for dimensions} \qquad d > 2l\,. \tag{4}$$

The cases $l = 1$ and $\gamma > 0$ for $d \geq 2$ or $\gamma > \frac{1}{2}$ for $d = 1$ respectively, have been settled in the original paper [1]. Their method extends immediately to arbitrary $l > 0$ for all $\gamma > \max\{0, \gamma_{\rm cr}\}$. The important special case $\gamma = 0$ for $d > 2l$ has been solved in [2] (for $l = 1$), in [3, 4] (for $l \in \mathbb{N}$) and in [5]. The techniques in the latter paper apply for all $l > 0$. The case $\gamma = \gamma_{\rm cr} > 0$ for $d < 2l$ has been proven in [6] for $l = 1$ and in [7] for $l \in \mathbb{N}$. In view of a remark by Simon [8] these methods extend actually to all $l > 0$ [9].

It has also been shown that for $l \in \mathbb{N}$ in the case of $d < 2l$ for $0 < \gamma \leq \gamma_{\rm cr}$ and for $\gamma = 0$ if $d = 2l$ a reverse bound

$$S_{d,\gamma}(V) \geq \tilde{R}(d, \gamma, l) S^{\rm cl}_{d,\gamma}(V) \tag{5}$$

holds true for all $0 \leq V \in L_{\gamma+\varkappa}(\mathbb{R}^d)$ with suitable positive constants $\tilde{R}(d, \gamma, l)$, see [10] for $d = l = 1$, $\gamma = \gamma_{\rm cr}$ and [11] for $d = l = 1$, $\gamma < \gamma_{\rm cr}$, as well as [7] for $l \in \mathbb{N}$ and $0 < \gamma = \gamma_{\rm cr}$ and [12] for $l \in \mathbb{N}$ and $0 < \gamma < \gamma_{\rm cr}$. The subtle case $\gamma = \gamma_{\rm cr} = 0$ has been settled in [13]. As a consequence for $l \in \mathbb{N}$, $\gamma = \gamma_{\rm cr} > 0$ and all non-negative $V \in L_1(\mathbb{R}^d)$ one has actually a two-sided bound

$$\tilde{R}(d, \gamma_{\rm cr}) S^{\rm cl}_{d,\gamma_{\rm cr}}(V) \leq S_{d,\gamma_{\rm cr}}(V) \leq R(d, \gamma_{\rm cr}) S^{\rm cl}_{d,\gamma_{\rm cr}}(V) \tag{6}$$

with some positive $\tilde{R}(d, \gamma_{\rm cr})$.

For non-integer $l > 0$ and $0 \leq \gamma \leq \gamma$cr the validity of (5) - and hence the validity of the lower bound in (6) - remains open so far.

2. Sharp Lieb-Thirring constants

We turn now to the optimal values of the constants $R(d, \gamma, l)$ in (1). The discussion of these quantities is governed by two basic facts: Namely, for fixed d and l the functions $R(d, \gamma, l)$ are non-increasing in γ and, moreover, $R(d, \gamma, l) \geq 1$. The first observation is due to Aizenman and Lieb [14], the second one is an immediate consequence of the large coupling asymptotics [b]

$$S_{d,\gamma}(\alpha V) = (1 + o(1)) S^{\rm cl}_{d,\gamma}(\alpha V) \quad \text{as} \quad \alpha \to +\infty\,. \tag{7}$$

Hence, if we have $R(d, \gamma_0, l) = 1$ for some value γ_0, then for this dimension d it also holds $R(d, \gamma, l) = 1$ for all $\gamma \geq \gamma_0$. Similary, one has $\tilde{R}(d, \gamma, l) \leq 1$ for all $0 < \gamma \leq \gamma_{\rm cr}$. Note that the Aizenman-Lieb trick does not work downwards for the lower bounds.

[b] This Weyl type formula can be verified by standard methods for sufficiently regular potentials. In all cases when (1) holds true, the asymptotic formula extends to all potentials with finite phase space average $S^{\rm cl}_{d,\gamma}(V)$.Further below we shall also mention some examples of potentials V with finite $S^{\rm cl}_{d,\gamma}(V)$, where both (1) and (7) fail.

The sharp values of $R(d,\gamma,l)$ are known only in the following two cases

$$R\left(1,\frac{1}{2},1\right)=2 \qquad \text{and} \qquad R\left(d,\gamma,1\right)=1 \quad \text{for all} \quad \gamma\geq\frac{3}{2},\ d\in\mathbb{N}\,. \tag{8}$$

In the first case $l=d=1$ and $\gamma=\gamma_{\mathrm{cr}}=\frac{1}{2}$ the constant $R\left(1,\frac{1}{2},1\right)=2$ corresponds to the asymptotic behaviour of the weak coupling bound state. Indeed, for smooth and compactly supported $V\geq 0$ one has exactly one negative eigenvalue for all sufficiently small $\alpha>0$ and (see [15])

$$S_{1,\frac{1}{2}}(\alpha V)=(1+o(1))S^{\mathrm{cl}}_{1,\frac{1}{2}}(\alpha V) \quad \text{as} \quad \alpha\to+0\,.$$

By scaling this corresponds to the fact that the constant $R\left(1,\frac{1}{2},1\right)=2$ is "achieved" for the Delta potential $V=\delta(x-x_0)$. This case has been settled in [16]. The second case in (8) corresponds to the large coupling Weyl formula (7). This result has been obtained for the one-dimensional case in [1, 14] and for arbitrary dimensions in [17].

In fact, for $l=d=1$ and $\gamma=\gamma_{\mathrm{cr}}=\frac{1}{2}$ the Weyl formula is sharp for the lower bound. That means $\tilde{R}\left(1,\frac{1}{2},1\right)=1$ and the two-sided estimate takes the form

$$S^{\mathrm{cl}}_{1,\frac{1}{2}}(V)\leq S_{1,\frac{1}{2}}(V)\leq 2S^{\mathrm{cl}}_{1,\frac{1}{2}}(V)$$

for all $0\leq V\in L_1(\mathbb{R})$.

There are various non-sharp upper and lower bounds on the constants $R(d,\gamma,1)$. In particular, one has $1<R(d,\gamma,1)$ for all $\gamma<1$ [18]. Moreover, $R(d,\gamma,1)\leq 2$ for $\frac{1}{2}\leq\gamma<1$ [19] and $R(d,\gamma,1)\leq 1.814$ for $1\leq\gamma<\frac{3}{2}$ [20, 21] as well as $R(2,1,1)>1$ and $R(1,\gamma,1)>1$ for $\frac{1}{2}\leq\gamma<\frac{3}{2}$ [1, 22].

Much less is known on the values of $R(d,\gamma,l)$ for $l\neq 1$. Not only is there no single case where the sharp value has been established, even natural conjectures based on the case $l=1$ seem to fail. For example, in the critical case $\gamma=\gamma_{\mathrm{cr}}=\frac{1}{2}$ for $d=l=1$ the sharp constant corresponds to the weak coupling behaviour or equivalently the Delta potential. Since for $\gamma=\gamma_{\mathrm{cr}}>0$ the weak coupling ground state exists and satisfies [7]

$$S_{d,\gamma_{\mathrm{cr}}}(\alpha V)=(1+o(1))\tau(d,l)S^{\mathrm{cl}}_{d,\gamma_{\mathrm{cr}}}(\alpha V) \quad \text{as} \quad \alpha\to+0\,,$$

where $\tau(d,l)=\frac{\pi\frac{d}{2l}}{\sin\left(\pi\frac{d}{2l}\right)}>1$. It seems reasonable to conjecture that $R(d,\gamma_{\mathrm{cr}},l)=\tau(d,l)$. This hypothesis fails. Indeed, in [23] it has been shown, that for $l\in\mathbb{N}$ and non-trivial, sufficiently regular $V\geq 0$ the operator $H(V)$ has exactly $m(d,l)=\binom{l+\left[\frac{d}{2}\right]}{d}$ weak coupling states. Since for weak coupling the higher states do all vanish with higher order in the coupling parameter than the ground state, this does not immediately imply a counter example. But on a closer look one can construct even for $d=1$ and $l=2$ a two Delta potential for which $S_{1,\frac{3}{4}}(V)>\tau(1,2)S^{\mathrm{cl}}_{1,\frac{3}{4}}(V)$. For that end one starts with a single Delta potential. Since the corresponding ground state of a 4th order operator changes sign, one can add a second Delta function in the nodal point of the ground state to the potential - and therefore a second negative eigenvalue to the operator - not spoiling the first one. A subtle play with the coupling yields the counter example which is essentially based on the presence of two negative eigenvalues [24]. Therefore it seems reasonable to put forward a

modified working conjecture that for $\gamma_{\rm cr} > 0$ one has $R(d, \gamma_{\rm cr}, l) = \tau(d, l)$ if and only if $m(d, l) = 1$ and $R(d, \gamma_{\rm cr}, l) > \tau(d, l)$ otherwise.

3. Further developments

Although the knowledge on sharp constants is now about the same as in the year 2000, the subject sparked quite a substantial amount of work on semiclassical spectral estimates during the past decade. Let me just mention a few important directions, which shall however not be discussed in detail below.

Let me first mention the amazing observation, that for $l = 1$ and $\gamma \geq 2$ the ratio $S_{d,\gamma}(\alpha V)/S^{\rm cl}_{d,\gamma}(\alpha V)$ is monotone increasing in α [25, 26]. Therefore, the proof of the Lieb-Thirring bound and the estimate for the corresponding constant can be pushed into the semiclassical limit. This is the first approach to sharp constants, which is directly applicable to higher dimensions and does not reduce the problem to a one-dimensional setting.

In [20, 21] techniques of mass transport have been applied to claim improved estimates on $R(d, 1, 1)$. Moreover, in [27] a beautiful connection between estimates on $R(d, 1, 1)$ and the so-called loop conjecture have been found.

A third line of work concerns improved Lieb-Thirring estimates with additional Hardy type terms [28–30].

Finally one should mention Lieb-Thirring estimates on graphs [31] and on metric trees [32, 33].

4. Logarithmic Lieb-Thirring estimates

We turn now to the case $d = 2l$, $l \in \mathbb{N}$ and $\gamma = \gamma_{\rm cr} = 0$. As mentioned above, in [13] the estimate (5) from below has been established, while the corresponding bound (1) from above fails. To see the latter fact one usually makes the following point: For $d = 2l$ the operator $H(\alpha V)$ has for any nontrivial $V \geq 0$ and any $\alpha > 0$ at least one negative bound state and $S_{0,d}(\alpha V) \geq 1$, while at the same time $S^{\rm cl}_{0,d}(\alpha V) \to 0$ as $\alpha \to +0$. Therefore (1) must fail for $\gamma = \gamma_{\rm cr} = 0$ as $\alpha \to +0$. This argument, although true of course, shows only a part of the full story. In fact, for $\gamma = \gamma_{\rm cr} = 0$ the bound (1) may fail even in the large coupling limit. Put $l = 1$, $d = 2l = 2$ and for $p > 1$ consider the potentials

$$V_p^{(\infty)}(r) = \frac{\chi_{r>e^2}(r)}{r^2 |\ln r|^2 |\ln|\ln r||^{\frac{1}{p}}} \quad \text{and} \quad V_p^{(0)}(r) = \frac{\chi_{r<e^{-2}}(r)}{r^2 |\ln r|^2 |\ln|\ln r||^{\frac{1}{p}}}, \quad r = |x|\,.$$

Note that $V_p^{(\infty)}, V_p^{(0)} \in L^1(\mathbb{R}^2)$ and therefore both $S^{\rm cl}_{0,2}(\alpha V_p^{(\infty)}) \sim \alpha$ and $S^{\rm cl}_{0,2}(\alpha V_p^{(0)}) \sim \alpha$ for $\alpha \to +\infty$. On the other hand it turns out that we have a non-Weyl high coupling asymptotics

$$S_{0,2}(\alpha V_p^{(\infty)}) \sim \alpha^p \quad \text{and even} \quad S_{0,2}(\alpha V_p^{(0)} - C) \sim \alpha^p \quad \text{as} \quad \alpha \to +\infty$$

for any $C \geq 0$, see [34, 35]. Hence, for $p > 1$ even a modified estimate $S_{0,2}(\alpha V_p^{(0)} - C_1) \leq C_2 + C_3 S^{\rm cl}_{0,2}(\alpha V_p^{(0)})$ fails for arbitrary $C_j > 0$.

In search for a replacement of a critical Lieb-Thirring bound for $d = 2$ and $l = 1$ one can now look on the weak coupling behaviour. Indeed, for sufficiently regular V one has again exactly one weak coupling state $-\lambda_1(\alpha V)$ satisfying

$$\frac{4\pi}{|\ln \lambda_1(\alpha V)|} = (1 + o(1))\alpha \int_{\mathbb{R}^2} V dx = (1 + o(1))CS^{\mathrm{cl}}_{0,2}(\alpha V) \quad \text{as} \quad \alpha \to +0.$$

This motivates to study sums $\sum_j F_s(\lambda_j(V))$, where

$$F_s(t) = \frac{1}{|\ln ts^2|} \quad \text{as} \quad 0 < t \le \frac{1}{es^2} \quad \text{and} \quad F_s(t) = 1 \quad \text{for} \quad 0 < \frac{1}{es^2} < t\,.$$

Note that $F_s(0+) = 0$ and the weak coupling result reads as follows

$$F_s(\varkappa_1(\alpha V)) \sim \frac{\alpha}{4\pi} \int V(x)dx \quad \text{as} \quad \alpha \to +0\,.$$

This supports the goal to estimate $\sum_j F_s(\lambda_j)$ by a term proportional to $\int V(x)dx$. On the other hand, for large t the function $F_s(t)$ coincides with the counting function and for $V = V_p^{(0)}$ as above we find

$$\sum_j F_s(\lambda_j(\alpha V_p^{(0)})) \ge S_{0,2}\left(\alpha V_p^{(0)} - \frac{1}{es^2}\right) \sim \alpha^p \quad \text{as} \quad \alpha \to +\infty.$$

Hence, a straightforward bound of $\sum_j F_s(\lambda_j(\alpha V))$ by $\alpha \int V dx = CS^{\mathrm{cl}}_{0,2}(\alpha V)$ is not possible. Our main result is as follows (joint work with H. Kovařík and S. Vugalter [36]):

Theorem 4.1. *Put $d = 2$, $l = 1$ and $V \ge 0$. Then for any $p > 1$ and $s > 0$ it holds*

$$\sum_j F_s(\lambda_j) \le c_1 \int_{|x|<s} V(x)|\ln |x|s^{-1}|dx + c_p \int_0^{+\infty} rdr \left(\int_0^{2\pi} |V(r,\theta)|^p d\theta\right)^{1/p},$$

where the constants c_1 and c_p are independent of s and V. If V is spherical symmetric, then there exists a constant c_0, such that

$$\sum_j F_s(\lambda_j) \le c_1 \int_{|x|<s} V(x)|\ln |x|s^{-1}|dx + c_0\|V\|_{L^1(\mathbb{R}^2)}\,.$$

The r.h.s. of these bounds is homogeneous of degree 1 in V, cf. also [37–39]. Hence, it reflects the (standard) correct order of the l.h.s. in the weak as well as in the strong coupling limit. Moreover, the finiteness of the r.h.s. fails for potentials $V = V_p^{(0)}$. and excludes non-Weyl asymptotics of deep eigenvalues. On the other hand, the theorem allows for potentials $V = V_p^{(\infty)}$. The non-Weyl asymptotics of the number of negative eigenvalues is compensated by the fact that these eigenvalues stay mainly close to the origin. In fact, the theorem gives estimates on the rate of accumulation of these eigenvalues.

It remains as an open question, whether a similar bound holds true for $l = 1/2$ in the dimension $d = 1$, or in general for $l = d/2$.

5. Setting of the problem: Berezin-Li-Yau inequalities

Let $\Omega \subset \mathbb{R}^d$ be an open domain. We consider $-\Delta_D^\Omega$ on $L^2(\Omega)$ with Dirichlet boundary conditions at $\partial\Omega$ defined in the form sense.[c] We assume the spectrum of $-\Delta_D^\Omega$ to be discrete, e.g. Ω is of finite volume, and denote by

$$0 < \lambda_1(\Omega) \le \lambda_2(\Omega) \le \lambda_3(\Omega) \le \cdots$$

the ordered sequence of the eigenvalues counting multiplicities. Let

$$n(\Omega, \Lambda) := \#\{\lambda_j(\Omega) < \Lambda\}, \quad \Lambda > 0,$$

denote the counting function of this spectrum. Along with the counting function we study the spectral averages

$$S_{d,\gamma}(\Omega, \Lambda) = \sum_n (\Lambda - \lambda_n)_+^\gamma = \gamma \int_0^\Lambda (\Lambda - \tau)^{\gamma-1} n(\Omega, \tau) d\tau\,, \quad \Lambda \ge 0,\ \gamma > 0$$

and

$$s_{d,\gamma}(\Omega, N) = \sum_{k=1}^N \lambda_k^\gamma = \gamma \int_0^\infty \tau^{\gamma-1} (N - n(\Omega, \tau))_+ d\tau\,, \quad \gamma > 0.$$

In 1912 Weyl proved [40] that for high energies the counting function behaves asymptotically as the corresponding classical phase space volume

$$n(\Omega, \Lambda) = (1 + o(1)) n^{cl}(\Omega, \Lambda) \quad \text{as} \quad \Lambda \to +\infty,$$

where

$$n^{cl}(\Omega, \Lambda) = \int_{x\in\Omega} \int_{\xi\in\mathbb{R}^d : |\xi|^2 < \Lambda} \frac{dx \cdot d\xi}{(2\pi)^d} = \frac{\omega_d}{(2\pi)^d} \mathrm{vol}(\Omega) \Lambda^{d/2} = L^{cl}_{d,0} \mathrm{vol}(\Omega) \Lambda^{d/2}\,.$$

Here ω_d stands for the volume of the unit sphere in $\mathbb{R}^d$. This formula holds for all domains with finite volume, see also [41]. An integration of this asymptotics gives

$$\begin{aligned} S_{d,\gamma}(\Omega, \Lambda) &= (1 + o(1))\gamma \int_0^\Lambda (\Lambda - \tau)^{\gamma-1} \frac{\omega_d}{(2\pi)^d} \mathrm{vol}(\Omega) \tau^{d/2} d\tau \\ &= (1 + o(1)) S^{cl}_{d,\gamma}(\Omega, \Lambda) \quad \text{as} \quad \Lambda \to +\infty \end{aligned}$$

with the corresponding classical phase space average

$$\begin{aligned} S^{cl}_{d,\gamma}(\Omega, \Lambda) &:= \int_{x\in\Omega} \int_{\xi\in\mathbb{R}^d} (\Lambda - |\xi|^2)_+^\gamma \frac{dx \cdot d\xi}{(2\pi)^d} = L^{cl}_{d,\gamma} \mathrm{vol}(\Omega) \Lambda^{\gamma + d/2}\,, \\ L^{cl}_{d,\gamma} &:= \frac{\Gamma(\gamma + 1)}{2^d \pi^{d/2} \Gamma(1 + \gamma + d/2)} = \gamma B\left(\gamma, 1 + \frac{d}{2}\right) L^{cl}_{d,0}\,. \end{aligned}$$

[c] From now on we put always $l = 1$ and drop it from the corresponding notation. In particular, $L^{\mathrm{cl}}_{d,\gamma} = L^{\mathrm{cl}}_{d,\gamma,1}$.

Analogously it holds

$$\begin{aligned} s_{d,\gamma}(\Omega,\Lambda) &= (1+o(1))\gamma \int_0^\infty \tau^{\gamma-1}\left(N - L^{cl}_{d,0}\mathrm{vol}(\Omega)\tau^{d/2}\right)_+ d\tau \\ &= (1+o(1))s^{cl}_{d,\gamma}(\Omega,N) \quad \text{as} \quad N\to+\infty\,, \\ s^{cl}_{d,\gamma}(\Omega,N) &= c(d,\gamma)\left(\mathrm{vol}(\Omega)\right)^{-\frac{2\gamma}{d}} N^{1+\frac{2\gamma}{d}}\,, \end{aligned}$$

with the asymptotical constant

$$c(d,\gamma) := \frac{2\gamma}{d}\left(L^{cl}_{d,0}\right)^{-\frac{2\gamma}{d}} B\left(\frac{2\gamma}{d},2\right) = \frac{d}{2\gamma+d}\left(L^{cl}_{d,0}\right)^{-\frac{2\gamma}{d}}\,.$$

6. Pólya-Berezin-Lieb-Li-Yau bounds

Again, the semiclassical quantities serve as universal bounds for the corresponding spectral quantities of the Dirichlet Laplacian. In particular, for arbitrary $d\in\mathbb{N}$ and $\gamma\geq 0$ it holds true:

$$n(\Omega,\Lambda) \leq r(d,0)n^{cl}(\Omega,\Lambda)\,, \quad \Lambda>0\,, \tag{9}$$

$$S_{d,\gamma}(\Omega,\Lambda) \leq r(d,\gamma)S^{cl}_{d,\gamma}(\Omega,\Lambda)\,, \quad \Lambda>0\,, \tag{10}$$

$$s_{d,\gamma}(\Omega,N) \geq \rho(d,\gamma)s^{cl}_{d,\gamma}(\Omega,N)\,, \quad N\in\mathbb{N}\,. \tag{11}$$

Here, of course, we have $n(\Omega,\Lambda)=S_{d,0}(\Omega,\Lambda)$ and $n^{cl}(\Omega,\Lambda)=S^{cl}_{d,0}(\Omega,\Lambda)$. In fact, the bounds (9)-(10) can formally be seen as a special case of (1) for potentials $V(x)=\Lambda$ for $x\in\Omega$ and $V(x)=-\infty$ otherwise. In particular, the bound (9) for $d\geq 3$ follows from [2–5], paper [2] covers also the estimate (9) for $d=2$.

But since in this special case the inequalities (9)-(10) hold true for all pairs γ, d with more subtle information on the constants involved, they are usually studied with separate methods. Let us point out the following known information on the constants r and ρ:

$$1 \leq r(d,0) \leq (1+2d^{-1})^{d/2} \tag{12}$$

$$r(d,\gamma) = 1 \quad \text{for} \quad \gamma\geq 1, \tag{13}$$

$$\rho(d,\gamma) = 1 \quad \text{for} \quad \gamma\leq 1. \tag{14}$$

The bound (10) with the constant (13) ist due to Berezin [42]. The estimate (11) with (14) has been proven independently by Li any Yau [43]. It also follows from (10) and (13) via Legendre transformation. Both results imply (9) with the upper bound from (12), see also [44].

Pólya proved with a really beautiful argument that $r(d,0)=1$ for tiling domains [45] and conjectured that in fact

$$r(d,0)=1 \quad \text{holds true for arbitrary domains.}$$

Pólya's conjecture remains open so far for general domains, even for the circle! For some generalizations of Pólyas result to product type domains see [44].

7. Pólya's conjecture in the presence of magnetic field

It is an admissible approach in mathematics to learn more abount an interesting but difficult problem by stuying modifications of the original setting. Here we shall include a magnetic field: Let $A(x)$ be a real-valued vector field and consider the magnetic Laplacian

$$(i\nabla + \mathscr{A}(x))^2_{D,\Omega}$$

on $\Omega \subset \mathbb{R}^d$ with Dirichlet boundary conditions at $\partial\Omega$. To distinguish the magnetic case we shall simply enter $\mathscr{A}$ into the notations introduced above.

This modification is motivated by the following observations. Firstly, the inclusion of a magnetic field does not change the phase space volume. Secondly, it is known that if A induces a constant magnetic field, then [46]

$$S_{d,\gamma}(\Omega, \Lambda; \mathscr{A}) \leq S^{cl}_{d,\gamma}(\Omega, \Lambda),$$

for all $\gamma \geq 1$. Moreover, if we restrict ourselves to $\gamma \geq \frac{3}{2}$ then this result extends to arbitrary magnetic fields A (with sufficient regularity to define the magnetic operator in the usual form sense) [17]. In both cases the presence of the magnetic field does not spoil neither the inequality nor the sharp value of the constant therein. Therefore it seems reasonable to ask, whether this behaviour extends to the case $\gamma < 1$ and, in particular, to the case of Pólya's conjecture $\gamma = 0$.

Our main result disproves Pólya's conjecture in the presence of a magnetic field (joint work with R. Frank and M. Loss [47]):

Theorem 7.1. *Put $d = 2$ and let $\mathscr{A} = \frac{B}{2}(x_2, -x_1)$ induce a constant magnetic field B. Then there exist constants R_γ independent of B, such that*

$$S_{2,\gamma}(\Omega, \Lambda, \mathscr{A}) \leq R_\gamma S^{cl}_{2,\gamma}(\Omega, \Lambda), \quad 0 \leq \gamma < 1,$$

where the optimal value of the B-independent constant R_γ is given by

$$R_\gamma = 2\left(\frac{\gamma}{1+\gamma}\right)^\gamma > 1 \quad \textit{for} \quad 0 \leq \gamma < 1\,.$$

The constant R_γ cannot be improved - not even for tiling domains! The example is provided on squares balancing the size of the square with the strength of the magnetic field in a suitable way.

An immediate lesson from this result is that one cannot prove Pólya's original conjecture by methods which extend to the magnetic case. A second lesson is that Pólya's proof is in fact not so much about phase space volume but about the density of states. Indeed, if one allows for B-dependent estimates, then for $0 \leq \gamma < 1$, $\mathscr{A} = \frac{B}{2}(x_2, -x_1)$ and tiling Ω it holds [47]

$$S_{2,\gamma}(\Omega, \Lambda, \mathscr{A}) \leq \mathfrak{B}_\gamma(B, \Lambda)\mathrm{vol}(\Omega)\,, \quad \mathfrak{B}_\gamma(B, \Lambda) = \frac{B}{2\pi}\sum_{k\geq 0}(\Lambda - B(2k+1))^\gamma_+\,, \tag{15}$$

and the constants $\mathfrak{B}_\gamma(B, \Lambda)$ are sharp. For $\gamma = 0$ the quantity $\mathfrak{B}_0(B, \Lambda)$ is just the density of states of the Landau Hamiltonian!

It remains open, whether an estimate (15) holds true for general domains.

8. Two-term spectral bounds

Weyl conjectured also a two-term asymptotical formula for the counting function

$$n(\Omega,\Lambda) = L^{cl}_{d,0}\mathrm{vol}(\Omega)\Lambda^{d/2} - \frac{1}{4}L^{cl}_{d-1,0}|\partial\Omega|\Lambda^{(d-1)/2} + o(\Lambda^{(d-1)/2}) \quad \text{as} \quad \Lambda\to+\infty.$$

Here the first term on the r.h.s. equals $n^{cl}(\Omega,\Lambda)$. This formula holds true under certain geometrical conditions on the domain [48]. Integrating this asymptotic formula gives

$$\begin{aligned} S_{d,\gamma}(\Omega,\Lambda) &= L^{cl}_{d,\gamma}\mathrm{vol}(\Omega)\Lambda^{\gamma+d/2} - \frac{1}{4}L^{cl}_{d-1,\gamma}|\partial\Omega|\Lambda^{\gamma+(d-1)/2} + o(\Lambda^{\gamma+(d-1)/2}),\\ s_{d,\gamma}(\Omega,N) &= c(d,\gamma)\,(\mathrm{vol}(\Omega))^{-\frac{2\gamma}{d}}\,N^{1+\frac{2\gamma}{d}}\\ &\quad + \frac{L^{cl}_{d-1,\gamma}(L^{cl}_{d,\gamma})^{-1-\frac{2\gamma-1}{d}}}{4(\frac{d-1}{2}+\gamma)}\cdot\frac{\gamma|\partial\Omega|}{(\mathrm{vol}(\Omega))^{1+\frac{2\gamma-1}{d}}}N^{1+\frac{2\gamma-1}{d}} + o(N^{1+\frac{2\gamma-1}{d}})\,. \end{aligned}$$

Again, the first terms on the r.h.s. equal $S^{cl}_{d,\gamma}(\Omega,\Lambda)$ and $s^{cl}_{d,\gamma}(\Omega,N)$, respectively. At least for $\gamma\geq 1$ the geometrical conditions on the domain Ω can largely be dropped [49].

Note that the signs of the lower order terms seem to suggest, that the spectral bounds (10)-(11) with sharp first order Weyl term (13)-(14) could possibly be improved by additional terms reflecting the second order corrections.

Trying to prove such bounds one should first note that any bound

$$S_{d,\gamma}(\Omega,\Lambda) \leq S^{cl}_{d,\gamma}(\Omega,\Lambda) - C\cdot|\partial\Omega|\Lambda^{\gamma+\frac{d-1}{2}}$$

must fail in general. Indeed, adding "needles" to a domain Ω one can increase the perimeter $|\partial\Omega|$ arbitrarily without changing the volume of Ω a lot, and the r.h.s. of this bound would turn even negative. Therefore, part of the problem is to replace $|\partial\Omega|$ by some other suitable geometric value.

9. Melas' bound

A first step towards this direction was made by Melas [50]. Let for an open domain $\Omega\subset\mathbb{R}^d$

$$J(\Omega) = \min_{y\in\mathbb{R}^d}\int_\Omega |x-y|^2dx$$

be its moment. Then the following bound holds true

$$s_{d,1}(\Omega,N) \geq c(d,1)\,(\mathrm{vol}(\Omega))^{-\frac{2}{d}}\,N^{1+\frac{2}{d}} + M(d)\frac{\mathrm{vol}(\Omega)}{J(\Omega)}N\,. \tag{16}$$

Via Legendre transformation this turns into [51]

$$S_{d,1}(\Omega,\Lambda) \leq S^{cl}_{d,1}\left(\Omega,\Lambda - M_d\frac{\mathrm{vol}(\Omega)}{J(\Omega)}\right)\,. \tag{17}$$

This bound is remarkable, since it works at the endpoint $\gamma=1$ of the scale, where the Li-Yau and the Berezin bounds are proven with sharp semiclassical constants. On the other hand, the correction term of order $O(N)$ is not of the expected order $O(N^{1+\frac{1}{d}})$. The same holds in the Berezin picture (17).

10. Improved Berezin bounds with remainder terms of correct order

Consider an open domain $\Omega \subset \mathbb{R}^d$. Choose a coordinate system in $\mathbb{R}^d$ and put $\mathbb{R}^d \ni x = (x', x_d) \in \mathbb{R}^{d-1} \times \mathbb{R}$. For fixed $x' \in \mathbb{R}^{d-1}$ the intersection of $\{(x', t), t \in \mathbb{R}\} \cap \Omega$ consists of at most countable many intervals. Let $\Omega_\Lambda(x')$ be the union of all such intervals, which are longer than $l_\Lambda := \pi\Lambda^{-1/2}$. The number of these intervals is denoted by $\varkappa(x', \Lambda)$. Put

$$\Omega_\Lambda = \bigcup_{x' \in \mathbb{R}^{d-1}} \Omega_\Lambda(x') \subset \Omega \quad \text{and} \quad d_\Lambda(\Omega) = \int_{x' \in \mathbb{R}^{d-1}} \varkappa(x', \Lambda) dx' \,.$$

That means Ω_Λ is the subset of Ω, where the intervals of Ω in x_d-direction are longer than l_Λ. The set Ω_Λ is increasing in Λ. The value $d_\Lambda(\Omega)$ is an effective measure of the projection of Ω_Λ on the x'-plane counting the number of sufficiently long intervals. It also increases in Λ. Since $\mathrm{vol}(\Omega_\Lambda) \geq l_\Lambda d_\Lambda(\Omega)$, the finiteness of $\mathrm{vol}(\Omega_\Lambda)$ implies finiteness of $d_\Lambda(\Omega)$. It holds [52]

Theorem 10.1. *Assume that for a given $\Lambda > 0$ we have $vol(\Omega_\Lambda) < \infty$. Then for any $\gamma \geq \frac{3}{2}$*

$$S_{d,\gamma}(\Omega, \Lambda) \leq L^{cl}_{d,\gamma} vol(\Omega_\Lambda) \Lambda^{\sigma + \frac{d}{2}} - \nu(d, \gamma) 4^{-1} L^{cl}_{d-1,\gamma} d_\Lambda(\Omega) \Lambda^{\sigma + \frac{d-1}{2}} \,. \tag{18}$$

The first term on the r.h.s. coincides with $S^{cl}_{d,\gamma}(\Omega_\Lambda; \Lambda)$, while the correction term is of the expected second Weyl order $O(\Lambda^{\sigma + \frac{d-1}{2}})$. But even the first term is already an improvement over the standard Berezin bound for $\gamma \geq \frac{3}{2}$. Indeed, instead of $\mathrm{vol}(\Omega)$ only the quantity $\mathrm{vol}(\Omega_\Lambda)$ appears: The bound counts only the volume of the part of the domain, where it is wide enough for sufficiently deep bound states to settle. In particular, one can apply (18) even for domains Ω of infinite volume as long as $\mathrm{vol}(\Omega_\Lambda)$ is finite. Moreover, the bound (18) extends to the case of arbitrary magnetic fields. However, the techniques applied (sharp Lieb-Thirring inequalities with operator-valued potentials) restrict ourselfs to the case $\gamma \geq \frac{3}{2}$. It would be of great interest to extend this type of results, both regarding the effective reduction of the domain to Ω_Λ as well as the appearance of a second order term, to the case $\gamma = 1$. [d]

One can also supply explicite estimates on the constants $\nu(d, \gamma)$. Namely, we have

$$0 < 4\varepsilon \left(\gamma + \frac{d-1}{2}\right) \leq \nu(d, \gamma) \leq 2 \,,$$

where

$$\varepsilon(\sigma) = \inf_{a \geq 1} \left(\frac{a}{2} B\left(\sigma + 1, \frac{1}{2}\right) - \sum_{k \geq 1} \left(1 - \frac{k^2}{a^2}\right)^\sigma_+ \right) .$$

[d] Such an estimate has been obtained for the discrete Laplacian in [53].

In particular, it holds [54] $\varepsilon(\sigma) = \frac{1}{2}B\left(\sigma+1, \frac{1}{2}\right)$ for $\sigma \geq 3$, and a numerical evaluation gives for the special case $d = 2$ and $\gamma = \frac{3}{2}$

$$1.91 < \nu\left(2, \frac{3}{2}\right) \leq 2\,.$$

For further applications of (18) to bounds for the heat kernel of the Dirichlet Laplacian see [54].

11. A more geometric second term

The bound (18) as stated above is of particular use, if the domain streches along one distinguished direction, like horn shaped domains, see [54]. Otherwise one would wish for a more intrinsic geometrical second term, which is independent of the choice of the coordinate system. Of course, one can average (18) over all directions, but this does not necessarily yield a more appealing bound.

Alternatively, one can "hide" the correction first in a Hardy type term and average afterwards. Indeed, for any $u \in \mathbb{S}^{d-1}$ and $\gamma \geq 3/2$ one can prove (joint work with L. Geisinger and A. Laptev [55]) that

$$S_{d,\gamma}(\Omega,\Lambda) \,\leq\, L^{cl}_{d,\gamma} \int_\Omega \left(\Lambda - \frac{1}{4\,d(x,u)^2}\right)_+^{\gamma+\frac{d}{2}} dx\,,$$

where

$$\theta(x,u) = \inf\{t>0 \,:\, x+tu \notin \Omega\} \quad \text{and} \quad d(x,u) = \inf\{\theta(x,u), \theta(x,-u)\}\,.$$

Averaging over the directions gives now rise to the following result. For $x \in \Omega$ let

$$\Omega(x) \,=\, \{y \in \Omega \,:\, x + t(y-x) \in \Omega\,,\ \forall\, t \in [0,1]\}$$

be the part of Ω that "can be seen" from x and let $\delta(x) \,=\, \inf\left\{|y-x| \,:\, y \notin \overline{\Omega(x)}\right\}$ denote the distance to the exterior of $\Omega(x)$. For fixed $\varepsilon > 0$ put

$$A_\varepsilon(x) \,=\, \left\{a \in \mathbb{R}^d \setminus \overline{\Omega(x)} \,:\, |x-a| < \delta(x) + \varepsilon\right\}$$

and for $a \in A_\varepsilon(x)$ set $B_x(a) = \{y \in \mathbb{R}^d \,:\, |y-a| < |x-a|\}$ and

$$\rho_a(x) \,=\, \frac{|B_x(a) \setminus \overline{\Omega(x)}|}{\omega_d |x-a|^d}\,,$$

where ω_d denotes the volume of the unit ball in $\mathbb{R}^d$. Moreover, we put

$$\rho(x) \,=\, \inf_{\varepsilon>0} \sup_{a \in A_\varepsilon(x)} \rho_a(x) \quad \text{and} \quad M_\Omega(\Lambda) \,=\, \int_{R_\Omega(\Lambda)} \rho(x)\, dx\,,$$

where $R_\Omega(\Lambda) \subset \Omega$ denotes the set $\{x \in \Omega \,:\, \delta(x) < 1/(4\sqrt{\Lambda})\}$. The function $\rho(x)$ depends on the behaviour of the boundary close to $x \in \Omega$. For example, $\rho(x)$ is small close to a cusp. On the other hand $\rho(x)$ is larger than $1/2$ in a strictly convex domain. By definition, the function $M_\Omega(\Lambda)$ gives an average of this behaviour over $R_\Omega(\Lambda)$, which is like a tube of width $1/(4\sqrt{\Lambda})$ around the boundary. Its decay for $\lambda \to \infty$ is related to the Minkowski dimension of the boundary.

The following result allows a geometric interpretation of the remainder term (joint work with L. Geisinger and A. Laptev [55]):

Theorem 11.1. *Let $\Omega \subset \mathbb{R}^d$ be an open set with finite volume and $\gamma \geq 3/2$. Then*

$$S_{d,\gamma}(\Omega,\Lambda) \leq L^{cl}_{d,\gamma}\, vol(\Omega)\Lambda^{\frac{d}{2}+\gamma} - L^{cl}_{d,\gamma}\, 2^{-d+1}\, \Lambda^{\frac{d}{2}+\gamma}\, M_\Omega(\Lambda) \quad \textit{for all} \quad \Lambda > 0\,. \tag{19}$$

12. Improving Melas' bound

As stated above, it is of interest to transfer Berezin-Li-Yau bounds with remainder terms of sharp order to the limit case $\gamma = 1$ when the first term with sharp constant is known. To understand the difficulties let us have a look on the idea behind the proof of the Li-Yau and Melas inequalities.

Let ψ_j be the o.n. eigenfunctions of $-\Delta^D_\Omega$. Put $\hat{\psi}_j(\xi) = (2\pi)^{-d/2}(\psi_j, e^{i\xi x})_{L^2(\Omega)}$ and $F(\xi) = \sum_{j=1}^N |\hat{\psi}_j(\xi)|^2 \geq 0$. Then

$$s_{d,1}(\Omega,N) = \int_{\mathbb{R}^d} |\xi|^2 F(\xi) d\xi = I(F) \tag{20}$$

$$N = \int F(\xi) d\xi, \tag{21}$$

$$F(\xi) = \sum_{j=1}^N |\hat{\psi}_j(\xi)|^2 \leq (2\pi)^{-d} \|e^{i\xi x}\|^2_{L^2(\Omega)} = (2\pi)^{-d}\mathrm{vol}(\Omega)\,. \tag{22}$$

An estimate on $s_{d,1}(\Omega,N) = \sum_{j=1}^N \lambda_j$ from below can be obtained minimizing $I(F)$ in (20) for $F \geq 0$ satisfying (21) and (22). A minimizer should be spherical symmetric and non-increasing in the radius and a straightforward application of the bathtub principle leads to the Li-Yau bound with $\rho(d,1) = 1$. Using the momentum of the domain Melas puts forward the additional information $|\nabla F| \leq 2(2\pi)^{-d}\sqrt{J(\Omega)\mathrm{vol}(\Omega)}$. Solving the modified optimization problem leads to his improvement of the bound (16). A quite similar approach has recently been applied in [56, 57] for the Stokes and the Klein-Gordon operator.

But this idea will not yield remainder terms of sharp order. In fact, the true second Weyl term is hidden in Bessel's inequality (22). To quantify it, one has to show that lower Dirichlet eigenfunctions cannot approximate a free wave on the domain too well, since these eigenfunctions must vanish at the boundary. For this one needs to deduce subtle pointwise estimates on Dirichlet eigenfunctions from integral energy estimates. In contrast to the discrete case [53] this proves to be quite difficult in the continuous case. We can provide the following result (joint work with H. Kovařík and S. Vugalter [58]):

Theorem 12.1. *Let $\Omega \subset \mathbb{R}^2$ be a polygon with n sides. Let l_j be the length of the $j-th$ side p_j of Ω and let d_j be the distance of the middle third of p_j to $\partial\Omega \setminus p_j$.*

Then for any $k \in \mathbb{N}$ and any $\alpha \in [0,1]$ we have

$$s_{2,1}(\Omega,N) \;\geq\; s_{2,1}^{cl}(\Omega,N) + \frac{4\alpha\, c_3}{vol(\Omega)^{\frac{3}{2}}}\, N^{\frac{3}{2}-\epsilon(N)} \sum_{j=1}^{n} l_j\, \Theta\left(N - \frac{9vol(\Omega)}{2\pi\, d_j^2}\right) + (1-\alpha)\, M(2)\frac{vol(\Omega)}{J(\Omega)}\, N,$$

where

$$\epsilon(N) = \frac{2}{\sqrt{\log_2(2\pi N/c_1)}}, \qquad c_1 = \sqrt{\frac{3\pi}{14}}\; 10^{-11}\,, \qquad c_3 = \frac{2^{-3}}{9\sqrt{2}\,36}\,(2\pi)^{\frac{5}{4}} c_1^{1/4}\,.$$

Minimizing the r.h.s. in $\alpha \in [0,1]$ this is an actual improvement on Melas' bound which corresponds to the case $\alpha = 0$. The second term on the r.h.s. is almost of the expected Weyl order. The result can be extended to non-polygons as well; for details see [58].

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THE OTHER PLENARY TALK ABSTRACTS

SHARP CONSTANTS IN INEQUALITIES ON THE HEISENBERG GROUP

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We derive the sharp constants for the inequalities on the Heisenberg group whose analogues on Euclidean space are the well known Hardy-Littlewood-Sobolev inequalities. Only one special case had been known previously, due to Jerison-Lee more than twenty years ago. From these inequalities we obtain the sharp constants for their duals, which are the Sobolev inequalities for the Laplacian and conformally invariant fractional Laplacians. The methodology is completely different from that used to obtain the Euclidean inequalities and can be used to give a new, rearrangement free, proof of the HLS inequalities. The talk is based on joint work with E. H. Lieb.

QUADRATIC FORMS WITHOUT SEMIBOUNDEDNESS

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The talk reviews some recent results on representation theorems for not semibounded quadratic forms. In particular, we discuss some unexpected properties of the Dirac operator. The talk is based on a joint work with L. Grubisić, K. Makarov, and I. Veselić.

QUANTUM ENTANGLEMENT IN RANDOM SYSTEMS

KAROL ŻYCZKOWSKI

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We analyze quantum entanglement in composite random systems. Due to the measure concentration phenomenon a typical random pure state of a bi-partite system is almost

maximally entangled. Taking various measures on the set of pure states one can induce by partial trace various probability measures in the set of mixed states on a reduced system. Recent results on random states generated according to the Bures measure and random graph states, which lead to Marchenko-Pastur or higher order Fuss-Catalan distributions of level density are reviewed.

PART B

Topical Sessions

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Session in honour of Ari Laptev

Session organizer:

Pavel Exner

One of the main purposes of this QMath conference was to celebrate the jubilee of our colleague and friend Ari Laptev.

Ari was born on August 10, 1950, in Kiev. He studied at the Leningrad State University when he made his PhD under the supervision of Michael Solomyak. The world was different in those times and one can get into trouble even for choosing a spouse from a wrong country. This indeed happened and as a result Ari had to spend five years in conditions which most members of the academic community today can hardly imagine.

His life changed when he came to Sweden in 1987 and could restart his career and demonstrate how brilliant a mathematician he was. Two decades later we can see clearly from over sixty papers, some of which had a profound influence of development of spectral theory, and no less from looking at the results of about dozen PhD students he had educated.

It is not only these results from which the his colleagues benefit. Ari organized a European congress in 2004 and served for the last four years as President of European Mathematical Society, and everybody who had the luck to work with him must admire the energy he puts into the service of the community.

On behalf his collaborators, friends, and all conference participants we wish him most of all to keep his attitude to life and science for many years to come, interesting new results and happiness in personal life.

SPECTRAL PROBLEMS IN SPACES OF CONSTANT CURVATURE

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Here, recent spectral properties of some linear and nonlinear problems in spaces of constant curvature are reviewed. In particular, isoperimetric inequalities for low eigenvalues of the Laplace–Beltrami operator with Dirichlet and Neumann boundary conditions on smooth bounded domains on both $\mathbb{S}^n$ and $\mathbb{H}^n$ are considered. Also, I consider the Brézis–Nirenberg problem in those spaces.

Keywords: Eigenvalues of the Laplacian; spaces of constant curvature; Brézis–Nirenberg problem.

1. Introduction

During the last decade, there has been an increasing interest in the properties of several spectral problems in spaces of constant curvature, in particular in problems defined on the n–dimensional sphere and also on the hyperbolic space. In general, most properties of the analog problems defined on the Euclidean Space, do hold in the hyperbolic case, and even in the case of $\mathbb{S}^n$ as long as the domains are restricted to live on a hemisphere. The situation changes, however, when the domains are allowed to extend beyond a hemisphere of $\mathbb{S}^n$. Here I only address, as examples, two completely different situations. The first one being the isoperimetric inequalities for the low lying Dirichlet and Neumann eigenvalues. The second being the analog of the Brézis–Nirenberg problem on both $\mathbb{S}^n$ and $\mathbb{H}^n$. In the case of $\mathbb{S}^n$, when the domain extends beyond the hemisphere, many interesting new features do appear. In the last few years there have also been many articles on universal inequalities for eigenvalues of the Laplace–Beltrami operator on spaces of constant curvature, as well as spectral problems for higher order operators on those spaces (in particular the study of the analog of the *clamped plate* problem and many others), I will not review those results here. In Section 2, I will review the isoperimetric problems for eigenvalues of the Laplacian and in Section 3, I will review the Brézis–Nirenberg problem in $\mathbb{S}^n$ and in $\mathbb{H}^n$. It is interesting to note (and that is the reason I am treating these two, certainly different problems, together) that for some of the same reasons the proof of the typical isoperimetric inequalities for low eigenvalues of the Laplacian fail in the case of geodesic caps that extend beyond the hemisphere in $\mathbb{S}^n$, one encounters a whole new class of unexpected solutions for the Brézis–Nirenberg problem on those domains.

2. Isoperimetric inequalities for eigenvalues of the Laplacian

Consider the eigenvalue problem,

$$-\Delta u = \lambda u, \qquad \text{in } \Omega \tag{1}$$

with $u = 0$ in $\partial\Omega$, where Ω is a bounded domain in $\mathbb{R}^n$. It is well known that this problem has a sequence of values of λ (the *Dirichlet eigenvalues*), i.e.,

$$0 < \lambda_1 < \lambda_2 \leq \lambda_3 \ldots,$$

for which (1) has a nontrivial solution. Associated with each λ_k there is an eigenfunction $u_k \in H_0^1(\Omega)$. Certainly, the eigenvalues $\lambda_k(\Omega)$ depend on the geometry of the domain. In 1877, Lord Rayleigh conjectured that among all domains of fixed area (in two dimensions) the circular domain has the lowest λ_1. Rayleigh's conjecture was proved independently by G. Faber (1923) and E. Krahn (1925). Moreover, Krahn extended this result to n dimensions. This fact is known as the Rayleigh–Faber–Krahn (RFK) inequality, which reads,

$$\lambda_1(\Omega) \geq \left(\frac{C_n}{|\Omega|}\right)^{2/n} j_{n/2-1,1}^2 = \lambda_1(\Omega^*), \tag{2}$$

where $j_{m,1}$ denotes the first positive zero of the Bessel function J_m and C_n is the volume of the unit sphere in n dimensions. Here, Ω^* denotes a ball of the same volume of Ω. Equality is obtained in (2) if and only if Ω is a ball. There are many different proofs of the RFK inequality. Perhaps the simplest is based on the use of the variational characterization of λ_1 together with properties of symmetric decreasing rearrangements of functions. The RFK inequality has been extended to many other situations. In particular to the Dirichlet problem for domains on $\mathbb{S}^n$ by E. Sperner [1], and domains on $\mathbb{H}^n$, by I. Chavel [2]. In 1992, A. Melas [3] proved the stability of the RFK inequality in the Euclidean space. Stability here refers to the fact that if for a bounded, convex domain in $\mathbb{R}^n$, $\lambda_1(\Omega)|\Omega|$ differs little from the value that this quantity assumes for the ball, then the domain is approximately a ball (Melas also proved the stability of the PPW inequality that I discuss below). The stability for the analog of the RFK inequality for domains on on $\mathbb{S}^n$ was proved by A. Avila [4].

Consider now the corresponding Neumann problem for a bounded smooth domain, $\Omega \subset \mathbb{R}^n$, $n \geq 2$. That is,

$$-\Delta u = \mu u, \qquad \text{in } \Omega, \tag{3}$$

and $\partial u/\partial n = 0$ in $\partial\Omega$. Then, there is a sequence of values, $0 = \mu_0(\Omega) < \mu_1(\Omega) \leq \mu_2(\Omega) \ldots$, for which there is a nontrivial solution of the Neumann problem. In 1954, G. Szegö proved the isoperimetric inequality (for the case $n = 2$):

$$\mu_1(\Omega) \leq \mu_1(\Omega^*) = \frac{\pi p_{1,1}^2}{A}, \tag{4}$$

where $p_{1,1} = 1.8412\ldots$ is the first positive zero of the derivative of $J_1(t)$. The analogous result for $n \geq 2$ was proven by H. Weinberger in 1956. The analog of the Szegö–Weinberger inequality $\mathbb{S}^n$ was proven by Mark Ashbaugh and myself in 1995, [5]. However, our proof only works for domains that are contained in a

hemisphere. Whether the corresponding result holds for domains that extend beyond a hemisphere, is still an open problem. In the case of the hyperbolic space, there are technical difficulties, but essentially the original proof of Weinberger (in the Euclidean case) can be carried through for any bounded domain in $\mathbb{H}^n$ [2, 5].

In this context, the next simplest inequality that one can consider concerns the ratio between the first two Dirichlet eigenvalues. In 1955, L. Payne, G. Pólya and H. Weinberger [PPW] proved the *universal* inequality $\lambda_2(\Omega)/\lambda_1(\Omega) \leq 3$ for bounded, smooth domains in $\mathbb{R}^2$. The PPW inequality in n dimensions reads, $\lambda_2(\Omega)/\lambda_1(\Omega) \leq (1 + 4/n)$. There is a vast literature on *universal inequalities* for eigenvalues of the Laplacian (i.e., inequalities between eigenvalues which are independent of the domain), including recent works of H.-C. Yang, and collaborators, Harrell and Stubbe, Harrell and Hermi, Ashbaugh and Hermi, Levitin and Parnovski. At the same time, PPW conjectured the bound,

$$\frac{\lambda_2(\Omega)}{\lambda_1(\Omega)} \leq \frac{\lambda_2(\Omega^*)}{\lambda_1(\Omega^*)} = \frac{j_{1,1}^2}{j_{0,1}^2} \approx 2,539, \qquad \text{for all } \Omega \subset \mathbb{R}^2, \text{ bounded.} \tag{5}$$

The PPW conjecture was proven by Mark Ashbaugh and myself [6–8]. The proof of the PPW inequality (5) is done in five steps: i) The first is to use a Rayleigh–Ritz variational estimate for the second Dirichlet eigenvalue (the so called *gap formula*); ii) in the second step one exploits the degeneracy of the second eigenvalue (for the conjectured maximizing domain), and then averages, using a Center of Mass argument to insure the necessary orthogonality; more technically, one uses a Brower Fixed Point Theorem at this stage; iii) in the third step, one guesses the right variational trial function (the guess is obviously based on the properties of the maximizing domain). Then, one has to prove monotonicity properties for functions associated to the trial function; iv) then one uses symmetrization (symmetric decreasing rearrangements), and, finally, v) a comparison theorem due to G. Chiti.

The analogous result for domains in $\mathbb{S}^n$ was proved in [9], but, again, only for domains contained in a hemisphere. It is still an open problem to determine whether a PPW inequality, like (5) is true for domains in $\mathbb{S}^n$ extending beyond a hemisphere. The main reason (but not the only one) that our proof fails for domains that extend beyond a hemisphere is that we cannot prove the monotonicity properties associated to the trial functions (i.e., the main part of step iii) in the proof of PPW). This failure relies on the fact that the Laplace–Beltrami operator (in geodesic ccordinates) acting on radial functions has a term proportional to the radial derivative and the coefficient changes sign when going beyond the hemisphere (see equation (9) below). On the contrary, for both the Euclidean and the hyperbolic cases the corresponding coefficient is of one sign.

Concerning the hyperbolic space, the corresponding result was proven by H. Linde and myself [10]. In the case of $\mathbb{H}^n$, one cannot hope to prove that $\lambda_2/\lambda_1(\Omega)$ is maximized by geodesic balls (this is in fact not true in general). The point here is that the ratio $\lambda_2(B)/\lambda_1(B)$, where B is a geodesic ball, is not a decreasing function of the radius of the ball, as needed to complete the analog of the Chiti's comparison argument (step 5 in the proof of the euclidean case). Notice, that this ratio is independent of the radius of the ball in the Euclidean case, and it has the right monotonicity property for domains in $\mathbb{S}^n$. Thus, in the $\mathbb{H}^n$ case what one proves is

that among all domains having a fixed $\lambda_1(\Omega)$ eigenvalue, it is the geodesic ball the one that maximizes λ_2. For some recent detailed reviews on isoperimetric inequalities for eigenvalues of the laplacian, see, e.g., [11, 12].

3. Brézis–Nirenberg problem in $\mathbb{S}^n$ and $\mathbb{H}^n$

Consider the boundary value problem

$$-\Delta u = \lambda u + u^5, \tag{6}$$

in $\Omega \subset R^3$, bounded, with Dirichlet boundary conditions. Brézis and Nirenberg [13] considered the problem of determining the range of values of the parameter λ for which the above problem has a positive solution, $u > 0$ in Ω. If the domain Ω is a ball (of radius R, say), that range is precisely given by

$$\frac{\lambda_1}{4} < \lambda < \lambda_1, \tag{7}$$

where $\lambda_1 = \pi^2/R^2$ is the first Dirichlet eigenvalue of the ball. For general domains, there exists a value $0 < \lambda_1^*(\Omega) < \lambda_1(\Omega)$, such that for $\lambda \in (\lambda_1^*, \lambda_1)$ the above problem has a positive solution. The proof of the Brézis–Nirenberg result goes in two steps:
i) Nonexistence: For $\lambda \geq \lambda_1$, just multiply (6) by the first Dirichlet eigenfunction of the domain, integrate in Ω and you are done. Moreover, when the domain is a ball, use a refinement of the Rellich–Pohozaev identity in order to show that there are no positive solutions for $\lambda \leq \lambda_1/4$.
ii) Existence: In order to show existence in the interval $(\lambda_1/4, \lambda_1)$ (for the case of the ball), one uses the Brézis–Lieb compactness argument [14].

The corresponding problem,

$$-\Delta_{\mathbb{S}^3} u = \lambda u + u^5 \tag{8}$$

for $u > 0$ on geodesic balls $D'(\theta^*)$ on $\mathbb{S}^3$ with Dirichlet boundary conditions was considered in [15]. Here, without loss of generality the geodesic ball is centered at the north pole, and θ^* is the azimuthal angle of the boundary of D'. Using a moving plane method (more precisely a moving spheres method) introduced by Padilla [16] one can prove that the positive solutions of (8) (when $\theta^* \leq \pi/2$, i.e., when D' lies inside a hemisphere) are radially symmetric, i.e., they only depend on the azimuthal angle θ. In geodesic coordinates, for radial functions,

$$\Delta_{\mathbb{S}^3} u = u''(\theta) + 2\cot\theta\, u'(\theta) \tag{9}$$

For domains lying inside a hemisphere the situation is similar to the Euclidean case. One has the following result:

Theorem 3.1 ([15]). *If $\lambda > -3/4$, there is a positive solution to (8), if and only if,*

$$\lambda_1^* = \frac{\pi^2 - 4{\theta^*}^2}{4{\theta^*}^2} < \lambda < \frac{\pi^2 - {\theta^*}^2}{{\theta^*}^2}.$$

If $\lambda \leq -3/4$, and $\theta^* \in (0, \pi/2]$ there are no positive solutions to (8).

As in the Euclidean case, the existence part relies on the Brézis–Lieb compactness result. The nonexistence part relies on a refined Rellich–Pohozaev argument. The picture for the geodesic balls contained in a hemisphere is not surprising. It is to be expected, after the results of Bandle and Peletier on best critical constants for the Sobolev embeddings in $\mathbb{S}^3$, in the case $\lambda = 0$ [17].

On the other hand, once we exceed the hemisphere, interesting new solutions start appearing. Originally, we proved the following result.

Theorem 3.2 ([15]). *Given any $\theta^* \in (\pi/2, \pi)$, there exist at least two non constant solutions of the Brézis–Nirenberg problem on $D' \subset \mathbb{S}^3$, as long as λ is sufficiently large (and negative).*

Later, Bandle and Stingelin [18] numerically found a double sequence of new positive solutions for domains exceeding the hemisphere. Then, independently, Chen and Wei [19], Brézis and Peletier [20], and Bandle and Wei [21, 22] completely classified all the positive solutions to this problem. In particular one has,

Theorem 3.3 ([20]). *Given any $\theta^* \in (\pi/2, \pi)$, there exists a constant $A_k > 0$ such that for $\lambda < -A_k$, the Brézis–Nirenberg problem has at least $2k$ solutions, such that at the North–Pole, $u(0) \in (0, |\lambda|^{1/4})$.*

While in the $\mathbb{S}^3$ case there is this rich set of solutions once we exceed a hemisphere, in the hyperbolic case the situation is completely analogous to the one for the euclidean space. The analogous problem for geodesic balls in the hyperbolic space $\mathbb{H}^3$ (in fact for $\mathbb{H}^n$, with $n \geq 3$) was considered in the Ph.D. Thesis of Silke Stapelkamp [23]. She considers the following realization of $\mathbb{H}^3$ (as the positive branch of an hyperboloid embedded in $\mathbb{R}^4$):

$$\mathbb{H}^3 = \left\{ x \in \mathbb{R}^4 \;\middle|\; x_1^2 + x_2^2 + x_3^2 - x_4^2 = 1, x_4 > 0 \right\}$$

and, moreover she considers the stereographic projection of $\mathbb{H}^3$ into $\mathbb{R}^3$ (in fact into the Euclidean space defined as $x_4 = 0$), from the point $(0, 0, 0, -1)$ in $\mathbb{R}^4$. Then, among many other results (including results for geodesic balls in $\mathbb{H}^n$, with $n \geq 4$), she proved the following theorem for geodesic balls in $\mathbb{H}^3$.

Theorem 3.4 ([23]). *Let D' be a geodesic ball in $\mathbb{H}^3$, with center at $(0, 0, 0, 1)$. Let $D = B(0, R)$, $0 < R < 1$ be the stereographic projection of D' into $\mathbb{R}^3$. Let,*

$$\lambda^* = 1 + \frac{\pi^2}{16(\tanh^{-1}(R))^2}. \tag{10}$$

Then,
i) If $\lambda \leq \lambda^*$, or $\lambda \geq \lambda_1$, the Brézis–Nirenberg problem on D' has only trivial solutions.
ii) Moreover, if $\lambda \in (\lambda^*, \lambda_1)$, there is a nontrivial positive solution to the Brézis–Nirenberg problem on D'.

Remark: Here, λ_1 denotes the first Dirichlet eigenvalue of the Laplace–Beltrami operator on $D' \subset \mathbb{H}^3$. It is clear from (10) that $\lambda^* \to 1$ as $R \to 1$. Moreover, one can check also that $\lambda_1(R) \to 1$ as $R \to 1$. The proof of this theorem follows the same steps as in the case of $\mathbb{R}^3$ and $\mathbb{S}^3$. In particular, it uses the fact that the positive

solutions of the Brézis–Nirenberg equation on $D' \subset \mathbb{H}^3$ are radial, which is proved using a generalization of the moving planes method. For higher dimensions, if D' is now any bounded domain in $\mathbb{H}^n$, $n \geq 4$, the Brézis–Nirenberg problem does not have nontrivial solutions if $\lambda \geq \lambda_1$, nor does it if it is star shaped, and $\lambda \leq n(n-2)/4$. On the other hand, there exists a nontrivial solution if $\lambda \in (n(n-2)/4, \lambda_1)$. The proof of existence relies on a concentration-compactness argument, while the nonexistence result for star shaped domains, when $\lambda < n(n-2)/4$, relies on a Rellich–Pohozaev argument.

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TWO-TERM SPECTRAL ASYMPTOTICS FOR THE DIRICHLET LAPLACIAN ON A BOUNDED DOMAIN

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Dedicated to Ari Laptev on the occasion of his 60th birthday

Let $-\Delta$ denote the Dirichlet Laplace operator on a bounded open set in $\mathbb{R}^d$. We study the sum of the negative eigenvalues of the operator $-h^2\Delta - 1$ in the semiclassical limit $h \to 0+$. We give a new proof that yields not only the first term of the asymptotic formula but also the second term involving the surface area of the boundary of the set. The proof is valid under weak smoothness assumptions on the boundary.

Keywords: Dirichlet Laplace operator; semiclassical limit; Weyl's law.

1. Introduction and main result

1.1. *Introduction*

Let Ω be a bounded open set in $\mathbb{R}^d$, $d \geq 2$. We consider the Dirichlet Laplace operator $-\Delta_\Omega$ defined as a self-adjoint operator in $L^2(\Omega)$ generated by the form

$$(v, -\Delta_\Omega v) \;=\; \int_\Omega |\nabla v(x)|^2 dx$$

with form domain $H^1_0(\Omega)$. Since Ω is bounded the embedding of $H^1_0(\Omega)$ into $L^2(\Omega)$ is compact and the spectrum of $-\Delta_\Omega$ is discrete. It consists of a series of positive eigenvalues $0 < \lambda_1 \leq \lambda_2 \leq \cdots$ accumulating at infinity only.

In general, the eigenvalues λ_k cannot be calculated explicitly and especially for large k it is difficult to evaluate them numerically. Therefore it is interesting to describe the asymptotic behavior of λ_k as $k \to \infty$. This is equivalent to the asymptotics of the negative eigenvalues of the operator

$$H_\Omega \;=\; -h^2\Delta_\Omega - 1$$

in the semiclassical limit $h \to 0+$.

The first general result is due to H. Weyl who studied the counting function

$$N_\Omega(h) \;=\; \sharp\{\lambda_k < h^{-2}\} = \mathrm{Tr}\,(H_\Omega)_-^0 \;.$$

In 1912 he showed that the first term of its semiclassical limit is given by the phase-space volume [11]: For any open bounded set $\Omega \subset \mathbb{R}^d$ the limit

$$N_\Omega(h) \;=\; C_d\,|\Omega|\,h^{-d} + o(h^{-d})$$

holds as $h \to 0+$, where

$$C_d \;=\; \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}(|p|^2-1)_-^0\,dp \;=\; \frac{\omega_d}{(2\pi)^d}$$

and ω_d denotes the volume of the unit ball in $\mathbb{R}^d$.

H. Weyl conjectured in [12] that this formula can be refined by a second term of order h^{-d+1} depending on the boundary of Ω. This stimulated a detailed analysis of the semiclassical limit of partial differential operators. We refer to the books [4, 6, 9] for general results and an overview over the literature. Eventually, the existence of a second term was proved by V. Ivrii by means of a detailed microlocal analysis [5]: If the boundary of Ω is smooth and if the measure of all periodic geodesic billiards is zero then the limit

$$N_\Omega(h) \;=\; C_d\,|\Omega|\,h^{-d} - \frac{1}{4}C_{d-1}\,|\partial\Omega|\,h^{-d+1} + o(h^{-d+1}) \tag{1}$$

holds as $h \to 0+$, where $|\partial\Omega|$ denotes the surface area of the boundary.

In this article we are interested in the sum of the negative eigenvalues

$$\mathrm{Tr}(H_\Omega)_- \;=\; \sum(h^2\lambda_k - 1)_- \;.$$

This quantity describes the energy of non-interacting, fermionic particles trapped in Ω and plays an important role in physical applications.

The asymptotic relation (1) immediately implies a refined formula for the semiclassical limit of $\mathrm{Tr}(H_\Omega)_-$: Suppose that the aforementioned geometric conditions on Ω are satisfied. Then integrating (1) yields

$$\mathrm{Tr}(H_\Omega)_- \;=\; L_d\,|\Omega|\,h^{-d} - \frac{1}{4}L_{d-1}|\partial\Omega|h^{-d+1} + o(h^{-d+1}) \tag{2}$$

as $h \to 0+$, with

$$L_d \;=\; \int_{\mathbb{R}^d}(|p|^2-1)_-\,dp \;=\; \frac{2}{d(d+2)}\,\frac{\omega_d}{(2\pi)^d}\,.$$

In the following we present a direct approach to derive the semiclassical limit of $\mathrm{Tr}(H_\Omega)_-$. We prove (2) without using the result for the counting function. Since we do not apply any microlocal methods the proof works under much weaker conditions.

1.2. *Main result*

Our main result holds without any global geometric conditions on Ω. We only require weak smoothness conditions on the boundary - namely that the boundary belongs to the class $C^{1,\alpha}$ for some $\alpha > 0$. That means, we assume that the local charts of Ω are differentiable and the derivatives are Hölder continuous with exponent α.

Theorem 1.1. *Let the boundary of Ω satisfy $\partial\Omega \in C^{1,\alpha}$, $0 < \alpha \leq 1$. Then the asymptotic limit*

$$\mathrm{Tr}(H_\Omega)_- \;=\; L_d\,|\Omega|\,h^{-d} - \frac{1}{4}L_{d-1}\,|\partial\Omega|\,h^{-d+1} + O\left(h^{-d+1+\alpha/(2+\alpha)}\right)$$

holds as $h \to 0+$.

Our work was stimulated by the question whether similar two-term formulae hold for non-local, non-smooth operators. This is unknown, since the microlocal methods leading to (1) are not applicable. Therefore it is necessary to use a direct approach.

Indeed, Theorem 1.1 can be extended to fractional powers of the Dirichlet Laplace operator [3]. The strategy of the proof is similar but dealing with non-local operators is more difficult and elaborate. In order to give a flavor of our techniques we confine ourselves in this article to the local case.

The question whether the second term of the semiclassical limit of $\mathrm{Tr}(H_\Omega)_-$ exists for Lipschitz domains Ω remains open.

1.3. *Strategy of the proof*

The proof of Theorem 1.1 is divided into three steps: First, we localize the operator H_Ω into balls, whose size varies depending on the distance to the complement of Ω. Then we analyze separately the semiclassical limit in the bulk and at the boundary.

To localize, let $d(u) = \inf\{|x-u| \,:\, x \notin \Omega\}$ denote the distance of $u \in \mathbb{R}^d$ to the complement of Ω. We set

$$l(u) \;=\; \frac{1}{2}\left(1 + \left(d(u)^2 + l_0^2\right)^{-1/2}\right)^{-1}\,,$$

where $0 < l_0 \leq 1$ is a parameter depending only on h. Indeed, we will finally choose l_0 proportional to $h^{2/(\alpha+2)}$.

In Section 3 we introduce real-valued functions $\phi_u \in C_0^\infty(\mathbb{R}^d)$ with support in the ball $B_u = \{x \in \mathbb{R}^d \,:\, |x-u| < l(u)\}$. For all $u \in \mathbb{R}^d$ these functions satisfy

$$\|\phi_u\|_\infty \;\leq\; C\,, \qquad \|\nabla\phi_u\|_\infty \leq C\,l(u)^{-1} \tag{3}$$

and for all $x \in \mathbb{R}^d$

$$\int_{\mathbb{R}^d} \phi_u^2(x)\,l(u)^{-d}\,du \;=\; 1\,. \tag{4}$$

Here and in the following the letter C denotes various positive constants that might depend on Ω, but that are independent of u, l_0 and h.

Proposition 1.1. *For $0 < l_0 \leq 1$ and $h > 0$ we have*

$$\left|\mathrm{Tr}(H_\Omega)_- - \int_{\mathbb{R}^d} \mathrm{Tr}\,(\phi_u H_\Omega \phi_u)_-\,l(u)^{-d}\,du\right| \;\leq\; C\,l_0^{-1}\,h^{-d+2}\,.$$

In view of this result, one can analyze the local asymptotics, i. e., the asymptotic behavior of $\mathrm{Tr}(\phi_u H_\Omega \phi_u)_-$ separately on different parts of Ω. First, in the bulk, where the influence of the boundary is not felt.

Proposition 1.2. *Assume that $\phi \in C_0^\infty(\Omega)$ is supported in a ball of radius $l > 0$ and that*

$$\|\nabla\phi\|_\infty \,\leq\, C\, l^{-1} \tag{5}$$

is satisfied. Then for $h > 0$ the estimate

$$\left| \mathrm{Tr}\,(\phi H_\Omega \phi)_- - L_d \int_\Omega \phi^2(x)\, dx\, h^{-d} \right| \,\leq\, C\, l^{d-2}\, h^{-d+2}$$

holds, with a constant depending only on the constant in (5).

Close to the boundary of Ω, more precisely, if the support of ϕ intersects the boundary, a term of order h^{-d+1} appears:

Proposition 1.3. *Assume that $\phi \in C_0^\infty(\mathbb{R}^d)$ is supported in a ball of radius $l > 0$ intersecting the boundary of Ω and that inequality (5) is satisfied.*

Then for all $0 < l \leq 1$ and $0 < h \leq 1$ the estimate

$$\left| \mathrm{Tr}\,(\phi H_\Omega \phi)_- - L_d \int_\Omega \phi^2(x)\, dx\, h^{-d} + \frac{1}{4} L_{d-1} \int_{\partial\Omega} \phi^2(x) d\sigma(x)\, h^{-d+1} \right| \,\leq\, r(l,h)$$

holds. Here $d\sigma$ denotes the $d-1$-dimensional volume element of $\partial\Omega$ and the remainder satisfies

$$r(l,h) \,\leq\, C \left(\frac{l^{d-2}}{h^{d-2}} + \frac{l^{2\alpha+d-1}}{h^{d-1}} + \frac{l^{d+\alpha}}{h^d} \right)$$

with a constant depending on Ω, $\|\phi\|_\infty$ and the constant in (5).

Based on these propositions we can complete the proof of the main result.

Proof of Theorem 1.1. In order to apply Proposition 1.3 to the operators $\phi_u H_\Omega \phi_u$, we need to estimate $l(u)$ uniformly. Assume that $u \in \mathbb{R}^d$ satisfies $B_u \cap \partial\Omega \neq \emptyset$. Then we have $d(u) \leq l(u)$, which by definition of $l(u)$ implies

$$l(u) \leq\, l_0/\sqrt{3}\,. \tag{6}$$

In view of (3) we can therefore apply Proposition 1.2 and Proposition 1.3 to all functions ϕ_u, $u \in \mathbb{R}^d$. Combining these results with Proposition 1.1 we get

$$\begin{aligned} &\left| \mathrm{Tr}\,(H_\Omega)_- - \frac{L_d}{h^d} \int_{\mathbb{R}^d} \int_\Omega \phi_u^2(x) dx\, \frac{du}{l(u)^d} + \frac{L_{d-1}}{4h^{d-1}} \int_{\mathbb{R}^d} \int_{\partial\Omega} \phi_u^2(x) d\sigma(x)\, \frac{du}{l(u)^d} \right| \\ &\leq\, C \left(l_0^{-1} h^{-d+2} + \int_{U_1} l(u)^{-2}\, du\, h^{-d+2} + \int_{U_2} r(l(u),h) l(u)^{-d}\, du \right), \end{aligned}$$

where $U_1 = \{u \in \Omega \,:\, B_u \cap \partial\Omega = \emptyset\}$ and $U_2 = \{u \in \mathbb{R}^d \,:\, B_u \cap \partial\Omega \neq \emptyset\}$. Now we change the order of integration and by virtue of (4) we obtain

$$\begin{aligned}&\left|\operatorname{Tr}(H_\Omega)_- - L_d\,|\Omega|\,h^{-d} + \frac{1}{4}L_{d-1}\,|\partial\Omega|\,h^{-d+1}\right| \\ &\leq C\left(l_0^{-1}h^{-d+2} + \int_{U_1} l(u)^{-2}\,du\,h^{-d+2} + \int_{U_2} r(l(u),h)l(u)^{-d}\,du\right). \qquad (7)\end{aligned}$$

It remains to estimate the remainder terms. Note that, by definition of $l(u)$, we have

$$l(u) \geq \frac{1}{4}\min\left(d(u),1\right) \quad \text{and} \quad l(u) \geq \frac{l_0}{4}$$

for all $u \in \mathbb{R}^d$. Together with (6) this implies

$$\int_{U_1} l(u)^{-2}du \leq Cl_0^{-1} \quad \text{and} \quad \int_{U_2} l(u)^a du \leq Cl_0^a \int_{\{d(u)\leq l_0\}} du \leq Cl_0^{a+1} \qquad (8)$$

for any $a \in \mathbb{R}$. Inserting these estimates into (7) we find that the remainder terms are bounded from above by a constant times

$$l_0^{-1}h^{-d+2} + l_0^{2\alpha}h^{-d+1} + l_0^{\alpha+1}h^{-d}\,.$$

Finally, we choose l_0 proportional to $h^{2/(\alpha+2)}$ and conclude that all error terms in (7) equal $O(h^{-d+1+\alpha/(2+\alpha)})$ as $h \to 0+$. □

The remainder of the text is structured as follows. In Section 2 we analyze the local asymptotics and outline the proofs of Propositions 1.2 and 1.3. In Section 3, we perform the localization and, in particular, prove Proposition 1.1.

2. Local asymptotics

To prove the propositions we need the following rough estimate, a variant of the Berezin-Lieb-Li-Yau inequality [2, 7, 8].

Lemma 2.1. *For any $\phi \in C_0^\infty(\mathbb{R}^d)$ and $h > 0$*

$$\operatorname{Tr}(\phi H_\Omega \phi)_- \leq L_d \int_{\mathbb{R}^d} \phi^2(x)\,dx\,h^{-d}\,.$$

Proof. Let us introduce the operator

$$H_0 = -h^2\Delta - 1\,,$$

defined with form domain $H^1(\mathbb{R}^d)$. The variational principle for sums of eigenvalues implies $\operatorname{Tr}(\phi H_\Omega \phi)_- \leq \operatorname{Tr}(\phi(H_0)_-\phi)_-$. Using the Fourier-transform one can derive an explicit expression for the kernel of $(H_0)_-$ and inserting this yields the claim. □

2.1. *Local asymptotics in the bulk*

First we assume $\phi \in C_0^\infty(\Omega)$. Then we have $\mathrm{Tr}\,(\phi H_\Omega \phi)_- = \mathrm{Tr}\,(\phi H_0 \phi)_-$, since the form domains of $\phi H_\Omega \phi$ and $\phi H_0 \phi$ coincide. Moreover, by scaling, we can assume $l = 1$. Thus, to prove Proposition 1.2, it suffices to establish the estimate

$$\left| \mathrm{Tr}\,(\phi H_0 \phi)_- - L_d \int_{\mathbb{R}^d} \phi^2(x)\, dx\, h^{-d} \right| \leq C h^{-d+2}$$

for $h > 0$. The lower bound follows immediately from Lemma 2.1. The upper bound can be derived in the same way as in the proof of Lemma 2.3 below. Indeed, by choosing the trial density matrix $\gamma = \chi(H_0)_-^0 \chi$ we find

$$\mathrm{Tr}\,(\phi H_0 \phi)_- \geq L_d \int_{\mathbb{R}^d} \phi^2(x)\, dx - C_d \int_{\mathbb{R}^d} (\nabla\phi)^2(x)\, dx\, h^{-d+2}$$

and the claim follows.

2.2. *Straightening the boundary*

Here we transform the operator H_Ω locally to an operator given on the half-space $\mathbb{R}^d_+ = \{y \in \mathbb{R}^d : y_d > 0\}$. There we define the operator H^+ in the same way as H_Ω, with form domain $H_0^1(\mathbb{R}^d_+)$.

Under the conditions of Proposition 1.3 let B denote the open ball of radius $l > 0$, containing the support of ϕ. Choose $x_0 \in B \cap \partial\Omega$ and let ν_{x_0} be the normed inner normal vector at x_0. We choose a Cartesian coordinate system such that $x_0 = 0$ and $\nu_{x_0} = (0, \ldots, 0, 1)$, and we write $x = (x', x_d) \in \mathbb{R}^{d-1} \times \mathbb{R}$ for $x \in \mathbb{R}^d$.

For sufficiently small $l > 0$ one can introduce new local coordinates near the boundary. Let D denote the projection of B on the hyperplane given by $x_d = 0$. Since the boundary of Ω is compact and in $C^{1,\alpha}$, there exists a constant $c > 0$, such that for $0 < l \leq c$ we can find a real function $f \in C^{1,\alpha}$ given on D, satisfying

$$\partial\Omega \cap B = \{(x', x_d) : x' \in D, x_d = f(x')\} \cap B\,.$$

The choice of coordinates implies $f(0) = 0$ and $\nabla f(0) = 0$. Since $f \in C^{1,\alpha}$ and the boundary of Ω is compact we can estimate

$$\sup_{x' \in D} |\nabla f(x')| \leq C\, l^\alpha\,, \tag{9}$$

with a constant $C > 0$ depending only on Ω, in particular independent of f.

Now we introduce new local coordinates given by a diffeomorphism $\varphi : D \times \mathbb{R} \to \mathbb{R}^d$. We set $y_j = \varphi_j(x) = x_j$ for $j = 1, \ldots, d-1$ and $y_d = \varphi_d(x) = x_d - f(x')$. Note that the determinant of the Jacobian matrix of φ equals 1 and that the inverse of φ is defined on $\mathrm{ran}\,\varphi = D \times \mathbb{R}$. There we define $\tilde{\phi} = \phi \circ \varphi^{-1}$ and extend it by zero to $\mathbb{R}^d$, such that $\tilde{\phi} \in C_0^1(\mathbb{R}^d)$ and $\|\nabla\tilde{\phi}\|_\infty \leq C l^{-1}$ holds.

Lemma 2.2. *For $0 < l \leq c$ and any $h > 0$ the estimate*

$$\left| \mathrm{Tr}(\phi H_\Omega \phi)_- - \mathrm{Tr}(\tilde{\phi} H^+ \tilde{\phi})_- \right| \leq C\, l^{d+\alpha}\, h^{-d} \tag{10}$$

holds. Moreover, we have

$$\int_\Omega \phi^2(x)\, dx = \int_{\mathbb{R}^d_+} \tilde{\phi}^2(y)\, dy \tag{11}$$

and

$$\left| \int_{\partial\Omega} \phi^2(x)\, d\sigma(x) - \int_{\mathbb{R}^{d-1}} \tilde{\phi}^2(y',0)\, dy' \right| \leq C\, l^{d-1+2\alpha}\,. \tag{12}$$

Proof. The definition of $\tilde{\phi}$ and the fact $\det J\varphi = 1$ immediately give (11). Using (9) we estimate

$$\int_{\partial\Omega} \phi^2(x) d\sigma(x) = \int_{\mathbb{R}^{d-1}} \tilde{\phi}^2(y',0)\sqrt{1+|\nabla f|^2}dy' \leq \int_{\mathbb{R}^{d-1}} \tilde{\phi}^2(y',0)dy' + Cl^{d-1+2\alpha}$$

from which (12) follows.

To prove (10) fix $v \in H_0^1(\Omega)$ with support in $\overline{B}$. For $y \in \operatorname{ran}\varphi$ put $\tilde{v}(y) = v \circ \varphi^{-1}(y)$ and extend $\tilde{v}$ by zero to $\mathbb{R}^d$. Note that $\tilde{v}$ belongs to $H_0^1(\mathbb{R}^d_+)$.

An explicit calculation shows

$$\left| (\tilde{v}, -\Delta_{\mathbb{R}^d_+}\tilde{v}) - (v, -\Delta_\Omega v) \right| \leq C\, l^\alpha\, (\tilde{v}, -\Delta_{\mathbb{R}^d_+}\tilde{v})\,.$$

Hence, we find

$$\operatorname{Tr}(\phi H_\Omega \phi)_- \leq \operatorname{Tr}(\tilde{\phi}(-(1-Cl^\alpha)h^2\Delta_{\mathbb{R}^d_+} - 1)\tilde{\phi})_-\,.$$

Set $\varepsilon = 2Cl^\alpha$ and assume l to be sufficiently small, so that $0 < \varepsilon \leq 1/2$ holds. Then

$$\begin{aligned}
\operatorname{Tr}(\phi H_\Omega \phi)_- &\leq \operatorname{Tr}(\tilde{\phi}(-(1-Cl^\alpha)h^2\Delta_{\mathbb{R}^d_+} - 1)\tilde{\phi})_- \\
&\leq \operatorname{Tr}(\tilde{\phi}(-h^2\Delta_{\mathbb{R}^d_+} - 1)\tilde{\phi})_- + \operatorname{Tr}(\tilde{\phi}(-(\varepsilon - Cl^\alpha)h^2\Delta_{\mathbb{R}^d_+} - \varepsilon)\tilde{\phi})_- \\
&\leq \operatorname{Tr}(\tilde{\phi}H^+\tilde{\phi})_- + \varepsilon \operatorname{Tr}(\tilde{\phi}(-(h^2/2)\Delta_{\mathbb{R}^d_+} - 1)\tilde{\phi})_-\,.
\end{aligned}$$

By Lemma 2.1 we have $\operatorname{Tr}(\tilde{\phi}(-(h^2/2)\Delta_{\mathbb{R}^d_+} - 1)\tilde{\phi})_- \leq Cl^d h^{-d}$ and we obtain

$$\operatorname{Tr}(\phi H_\Omega \phi)_- \leq \operatorname{Tr}(\tilde{\phi}H^+\tilde{\phi})_- + C\, l^{d+\alpha}\, h^{-d}\,.$$

Finally, by interchanging the roles of H_Ω and H^+, we get an analogous upper bound and the proof of Lemma 2.2 is complete. □

2.3. *Local asymptotics in half-space*

In view of Lemma 2.2 we can reduce Proposition 1.3 to a statement concerning the operator H^+, given on the half-space $\mathbb{R}^d_+$. Indeed, to prove Proposition 1.3, it suffices to establish the following result.

Lemma 2.3. *Assume that $\phi \in C_0^1(\mathbb{R}^d)$ is supported in a ball of radius $l > 0$ and that (5) is satisfied. Then for $h > 0$ the estimate*

$$\left| \operatorname{Tr}\left(\phi H^+ \phi\right)_- - \frac{L_d}{h^d}\int_{\mathbb{R}^d_+} \phi^2(x)dx + \frac{L_{d-1}}{4h^{d-1}}\int_{\mathbb{R}^{d-1}} \phi^2(x',0)dx' \right| \leq Cl^{d-2}h^{-d+2}$$

holds with a constant depending only on the constant in (5).

Proof. On $\mathbb{R}^d_+$ we can rescale ϕ and assume $l = 1$. In a first step we prove the estimate

$$\left| \mathrm{Tr}\left(\phi H^+ \phi\right)_- - \frac{L_d}{h^d} \int_{\mathbb{R}^d_+} \phi^2(x) dx + \int_{\mathbb{R}^d_+} \phi^2(x) \int_{\mathbb{R}^d} \cos(2\xi_d x_d h^{-1}) (|\xi|^2 - 1)_- \frac{d\xi\, dx}{(2\pi h)^d} \right| \leq C\, h^{-d+2}\,. \tag{13}$$

To derive a lower bound we use the inequality $\mathrm{Tr}\,(\phi H^+ \phi)_- \leq \mathrm{Tr}\,(\phi (H^+)_- \phi)$ and diagonalize the operator $(H^+)_-$, applying the Fourier-transform in the x'-coordinates and the sine-transform in the x_d-coordinate. This yields

$$\mathrm{Tr}(\phi H^+ \phi)_- \;\leq\; \int_{\mathbb{R}^d_+} \phi^2(x) \int_{\mathbb{R}^d} 2\sin^2(\xi_d x_d h^{-1}) \left(|\xi|^2 - 1\right)_- \frac{d\xi\, dx}{(2\pi h)^d}$$

and the lower bound follows from the identity

$$2\sin^2(\xi_d x_d h^{-1}) \;=\; 1 - \cos(2\xi_d x_d h^{-1})\,. \tag{14}$$

To prove the upper bound, define the operator $\gamma = \chi (H^+)^0_- \chi$ with kernel

$$\gamma(x,y) \;=\; \frac{2}{(2\pi h)^d}\, \chi(x) \int_{|\xi|<1} e^{i\xi'(x'-y')/h}\, \sin(\xi_d x_d h^{-1}) \sin(\xi_d y_d h^{-1}) d\xi\, \chi(y)\,,$$

where χ denotes the characteristic function of an open ball containing the support of ϕ. Thus, γ is a trace-class operator, satisfying $0 \leq \gamma \leq 1$ and by the variational principle it follows that

$$\begin{aligned}
&\mathrm{Tr}(\phi H^+ \phi)_- \\
&\geq\; -\mathrm{Tr}(\gamma \phi H^+ \phi) \\
&=\; -2 \int_{|\xi|<1} \left(h^2 \|\nabla e^{i\xi'\cdot/h} \sin(\xi_d \cdot h^{-1}) \phi\|^2_{L^2(\mathbb{R}^d_+)} - \left\|\sin(\xi_d \cdot h^{-1})\phi\right\|^2_{L^2(\mathbb{R}^d_+)} \right) \frac{d\xi}{(2\pi h)^d} \\
&\geq\; \int_{\mathbb{R}^d} \left(|\xi|^2 - 1\right)_- \int_{\mathbb{R}^d_+} \phi^2(x)\, 2\sin^2(\xi_d x_d h^{-1}) \frac{dx\, d\xi}{(2\pi h)^d} - Ch^{-d+2}\,.
\end{aligned}$$

In view of (14) this gives an upper bound and we established (13).

We proceed to analyzing the term in (13) which contains the cosine. We substitute $x_d = th$ and write

$$\begin{aligned}
&\int_{\mathbb{R}^d_+} \phi^2(x) \int_{\mathbb{R}^d} \cos(2\xi_d x_d h^{-1}) \left(|\xi|^2 - 1\right)_- \frac{d\xi\, dx}{(2\pi h)^d} \\
&= \frac{1}{(2\pi)^d} \int_0^\infty \int_{\mathbb{R}^{d-1}} \phi^2(x', th) dx' \int_{\mathbb{R}^d} \cos(2\xi_d t) \left(|\xi|^2 - 1\right)_- d\xi\, dt\, h^{-d+1}\,.
\end{aligned} \tag{15}$$

Note that

$$\frac{1}{(2\pi)^d} \int_0^\infty \int_{\mathbb{R}^d} \cos(2\xi_d t) \left(|\xi|^2 - 1\right)_- d\xi\, dt \;=\; \frac{1}{4} L_{d-1}\,. \tag{16}$$

Moreover, in [1, (9.1.20)] it is shown that

$$\int_{\mathbb{R}^d} \cos(2\xi_d t) \left(|\xi|^2 - 1\right)_- d\xi = C \int_0^1 \cos(2\xi_d t)(1-\xi_d^2)^{(d+1)/2} d\xi_d = C \frac{J_{d/2+1}(2t)}{t^{d/2+1}}\,,$$

where $J_{d/2+1}$ denotes the Bessel function of the first kind. We remark that $|J_{d/2+1}(2t)|$ is proportional to $t^{d/2+1}$ as $t \to 0+$ and bounded by a constant times $t^{-1/2}$ as $t \to \infty$, see [1, (9.1.7) and (9.2.1)]. It follows that

$$\int_0^\infty t \left| \int_{\mathbb{R}^d} \cos(2\xi_d t) \left(|\xi|^2 - 1 \right)_- d\xi \right| dt \;\le\; C \int_0^\infty t^{-d/2} |J_{d/2+1}(2t)|\, dt \;\le\; C\,. \quad (17)$$

In view of (15), (16) and (17) we find

$$\left| \int_{\mathbb{R}^d_+} \phi^2(x) \int_{\mathbb{R}^d} \cos(2\xi_d x_d h^{-1}) \left(|\xi|^2 - 1 \right)_- \frac{d\xi\, dx}{(2\pi h)^d} - \frac{L_{d-1}}{4h^{d-1}} \int_{\mathbb{R}^{d-1}} \phi^2(x', 0) dx' \right| \le C h^{-d+2}\,.$$

Inserting this into (13) proves Lemma 2.3. □

Proposition 1.3 is a consequence of Lemma 2.2 and Lemma 2.3.

3. Localization

Here we construct the family of localization functions $(\phi_u)_{u\in\mathbb{R}^d}$ and prove Proposition 1.1. The key idea is to choose the localization depending on the distance to the complement of Ω, see [4, Theorem 17.1.3] and [10].

Fix a real-valued function $\phi \in C_0^\infty(\mathbb{R}^d)$ with support in $\{|x| < 1\}$ and $\|\phi\|_2 = 1$. For $u, x \in \mathbb{R}^d$ let $J(x,u)$ be the Jacobian of the map $u \mapsto (x-u)/l(u)$. We define

$$\phi_u(x) \;=\; \phi\left(\frac{x-u}{l(u)} \right) \sqrt{J(x,u)}\, l(u)^{d/2}\,,$$

such that ϕ_u is supported in $\{x : |x-u| < l(u)\}$. According to [10], the functions ϕ_u satisfy (3) and (4) for all $u \in \mathbb{R}^d$.

To prove the upper bound in Proposition 1.1, put

$$\gamma \;=\; \int_{\mathbb{R}^d} \phi_u \; (\phi_u H_\Omega \phi_u)_-^0 \; \phi_u\, l(u)^{-d}\, du\,.$$

Obviously, $\gamma \ge 0$ holds and in view of (4) also $\gamma \le 1$. The range of γ belongs to $H_0^1(\Omega)$ and by the variational principle it follows that

$$-\mathrm{Tr}(H_\Omega)_- \;\le\; \mathrm{Tr}\,\gamma H_\Omega \;=\; -\int_{\mathbb{R}^d} \mathrm{Tr}\,(\phi_u H_\Omega \phi_u)_-\, l(u)^{-d}\, du\,.$$

To prove the lower bound we make use of the IMS-formula

$$\frac{1}{2}\left(f, \phi^2(-\Delta) f\right) + \frac{1}{2}\left(f, -\Delta\phi^2 f\right) \;=\; \left(f, \phi(-\Delta)\phi f\right) - \left(f, f(\nabla\phi)^2\right)\,,$$

valid for $\phi \in C_0^\infty(\mathbb{R}^d)$ and $f \in H_0^1(\Omega)$. Combining this identity with (4) yields

$$(f, -\Delta f) \;=\; \int_{\mathbb{R}^d} \left(\left(f, \phi_u(-\Delta)\phi_u f\right) - \left(f, (\nabla\phi_u)^2 f\right) \right) l(u)^{-d}\, du\,. \quad (18)$$

Using (3) and (4) one can show [10]

$$\int_{\mathbb{R}^d} (\nabla\phi_u)^2(x) l(u)^{-d}\, du \;\le\; C \int_{\mathbb{R}^d} \phi_u^2(x)\, l(u)^{-d-2}\, du\,.$$

We insert this into (18) and deduce

$$\operatorname{Tr}(H_\Omega)_- \leq \int_{\Omega^*} \operatorname{Tr}\left(\phi_u\left(-h^2\Delta - 1 - Ch^2 l(u)^{-2}\right)\phi_u\right)_- \, l(u)^{-d}\, du\,,$$

where $\Omega^* = \{u \in \mathbb{R}^d : \operatorname{supp}\phi_u \cap \Omega \neq \emptyset\}$. To estimate the localization error we use Lemma 2.1. For any $u \in \mathbb{R}$, let ρ_u be another parameter $0 < \rho_u \leq 1/2$ and estimate

$$\begin{aligned}
&\operatorname{Tr}\left(\phi_u\left(-h^2\Delta - 1 - Ch^2 l(u)^{-2}\right)\phi_u\right)_- \\
&\leq \operatorname{Tr}\left(\phi_u(-h^2\Delta - 1)\phi_u\right)_- + C\operatorname{Tr}\left(\phi_u\left(-\rho_u h^2\Delta - \rho_u - h^2 l(u)^{-2}\right)\phi_u\right)_- \\
&\leq \operatorname{Tr}\left(\phi_u H_\Omega \phi_u\right)_- + C\, l(u)^d (\rho_u h^2)^{-d/2}\left(\rho_u + h^2 l(u)^{-2}\right)^{1+d/2}\,.
\end{aligned}$$

With ρ_u proportional to $h^2 l(u)^{-2}$ we find

$$\operatorname{Tr}(H_\Omega)_- \leq \int_{\Omega^*} \operatorname{Tr}\left(\phi_u H_\Omega \phi_u\right)_- \, l(u)^{-d} du + Ch^{-d+2}\int_{\Omega^*} l(u)^{-2} du\,.$$

In view of (8) the last integral is bounded by a constant times l_0^{-1} and the proof of Proposition 1.1 is complete.

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ON THE ENERGY OF THE MINIMIZERS OF THE GINZBURG-LANDAU FUNCTIONAL FOR EXTERIOR MAGNETIC FIELDS BETWEEN H_{C_2} AND H_{C_3}

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Dedicated to Ari Laptev

Superconductivity for Type II superconductors in external magnetic fields of magnitude between the second and third critical fields is known to be restricted to a narrow boundary region. The profile of the superconducting order parameter in the Ginzburg-Landau model is expected to be governed by an effective one-dimensional model. This is known to be the case for external magnetic fields sufficiently close to the third critical field. In this text we announce such a result on a larger interval of validity. These results have been obtained in collaboration with Soeren Fournais and Mikael Persson and the complete proofs will appear elsewhere.

Keywords: Spectral theory; superconductivity.

1. Introduction

When studying superconductivity in the framework of the Ginzburg-Landau theory and when varying the strength H of the applied magnetic field, one meets in the case of a type II material[a], three critical values. When $0 \leq H$ is small enough, the wave function ψ, whose modulus represents the density of presence of the Cooper pairs, does not vanish (in the physical language, is superconducting). When increasing H, the first critical field H_{C_1} is where a vortex of the wave function appears and will not concern us in the present text. At the second critical field H_{C_2}, superconductivity becomes essentially restricted to the boundary and ψ is weak in the interior. At the third critical field H_{C_3}, superconductivity disappears completely. For $H > H_{C_3}$, ψ is actually identically 0. In this talk we will discuss superconductivity in the zone between H_{C_2} and H_{C_3} in the case when the Ginzburg-Landau parameter κ tends to $+\infty$.

[a]This means that its characteristic Ginzburg-Landau constant κ is sufficiently large.

2. Main results

But let us describe our problem more mathematically. A complete presentation of the theory is given in the book of Etienne Sandier and Sylvia Serfaty [10] for H close to $H_{C_3(\kappa)}$ and in the recent book of the author with Soeren Fournais [4] which presents the state of the art till say 2008 for H close to $H_{C_3(\kappa)}$. The Ginzburg-Landau model of superconductivity for a material represented by a bounded open set Ω in $\mathbb{R}^2$ is the functional associating with a pair $(\psi, \mathbf{A})$ an energy $\mathscr{E}[\psi, \mathbf{A}]$ which is defined by:

$$\mathscr{E}[\psi, \mathbf{A}] = \int_\Omega |(\nabla - i\kappa H \mathbf{A})\psi|^2 - \kappa^2|\psi|^2 + \tfrac{\kappa^2}{2}|\psi|^4 + (\kappa H)^2|\mathrm{curl}(\mathbf{A} - \mathbf{F})|^2 \, dx \,. \quad (1)$$

Here $\psi \in W^{1,2}(\Omega)$[b] is a complex valued wave function, $\mathbf{A} \in W^{1,2}(\Omega, \mathbb{R}^2)$ a vector potential, κ the Ginzburg-Landau parameter and H is the strength of the applied magnetic field. The potential $\mathbf{F} : \Omega \to \mathbb{R}^2$ is the unique vector field satisfying,

$$\mathrm{Curl}\, \mathbf{F} = 1 \,, \quad \mathrm{Div}\, \mathbf{F} = 0 \quad \text{in } \Omega \,, \qquad\qquad N \cdot \mathbf{F} = 0 \quad \text{on } \partial\Omega \,, \quad (2)$$

where N is the unit inward normal vector of $\partial\Omega$.

With this notation, the critical fields behave as follows for large κ:

$$H_{C_2} \approx \kappa + o(\kappa), \qquad H_{C_3} \approx \frac{\kappa}{\Theta_0} + o(\kappa), \quad (3)$$

where $\Theta_0 \approx 0.59$ is a universal "spectral" constant discovered by De Gennes (see below).

Therefore, when we study the Ginzburg-Landau functional for a κ-dependent external field, satisfying for some κ-independent $b \in]1, \Theta_0^{-1}[$

$$H(\kappa) = b\kappa \,, \quad (4)$$

superconductivity should be as κ is large a boundary phenomenon. This was exhibited in a weak sense by X. Pan in [9] who proves:

Theorem 2.1. *(see [9])*
For any $b \in \left]1, \Theta_0^{-1}\right[$, there exists a constant E_b, such that, for $H = \kappa b$,

$$\inf_{(\psi,\mathbf{A}) \in W^{1,2}(\Omega) \times W^{1,2}(\Omega;\mathbb{R}^2)} \mathscr{E}_{\kappa,H}[\psi, \mathbf{A}] = -\sqrt{\kappa H} E_b |\partial\Omega| + o(\kappa), \quad (5)$$

as $\kappa \to \infty$.

X. Pan also indicates that superconductivity is uniformly distributed along the boundary. However, the constant E_b is only defined as a limit and its calculation is not easy. A number of conjectures related to the calculation of E_b are given in [9]. In a paper of Almog-Helffer [1] (see also [4, Chapter 14]), the constant E_b is determined for b in the vicinity of Θ_0^{-1}. From the analysis of these two references, it turns out that the determination of the constant in this *non-linear* problem can be reduced to the positivity of a *linear* operator which will be defined below, after

[b] $W^{1,2}(\Omega) := \{u \in L^2(\Omega) \,, \nabla u \in L^2(\Omega)^2\}$ is the standard Sobolev space.

the introduction of a family of reduced functionals.
Having introduced the space $\mathscr{B}^1(\mathbb{R}^+)$ as

$$\mathscr{B}^1(\mathbb{R}^+) = \{\phi \in L^2(\mathbb{R}^+) \,:\, \phi' \in L^2(\mathbb{R}^+) \text{ and } t\phi \in L^2(\mathbb{R}^+)\}, \tag{6}$$

we consider, for $z \in \mathbb{R}$ and $\lambda > 0$, the functional $\mathscr{F}_{z,\lambda}$ which is defined for $\phi \in \mathscr{B}^1$ by,

$$\mathscr{F}_{z,\lambda}(\phi) := \int_0^{+\infty} |\phi'(t)|^2 + (t-z)^2|\phi(t)|^2 + \frac{\lambda}{2}|\phi(t)|^4 - \lambda|\phi(t)|^2\, dt\,. \tag{7}$$

We then denote by $f_{z,\lambda}$ the non-negative minimizer of $\mathscr{F}_{z,\lambda}$.

For $\lambda > 0$, we minimize $\mathscr{F}_{z,\lambda}(f_{z,\lambda})$ over z and denote a minimum[c] by $\zeta(\lambda)$. One can show that such a minimum exists when $\lambda \in]\Theta_0, 1]$. By definition of $f_{\zeta(\lambda),\lambda}$,

$$\mathscr{F}_{z,\lambda}(\phi) \geq \mathscr{F}_{\zeta(\lambda),\lambda}(f_{\zeta(\lambda),\lambda}), \tag{8}$$

for all $(z, \phi) \in \mathbb{R} \times \mathscr{B}^1(\mathbb{R}^+)$.

We also introduce a linear operator $\mathfrak{k}_\lambda$. Define, for $\nu \in \mathbb{R}$, $\lambda \in \mathbb{R}^+$, the operator $\mathfrak{k}_\lambda = \mathfrak{k}_\lambda(\nu)$ to be the Neumann realization of

$$\mathfrak{k}_\lambda(\nu) = -\frac{d^2}{dt^2} + (t-\nu)^2 + \lambda f_{\zeta(\lambda),\lambda}(t)^2, \tag{9}$$

on $L^2(\mathbb{R}^+)$. We denote by $\{\lambda_j(\nu)\}_{j=1}^\infty$ the spectrum of $\mathfrak{k}_\lambda(\nu)$ and by $\{v_j(t;\nu)\}_{j=1}^\infty$ some orthonormal basis of associated real eigenfunctions.

It follows from [1, 4] that

Theorem 2.2.
Let $\lambda \in]\Theta_0, 1[$. Suppose that there exists a minimum $\zeta(\lambda)$ such that for the corresponding choice of $\mathfrak{k}_\lambda(\nu)$ we have

$$\lambda \leq \inf_{\nu\in\mathbb{R}} \lambda_1(\nu)\,. \tag{10}$$

Then

$$E_{\lambda^{-1}} = \frac{\lambda}{2}\|f_{\zeta(\lambda),\lambda}\|^4_{L^4(\mathbb{R}^+)}. \tag{11}$$

It is also proved in [1, 4] (see Proposition 14.2.13 in [4]) that

Theorem 2.3.
There exists $\epsilon > 0$ such that (10) *is satisfied for $\lambda \in]\Theta_0, \Theta_0 + \epsilon[$.*

Our main goal is to give explicit bounds on the optimal ϵ. Let us start with a weaker result. A minimizer $f_{z,\lambda}$ of the functional $\mathscr{F}_{z,\lambda}$ will be a solution to the Euler-Lagrange equation for the minimization problem (7)

$$-u'' + (t-z)^2 u + \lambda|u|^2 u = \lambda u, \qquad u'(0) = 0. \tag{12}$$

In particular, when $\nu = \zeta(\lambda)$, we have $\lambda_1(\nu) = \lambda$, since by (12) with $z = \zeta(\lambda)$, the minimizer $f_{\zeta(\lambda),\lambda}$ is a positive eigenfunction of $\mathfrak{k}_\lambda(\zeta(\lambda))$ with corresponding

[c]This minimum is not necessarily unique but we will describe the argument in the case it is unique.

eigenvalue λ. Clearly, $\nu = \zeta(\lambda)$ is a critical point for $\lambda_1(\nu)$. Our first result is a local analysis around $\nu = \zeta(\lambda)$, which says:

Theorem 2.4.
Let $\Theta_0 < \lambda \leq 1$. Then $\lambda_1(\nu)$ has a local minimum for $\nu = \zeta(\lambda)$, i.e., there exist positive constants δ_λ and c_λ such that for all $|\nu - \zeta(\lambda)| < \delta_\lambda$ it holds that

$$\lambda_1(\nu) \geq \lambda + c_\lambda(\nu - \zeta(\lambda))^2.$$

This local analysis is completed by an analysis for ν large:

Theorem 2.5.
Let $\lambda > \Theta_0$, $z \in \mathbb{R}$, and let $f_{z,\lambda}$ be a positive minimizer of $\mathscr{F}_{z,\lambda}$. Define

$$\lambda_1(\nu; z) := \inf \mathrm{Spec}\Big\{ -\frac{d^2}{dt^2} + (t-\nu)^2 + \lambda f_{z,\lambda}^2 \Big\}, \tag{13}$$

where we consider the Neumann realization on $L^2(\mathbb{R}^+)$ of the operator.
Then, $\lambda_1(\nu; z) \to 1$ as $\nu \to +\infty$. Furthermore, there exists $\nu_0 = \nu_0(\lambda, z) > 0$ such that

$$\lambda_1(\nu; z) > 1, \tag{14}$$

for all $\nu \geq \nu_0$.

We conclude by our answer to the main question, only stating the numerical value, which we have obtained for the ϵ, whose existence was proved in Theorem 2.3.

Theorem 2.6.
Let $\Theta_0 \leq \lambda \leq 0.80$. Then (10) *holds, i.e.* $\inf_{\nu \in \mathbb{R}} \lambda_1(\nu) \geq \lambda$.

The proof is based on various tricky spectral estimates for various basic operators like $\mathfrak{k}_\nu$ composed in the last step with some numerics. Very roughly, this is a mixture between arguments used for the proof of the Feynman-Hellmann formula, the Temple inequality which gives a lower bound of the gap between the two first eigenvalues, the virial theorem and what is called Dauge-Helffer formula (related to the Hadamard's formula relative to the variation of the eigenvalues of the Dirichlet Laplacian when deforming the domain) and involves mainly the groundstate energy and the second eigenvalue of these operators. Some typical estimates will be presented in the last section. Note that some of these techniques have been efficiently used in [6] and [7] for connected problems on the family of anharmonic oscillators $D_t^2 + (t^k - z)^2$ ($k \geq 2$, $z \in \mathbb{R}$).

3. About some techniques used in the proof

We first recall a few properties of the de Gennes operator, which was playing the key role in the explanation of the so-called onset of superconductivity.

3.1. *Reminder for the de Gennes operator*

Define

$$\mathfrak{h}(\xi) = -\frac{d^2}{dt^2} + (t-\xi)^2, \tag{15}$$

in $L^2(\mathbb{R}^+)$ with Neumann boundary conditions at 0. We will denote the eigenvalues of this operator by $\{\mu_j(\xi)\}_{j=1}^{\infty}$ and corresponding (real normalized) eigenfunctions by $u_j(t) = u_j(t;\xi)$. A basic identity from perturbation theory (Feynman-Hellmann) is

$$\mu_j'(\xi) = -2\int_0^{+\infty} (t-\xi)|u_j(t;\xi)|^2\, dt. \tag{16}$$

An integration by parts yields the useful alternative formula from Dauge-Helffer [3]:

$$\mu_j'(\xi) = (\mu_j(\xi) - \xi^2)|u_j(0;\xi)|^2\,. \tag{17}$$

From this we deduce that μ_j has a unique minimum attained at $\xi_0^{(j)}$ satisfying $\mu_j(\xi_0^{(j)}) = (\xi_0^{(j)})^2$. By definition

$$\Theta_0 = \inf_{\xi\in\mathbb{R}} \mu_1(\xi) = \mu_1(\xi_0^{(1)}) = (\xi_0^{(1)})^2. \tag{18}$$

3.2. *A virial-type result*

The function $f_{\zeta,\lambda}$ satisfies the Euler-Lagrange equation (12). Since, $\zeta = \zeta(\lambda)$ is a minimum for the non-linear energy, we get

$$\int_0^{+\infty} (t-\zeta) f_{\zeta,\lambda}^2\, dt = 0. \tag{19}$$

In particular $\zeta(\lambda) > 0$.

Moreover, multiplying (12) by $f_{\zeta,\lambda}$ and integrating, we obtain

$$\|f_{\zeta,\lambda}'\|_2^2 + \|(t-\zeta)f_{\zeta,\lambda}\|_2^2 + \lambda\|f_{\zeta,\lambda}\|_4^4 = \lambda\|f_{\zeta,\lambda}\|_2^2\,. \tag{20}$$

The virial type argument consists in using the invariance by a dilation δ_t of the problem which leads to the property that the corresponding eigenvalues are constants. Differentiating with respect to t and using the Feynman-Hellmann formula leads to useful identities.

Lemma 3.1.
Assume that $\Theta_0 \le \lambda \le 1$ *and that* $(\zeta, f_{\zeta,\lambda})$ *is a minimizer of the functional* (7). *Then*

$$\|f_{\zeta(\lambda),\lambda}'\|_2^2 - \|(t-\zeta(\lambda))f_{\zeta(\lambda),\lambda}\|_2^2 + \frac{\lambda}{4}\|f_{\zeta(\lambda),\lambda}\|_4^4 = 0\,, \tag{21}$$

$$2\|f_{\zeta(\lambda),\lambda}'\|_2^2 + \frac{5\lambda}{4}\|f_{\zeta(\lambda),\lambda}\|_4^4 = \lambda\|f_{\zeta(\lambda),\lambda}\|_2^2\,, \tag{22}$$

and

$$2\|(t-\zeta(\lambda))f_{\zeta(\lambda),\lambda}\|_2^2 + \frac{3\lambda}{4}\|f_{\zeta(\lambda),\lambda}\|_4^4 = \lambda\|f_{\zeta(\lambda),\lambda}\|_2^2\,. \tag{23}$$

3.3. *Bounds on ζ*

The localization of the possibly non unique $\zeta(\lambda)$ plays an important role at various steps in the proof.

Lemma 3.2. *Let $\Theta_0 < \lambda \leq 1$. It holds that*

$$\sqrt{\lambda/2} \leq \zeta(\lambda) \leq \sqrt{\lambda}. \tag{24}$$

Proof. X. Pan has proved in [9] that

$$f_{\zeta,\lambda}(0)^2 = \frac{2}{\lambda}\big(\lambda - \zeta^2\big). \tag{25}$$

This implies the right hand side inequality. Moreover, it is standard that the minimizer $f_{\zeta,\lambda}$ satisfies $\|f_{\zeta,\lambda}\|_\infty \leq 1$, and this implies together with (25) the left hand side inequality. □

3.4. *Proof of Theorem 2.4*

The statement that $\nu = \zeta(\lambda)$ is a local minimum is finally the consequence of this universal estimate

$$\lambda_1(\nu) \geq \lambda + (\nu-\zeta)^2 \left[\frac{\mu_2(\nu) - \big(3\lambda - \frac{\lambda - \Theta_0}{|\zeta|^{1/2}\|u_1(\cdot,\xi_0)\|_4^2}\big) - (\nu-\zeta)^2}{\lambda_2(\nu) - \lambda - (\nu-\zeta)^2} \right], \tag{26}$$

together with a lower bound of $\mu_2(\zeta(\lambda))$.

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DECAY LAW FOR RESONANCES PRODUCED BY PERTURBATION OF UNSTABLE EIGENVALUES CLOSE TO A THRESHOLD

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Dedicated to Ari Laptev on the occasion of his 60th birthday

We report results concerning the decay laws for resonances produced by perturbation of unstable bound states close to a threshold. The model Hamiltonian is of the form

$$H_\varepsilon = \begin{bmatrix} H_{\rm op} & 0 \\ 0 & E_0 \end{bmatrix} + \varepsilon \begin{bmatrix} 0 & W_{12} \\ W_{21} & 0 \end{bmatrix} \quad \text{on} \quad \mathscr{H} = \mathscr{H}_{\rm op} \oplus \mathbf{C},$$

appearing in the study of Feshbach resonances. The operator $H_{\rm op}$ is assumed to have the properties of a Schrödinger operator in odd dimensions, with a threshold at zero. We consider for ε small the survival probability $|\langle \Psi_0, e^{-itH_\varepsilon}\rangle \Psi_0|^2$, where Ψ_0 is the eigenfunction corresponding to E_0 for $\varepsilon = 0$. For E_0 in a small neighborhood of the origin *independent of* ε, the survival probability amplitude is expressed in terms of some special functions related to the error function, up to error terms vanishing as $\varepsilon \to 0$. This allows for a detailed study of the crossover from exponential to non-exponential decay laws, and then to the bound state regime, as the position of the resonance is tuned across the threshold.

Keywords: Decay law; non-exponential decay; Fermi Golden Rule.

1. Introduction

This article is concerned with the decay laws for resonances produced by perturbation of unstable bound states. The problem has a long and distinguished history in quantum mechanics, and there is an extensive body of literature about

decay laws for resonances in general, both at the level of theoretical physics (see e.g. [10, 11, 23, 27–29] and references therein), and at the level of rigorous mathematical physics (see e.g. [3–6, 9, 13, 17–19, 25, 31, 32] and references therein). It started with the computation by Dirac of the decay rate in second order time-dependent perturbation theory, leading to the well known exponential decay law, $e^{-\Gamma t}$. Here Γ is given by the famous "Fermi Golden Rule" (FGR), $\Gamma \sim |\langle \Psi_0, \varepsilon W \Psi_{\mathrm{cont},E_0} \rangle|^2$, where Ψ_0, E_0 are the unperturbed bound state eigenfunction and energy, respectively, and Ψ_{cont,E_0} is the continuum "eigenfunction", degenerate in energy with the bound state. The FGR formula met with a fabulous success, and as a consequence, the common wisdom is that the decay law for the resonances produced by perturbation of non-degenerate bound states is exponential, at least in the leading non-trivial order in the perturbation strength.

However, it has been known for a long time, at least for semi-bounded Hamiltonians, that the decay law cannot be purely exponential; there must be deviations at least at short and long times. This implies that, in more precise terms, the question is whether the decay law is exponential up to errors vanishing as the perturbation strength tends to zero. So at the rigorous level the *crucial problem* is the *estimation of the errors*. This proved to be a hard problem, and only during the past decades consistent rigorous results have been obtained. The generic result is that (see [3, 4, 13, 17, 25] and references therein) the decay law is indeed (quasi)exponential, i.e. exponential up to error terms vanishing in the limit $\varepsilon \to 0$, as long as the resolvent of the unperturbed Hamiltonian is sufficiently smooth, when projected onto the subspace orthogonal to the eigenvalue under consideration. For most cases of physical interest this turns out to be the case, as long as the unperturbed eigenvalue lies in the continuum, far away from the threshold energies.

The problem with the exponential decay law appears for bound states situated near a threshold, since in this case the projected resolvent might not be smooth, or may even blow up, when there is a zero resonance at the threshold, see e.g. [15–17] and references therein. As it has been pointed out in [2, 12] at threshold the FGR formula does not apply. Moreover, the fact that the non-smoothness of the resolvent opens the possibility of a non-exponential decay at all times has been mentioned at the heuristic level [21, 23].

Let us mention that the question of the decay law for near threshold bound states is more than an academic one. While having the bound state in the very neighborhood of a threshold is a non-generic situation, recent advances in experimental technique have made it possible to realize this case for the so-called Feshbach resonances, where (with the aid of a magnetic field) it is possible to tune the energy of the bound state (and then the resonance position) throughout a neighborhood of the threshold energy.

The decay law for the case, when the resonance position is close to the threshold, has been considered at the rigorous level in [17–19], but only under the condition that the shift in the energy due to perturbation is sufficiently large, such that the resonance position is at a distance of order ε from the threshold. In this case it turns out that the decay law is still exponential, but the FGR has to be modified.

In this paper we report rigorous results for the case, when the resonance position is *anywhere* in a small ε-*independent* neighborhood of the threshold. To approximate

the survival probability amplitude we use an appropriate ansatz, close in the spirit to the well known Lorentzian approximation for perturbed eigenvalues far from the threshold, but with a functional form taking into account the behavior of the resolvent near the threshold. The main technical result is the control of the error due to this approximation. The approximated survival probability amplitude is expressed in terms of some special functions, related to the error function, replacing the exponential function in the decay law. As a result, we are able to obtain a rigorous and detailed description of the crossover of the decay law, as the resonance position is tuned through the threshold from positive to negative energies via tuning of E_0: Exponential decay with the usual FGR decay rate, to exponential decay with the modified FGR decay rate, then to non-exponential decay, and finally to bound state behaviour.

In what follows we present the guiding heuristics discussion, and some of the main results. The proofs, additional results, and other details are contained in [7, 8].

2. Generalities

We develop the theory in a somewhat abstract setting, which is applicable to two channel Schrödinger operators in odd dimensions, as they appear for example in the theory of Feshbach resonances (see e.g. [22, 30], and references therein).

Consider

$$H = \begin{bmatrix} H_{\rm op} & 0 \\ 0 & H_{\rm cl} \end{bmatrix} \quad \text{on } \mathscr{H} = \mathscr{H}_{\rm op} \oplus \mathscr{H}_{\rm cl}.$$

In concrete cases $\mathscr{H}_{\rm op} = L^2(\mathbf{R}^3)$ (or $L^2(\mathbf{R}_+)$ in the spherically symmetric case), and $H_{\rm op} = -\Delta + V_{\rm op}$ with $\lim_{|\mathbf{x}|\to\infty} V_{\rm op}(\mathbf{x}) = 0$. $H_{\rm op}$ describes the "open" channel. As for the "closed" channel, one starts again with a Schrödinger operator, but with $\lim_{|\mathbf{x}|\to\infty} V_{\rm cl}(\mathbf{x}) = V_{{\rm cl},\infty} > 0$. One assumes that $H_{\rm cl}$ has bound states below $V_{{\rm cl},\infty}$, which may be embedded in the continuum spectrum of $H_{\rm op}$. Only these bound states are relevant for the problem at hand. Thus one can retain only one isolated eigenvalue (or a group of almost degenerate eigenvalues isolated from the rest of the spectrum); the inclusion of the rest of the spectrum of $H_{\rm cl}$ merely "renormalizes" the values of some coefficients, without changing the qualitative picture. In this paper we shall consider only non-degenerate eigenvalues, i.e. we shall take $H_{\rm cl} = E_0$ in $\mathscr{H}_{\rm cl} = \mathbf{C}$, such that

$$H = \begin{bmatrix} H_{\rm op} & 0 \\ 0 & E_0 \end{bmatrix}, \tag{1}$$

on

$$\mathscr{H} = \mathscr{H}_{\rm op} \oplus \mathbf{C} = \left\{ \Psi = \begin{bmatrix} \psi \\ \beta \end{bmatrix} \,\middle|\, \psi \in \mathscr{H}_{\rm op},\, \beta \in \mathbf{C} \right\}.$$

In addition to the spectrum of $H_{\rm op}$ the operator H has a bound state $\Psi_0 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ at E_0.

The problem is to study the fate of E_0, when an interchannel perturbation

$$\varepsilon W = \varepsilon \begin{bmatrix} 0 & W_{12} \\ W_{21} & 0 \end{bmatrix}, \ \varepsilon > 0, \tag{2}$$

is added to H, i.e. the total Hamiltonian is

$$H_\varepsilon = H + \varepsilon W. \tag{3}$$

We assume that W is a bounded self-adjoint operator.

The quantity to be studied is the so-called survival probability amplitude

$$A_\varepsilon(t) = \langle \Psi_0, e^{-itH_\varepsilon}\Psi_0 \rangle. \tag{4}$$

As in [17–19] we shall follow the approach in [12, 31] to write down a workable formula for $A_\varepsilon(t)$, i.e. we use the Stone formula to express the compressed evolution in terms of the compressed resolvent, and then we use the Schur-Livsic-Feshbach-Grushin (SLFG) partition formula to express the compressed resolvent as an inverse. One arrives at the following basic formula for $A_\varepsilon(t)$,

$$A_\varepsilon(t) = \lim_{\eta \searrow 0} \frac{1}{\pi} \int_{-\infty}^{\infty} e^{-itx} \operatorname{Im} F(x + i\eta, \varepsilon)^{-1} dx \tag{5}$$

with

$$F(z, \varepsilon) = E_0 - z - \varepsilon^2 g(z), \ g(z) = \langle \Psi_0, WQ^*(H_{\text{op}} - z)^{-1} QW\Psi_0 \rangle. \tag{6}$$

Here Q is the projection onto the orthogonal complement of the bound state Ψ_0, and it is viewed as an operator from $\mathscr{H}$ to $\mathscr{H}_{\text{op}}$.

Since we are interested in the form of $A_\varepsilon(t)$, when E_0 is near a threshold of H_{op}, we shall assume that 0 is a threshold of H_{op}, and that E_0 is close to zero. To insure nontriviality we require $QW\Psi_0 \neq 0$.

Assumption 2.1.

(i) There exists $a > 0$, such that $(-a, 0) \subset \rho(H_{\text{op}})$ (the resolvent set) and $[0, a] \subset \sigma_{\text{ess}}(H_{\text{op}})$.
(ii) $|E_0| \leq \frac{1}{2}$.

From Assumption 2.1 and Eq. (6) one gets:

Proposition 2.1.

(i) $g(z)$ is analytic in $\mathbf{C} \setminus \{(-\infty, -a] \cup [0, \infty)\}$.
(ii) $g(z)$ is real and strictly increasing on $(-a, 0)$.
(iii) $\operatorname{Im} g(z) > 0$ for $\operatorname{Im} z > 0$.

Since we are interested in the case, where E_0 is tuned past the threshold, we need assumptions about the behavior of the function $g(z)$ in a neighborhood of the origin.

Assumption 2.2. *For $\operatorname{Re}\kappa \geq 0$ and $z \in \mathbf{C} \setminus [0, \infty)$ we let $\kappa = -i\sqrt{z}$. Let for $a > 0$, $D_a = \{z \in \mathbf{C} \setminus [0, \infty) \,|\, |z| < a\}$. Then for $z \in D_a$*

$$g(z) = \sum_{j=-1}^{4} \kappa^j g_j + \kappa^5 r(\kappa), \ \frac{d}{dz} g(z) = -\frac{1}{2\kappa} \sum_{j=-1}^{4} j\kappa^{j-1} g_j + \kappa^3 s(\kappa), \tag{7}$$

where $\sup_{z\in D_a}\{|r(\kappa)|, |s(\kappa)|\} < \infty$. *Furthermore, we assume that* $\lim_{\mathrm{Im}\, z\searrow 0}(g(z) - g_{-1}\kappa^{-1})$ *exists and is continuous on* $(-a, a)$.

Notice that due to Proposition 2.1 (ii), the coefficients g_j are real. Assumption 2.2 includes the case, when $H_{\mathrm{op}} = -\Delta + V_{\mathrm{op}}$ in odd dimensions. For the expansions of the resolvent of $-\Delta + V_{\mathrm{op}}$ leading to Eq. (7) the reader is sent to [14–18, 26, 33]. Examples of expansions with the corresponding explicit expressions for coefficients g_j are given in the Appendix to [17], with references to the literature.

Since the form of the decay law depends strongly upon the behaviour of $g(z)$ near 0, we divide the considerations into three cases.

(1) The *singular* case, in which $g_{-1} \neq 0$. In the Schrödinger case this corresponds to the situation, when H_{op} has a zero resonance at the threshold (see e.g. [15, 17]). Let us recall that the free particle in one dimension belongs to this class. From Proposition 2.1(iii) follows that $g_{-1} > 0$.
(2) The *regular* case, in which $g_{-1} = 0$ and $g_1 \neq 0$. We note that $g_{-1} = 0$ is the generic case for Schrödinger operators in one and three dimensions. Again from Proposition 2.1(iii) one has $g_1 < 0$. Let us remark that the behavior $\mathrm{Im}\, g(x+i0) \sim x^{1/2}$ as $x \to 0$ is nothing but the famous Wigner threshold law [24, 30].
(3) The *smooth* case, in which $g_{-1} = g_1 = 0$. This case occurs for free Schrödinger operators in odd dimensions larger that three, and in the spherical symmetric case for partial waves $\ell \geq 1$, see [17, 18]. Notice that in this case $\frac{d}{dz}g(z)$ is uniformly bounded in D_a.

Throughout the paper H_{op} and W are kept fixed, while E_0 and ε are parameters. In stating the results we use the following notation:

(i) $A \lesssim B$ means that there exists a constant c such that $A \leq cB$. An analogous definition holds for $A \gtrsim B$.
(ii) $A \simeq B$ means that both $A \lesssim B$ and $A \gtrsim B$ hold.
(iii) $A \cong B$ means that A and B are equal to leading order in a parameter, e.g. $A = B + \delta(\varepsilon)$ with $\lim_{\varepsilon\searrow 0}\delta(\varepsilon) = 0$.

3. Heuristics

For E_0 outside a small (possibly ε-dependent) neighborhood of the origin, the situation is well understood, both at the heuristic level, and at the rigorous level. Indeed, for negative E_0, using the analytic perturbation theory, one can show that

$$|A_\varepsilon(t) - e^{-itE_\varepsilon}| \lesssim \varepsilon^2, \tag{8}$$

where E_ε is the perturbed eigenvalue, which coincides with E_0 in the limit $\varepsilon \to 0$. As a consequence, the survival probability remains close to one uniformly in time.

On heuristic grounds, if E_0 is positive, i.e. embedded in the essential spectrum of H_{op}, Ψ_0 turns into a metastable decaying state. The main problem is to compute the "decay law", i.e. $|A_\varepsilon(t)|^2$, up to error terms vanishing in the limit $\varepsilon \to 0$. For eigenvalues embedded in the continuum spectrum the heuristics for the exponential decay law $|A_\varepsilon(t)|^2 \cong e^{-2\Gamma(\varepsilon)t}$ runs as follows.

Suppose $F(z, \varepsilon)$ is sufficiently smooth, as z approaches the real line from above, $F(x+i0, \varepsilon)$, for x in a neighborhood of E_0. Let $F(x+i0, \varepsilon) = R(x, E_0, \varepsilon) + iI(x, \varepsilon)$.

Then the main contribution to the integral in Eq. (5) comes from the neighborhood of the point $x_0(E_0, \varepsilon)$ where $R(x, E_0, \varepsilon) = 0$ and in this neighborhood (to simplify the notation we omit in what follows the dependence of $R(x, E_0, \varepsilon)$, $I(x, \varepsilon)$, and $x_0(E_0, \varepsilon)$ on E_0 and ε).

$$F(x + i0, \varepsilon) \cong x_0 - x + iI(x_0), \tag{9}$$

and then

$$\operatorname{Im} F(x, \varepsilon)^{-1} \cong \frac{-I(x_0)}{(x - x_0)^2 + I(x_0)^2}, \tag{10}$$

i.e. it has a Lorentzian peak shape leading to

$$|A_\varepsilon(t)|^2 \cong e^{-2|I(x_0)|t}. \tag{11}$$

In the cases where the resolvent has an analytic continuation through the positive semi-axis [12], the resonance is defined as the zero, $z_r = x_r + iy_r$, of $F(z, \varepsilon)$ situated near E_0 in the lower half plane. In the case, where we have smoothness, but not analyticity, we take $x_0 + iI(x_0)$ as the "resonance". Using the form of $F(z, \varepsilon)$ given in Eq. (6) one can show that

$$|x_0 + iI(x_0) - z_r| \lesssim \varepsilon^2 |y_r|, \tag{12}$$

for ε sufficiently small. We note that the estimate Eq. (12) agrees with the general uniqueness result in [20].

The problem with the energies near the threshold is that $F(x + i0, \varepsilon)$ might not be smooth and can even blow up (see Assumption 2.2), if the open channel has a zero resonance at the threshold. Then a Lorentzian approximation might break down. For the case at hand, elaborating on a heuristic argument in [21], one can quantify at the heuristic level how far from the origin $x_0 > 0$ must be in order to have a chance for an exponential decay law: The contribution of the tail at negative x of the Lorentzian must be negligible. Since

$$\int_{-\infty}^{0} \frac{|I(x_0)|}{(x - x_0)^2 + I(x_0)^2} dx \simeq \frac{|I(x_0)|}{x_0}, \tag{13}$$

one gets the condition

$$|I(x_0)| \ll x_0. \tag{14}$$

Consider first the condition Eq. (14) in the *singular* case. For $x > 0$ small enough

$$I(x) \cong -g_{-1}\varepsilon^2 x^{-1/2},$$

and the condition Eq. (14) gives $g_{-1}\varepsilon^2 x_0^{-1/2} \ll x_0$, i.e. $x_0 \gg \varepsilon^{4/3}$. If we take (by adjusting E_0!) $x_0 = b\varepsilon^p$, then one obtains, for $0 \leq p < 4/3$, the exponential decay law (see Eq. (11))

$$|A_\varepsilon(t)|^2 \cong e^{-2g_{-1}b^{-1/2}\varepsilon^{2-p/2}t}. \tag{15}$$

Notice that for $p = 0$ (i.e. the resonance stays away from the threshold as $\varepsilon \to 0$), Eq. (15) is nothing but the usual Fermi Golden Rule (FGR) formula. However, for $p > 0$, but not very large (i.e. the resonance position approaches zero as $\varepsilon \to 0$, but

not too fast), one gets a "modified FGR formula", for which the ε-dependence of the resonance width is $\varepsilon^{2-p/2}$ instead of the usual ε^2-dependence.

For the *regular* case, a similar argument leads to the condition

$$x_0 \gg \varepsilon^4, \tag{16}$$

and a decay law

$$|A_\varepsilon(t)|^2 \cong e^{-2|g_1|b^{1/2}\varepsilon^{2+p/2}t}. \tag{17}$$

Finally, in the *smooth* case the condition Eq. (14) reads

$$\varepsilon^2 x_0^{1/2} \ll 1, \tag{18}$$

which holds true irrespective of how close to zero x_0 is. In other words, in the smooth case one observes an exponential decay law (with a resonance width vanishing as $x_0 \to 0$), as the resonance position is tuned past the threshold, via the tuning of the eigenvalue E_0.

For the regular and smooth cases the above heuristics in substantiated by the following two cases of the results in [17] (see also [4, 31]).

Theorem 3.1. *(i) Assume that $F(z,\varepsilon)$ is $\frac{1}{2}$-Hölder continuous uniformly for $z \in D_a$ and ε sufficiently small. Then for $|I(x_0)| \geq const.\varepsilon^\gamma$, $2 \leq \gamma < 4$,*

$$|A_\varepsilon(t) - e^{-it(x_0+iI(x_0))}| \lesssim const.\varepsilon^\delta, \quad \delta = 2 - \frac{\gamma}{2}. \tag{19}$$

(ii) Assume that $F(z,\varepsilon)$ is Lipschitz continuous uniformly for $z \in D_a$ and ε sufficiently small. Then

$$|A_\varepsilon(t) - e^{-it(x_0+iI(x_0))}| \lesssim \varepsilon^2 |\ln \varepsilon|. \tag{20}$$

Indeed, the smooth case is covered by Theorem 3.1(ii). In the regular case, as far as $x_0 \gg \varepsilon^4$ (see Eq. (16)), we get from Eq. (6) and Eq. (7) that $|I(x_0| \gg \varepsilon^4$, and one can apply Theorem 3.1(i).

However, neither the above heuristics nor previous results give any hint about the form of the decay low in the singular and regular case, when x_0 is very close to the threshold. Our result is that in this case the decay law is definitely non-exponential. Due to lack of space only results in the *regular case* are presented. The results in the singular case (which can be found in [7, 8]) are similar, in spite of the fact that the proofs are a bit more complicated, due to the singularity of $g(z)$ at threshold.

4. The model function, regular case

We recall first (see previous section) that in the case of embedded eigenvalues (i.e. $p = 0$) the "model function" approximating $F(z,\varepsilon)$ is the linear function $L(z) = \alpha + i\beta - z$, where the constants α and β are fixed by the condition that $F(x_0 + i0, \varepsilon) = L(x_0 + i0)$ i.e. F and L *coincide* at $x_0(\varepsilon)$.

In the regular case we replace $F(z,\varepsilon)$ for all $p \in (0,\infty)$ by the "model function"

$$H_r(z) = \alpha - z + \varepsilon^2 \beta\kappa, \tag{21}$$

resembling the expansion of $F(z,\varepsilon)$ around the threshold. The free parameters are fixed by the condition that F and H_r coincide at the zeroes of F. There are two real parameters α and β, to be determined. In the case $E_1 = E_0 - g_0\varepsilon^2 \geq 0$ (when the zero of $R(x)$ is positive) the condition used is $F(x_0,\varepsilon) = H_r(x_0)$. In the case $E_1 < 0$ (when the zero, x_b, of $R(x)$ is negative and gives the energy of the bound state) the conditions used are $F(x_b,\varepsilon) = H_r(x_b)$ together with $\frac{d}{dx}F(x_b,\varepsilon) = \frac{d}{dx}H_r(x_b)$. Thus in the case $E_1 < 0$ our conditions determining α and β give as a result that the residues at the pole x_b of $\dfrac{1}{F(x,\varepsilon)}$ and $\dfrac{1}{H_r(x)}$ are equal.

5. Main results; error analysis

We are now in a position to formulate the main technical result: For ε sufficiently small and E_0 in an ε-independent neighborhood of the threshold, the error in $A_\varepsilon(t)$ due to the replacement of $F(z,\varepsilon)$ with the model function $H_r(z)$, as given by Eq. (21), vanishes in the limit $\varepsilon \to 0$.

Theorem 5.1. *Assume $g_{-1} = 0$, $g_1 \neq 0$. There exists c, $\frac{a}{2} \geq c > 0$, such that for sufficiently small ε, $|E_0| \leq c$, and all $t \geq 0$, we have*

$$\begin{aligned}\Big|A_\varepsilon(t) - \lim_{\eta\searrow 0}\frac{1}{\pi}\int_{-\infty}^{\infty} e^{-itx}\,\mathrm{Im}\,H_r(x+i\eta)^{-1}dx\Big| \\ \lesssim \begin{cases}\varepsilon^2(1+x_0^{1/2}|\ln\varepsilon|), & \text{for } E_1 > 0,\\ \varepsilon^2, & \text{for } E_1 \leq 0.\end{cases}\end{aligned} \tag{22}$$

6. Crossover from exponential to non-exponential decay laws

The contribution of the negative semi-axis in $\lim_{\eta\searrow 0}\frac{1}{\pi}\int_{-\infty}^{\infty} e^{-itx}\,\mathrm{Im}\,H_r(x+i\eta)^{-1}dx$ is just the residue at the zero, x_b, of $H_r(z)$ (when it exists). Accordingly

$$\lim_{\eta\searrow 0}\frac{1}{\pi}\int_{-\infty}^{\infty} e^{-itx}\,\mathrm{Im}\,H_r(x+i\eta)^{-1}dx = -\frac{1}{\frac{d}{dx}H_r(x_b)}e^{-itx_b} + \hat{A}_{\varepsilon,r}(t) \tag{23}$$

with

$$\hat{A}_{\varepsilon,r}(t) \equiv \frac{1}{\pi}\int_0^{\infty} e^{-itx}\,\mathrm{Im}\,H_r(x+i0)^{-1}dx. \tag{24}$$

Since H_r has a simple functional form with only two free parameters, the integral in the r.h.s of Eq. (24) can be evaluated numerically or expressed in closed form in terms of special functions:

$$\mathscr{I}_1(z) = \frac{2z}{i\pi}\int_0^{\infty}\frac{e^{-ix^2}}{x^2-z^2}dx, \quad \mathscr{I}_p(z) = \frac{1}{(p-1)!}\frac{d^{p-1}}{dz^{p-1}}\mathscr{I}_1(z), \quad p > 1, \tag{25}$$

closely related to the error function.

Passing to the variable $k = \sqrt{z} = i\kappa$ we get

$$\hat{A}_{\varepsilon,r}(t) = \frac{1}{i\pi}\int_{-\infty}^{\infty}\frac{e^{-itk^2}}{P_r(\kappa)}k dk,\ P_r(\kappa) = \kappa^2 + \varepsilon^2\beta\kappa + \alpha. \tag{26}$$

When the zeroes of P_r are distinct (the other case can be recovered as a limit) a partial fraction decomposition yields the following result.

Proposition 6.1.

$$\hat{A}_{\varepsilon,r}(t) = -\sum_{j=1}^{2} q_j \mathscr{I}_1(i\kappa_j\sqrt{t}), \tag{27}$$

where

$$\kappa_j = \tfrac{1}{2}\big(-\varepsilon^2\beta - (-1)^j\sqrt{\varepsilon^4\beta^2 - 4\alpha}\big), \quad j = 1, 2, \tag{28}$$

are the roots of $P_r(\kappa)$*, and*

$$q_j = \tfrac{1}{2}\big(1 + (-1)^j\frac{\varepsilon^2\beta}{\sqrt{\varepsilon^4\beta^2 - 4\alpha}}\big), \quad j = 1, 2, \tag{29}$$

are the corresponding residues of $\dfrac{\kappa}{P_r(\kappa)}$.

As a consequence of Proposition 6.1 we can now discuss the various regimes.

The exponential regime

According to the heuristics, if we set $\alpha = b\varepsilon^p$, $b > 0$, then for $p \in [0, 4)$ the decay law is still exponential. Notice that as $\varepsilon \to 0$ we have $\varepsilon^2/\sqrt{\alpha} \simeq \varepsilon^{2-\frac{p}{2}}$.

Proposition 6.2. *(i) For* $p \in [0, 4)$*:*

$$\hat{A}_{\varepsilon,r}(t) = 2q_2 e^{i\kappa_2^2 t} - \frac{\beta}{2}\frac{\varepsilon^2}{\sqrt{\alpha}}\overline{\mathscr{I}_3(i\sqrt{\alpha t})} + \mathscr{O}(\varepsilon^{4-p}), \tag{30}$$

and up to error terms as in Theorem 5.1 we have $A_\varepsilon(t) = \hat{A}_{\varepsilon,r}(t)$.
(ii) For $p \in (0, 4)$ *we have* $|A_\varepsilon(t)|^2 = e^{-2|g_1|b^{1/2}\varepsilon^{2+\frac{p}{2}}t}$*, up to errors vanishing as* $\varepsilon \to 0$.

Note that the exponential law becomes less and less accurate due to the error term, as p approaches 4 from below. Thus one needs to compute corrections. Proposition 6.2 gives only the first order correction in $\varepsilon^2/\sqrt{\alpha}$, but the method of proof provides also the higher order corrections. Due to Eq. (6) and Eq. (7) we have (see [25] for the notation)

$$|g_1|b^{1/2}\varepsilon^{2+\frac{p}{2}} = |I(x_0)| = \pi\varepsilon^2\langle\Psi_0, WQ^*\delta(H_{\rm op} - x_0)QW\Psi_0\rangle$$

to leading order in ε, and the exponential decay is correctly described by the "modified FGR", in which one uses the standard formula, but computed at the position x_0 of the resonance, instead of at E_0.

The bound state regime

If $\alpha = -b\varepsilon^p$, $b > 0$, then for $p \in [0, 4)$ one expects (see the heuristics) a bound state regime, i.e. to leading order the contribution comes from the bound state. The result below provides the mathematical substantiation as well as the first order correction. Again, the proof gives the means to compute higher order corrections.

As in the previous case, as $\varepsilon \to 0$, we have $\varepsilon^2/\sqrt{|\alpha|} \simeq \varepsilon^{2-\frac{p}{2}}$. Note that $\kappa_1 > 0$, and there is a contribution from the pole of $\dfrac{1}{H_r(z)}$ at $x_b = -\kappa_1^2$.

Proposition 6.3.

$$\hat{A}_{\varepsilon,r}(t) = -i\frac{\beta}{2}\frac{\varepsilon^2}{\sqrt{|\alpha|}}\mathscr{I}_3(i\sqrt{|\alpha|t}) + \mathscr{O}(\varepsilon^{(4-p)}), \tag{31}$$

and up to error terms as in Theorem 5.1 we have

$$A_\varepsilon(t) = \hat{A}_{\varepsilon,r}(t) + \Big(1 - i\frac{\beta}{2}\frac{\varepsilon^2}{\sqrt{|\alpha|}}\Big)e^{i\kappa_1^2 t}. \tag{32}$$

To leading order one obtains the bound state behavior $|A_\varepsilon(t)|^2 = 1$.

The non-exponential regime

We come now to the most interesting part of our analysis, when

$$|\alpha| = b\varepsilon^p, \quad b > 0, \quad \text{with} \quad p \geq 4. \tag{33}$$

According to the heuristics, for these values of p the decay law is neither (quasi)-exponential nor bound state like. We consider two cases separately.

Case 1: The threshold regime given by $p > 4$.

In this case the survival probability amplitude is given by

Proposition 6.4. *Up to errors as in Theorem 5.1 we have*

$$A_\varepsilon(t) = e^{is}\big(1 - \mathrm{erf}(e^{i\pi/4}s^{1/2})\big) + \mathscr{O}(\varepsilon^{p-4}), \tag{34}$$

where $\mathrm{erf}(u)$ *is the usual error function [1] and* $s = \beta^2\varepsilon^4 t$.

The result Eq. (34) implies that the decay law is non-exponential for all $p > 4$, and that the leading term is independent of α and equals the threshold case $x_0 = 0$. It follows also that the threshold decay time scale in the regular case is $t \sim \varepsilon^{-4}$ for all $p > 4$. Note that the "modified FGR" gives a decay time scale $t \sim \varepsilon^{-(2+\frac{p}{2})}$, such that in this case it breaks down even at the time scale level.

Case 2: The "crossover regime", which is given by $p = 4$.

In this case, in scaled variables $s = \varepsilon^4\beta^2 t$, $\quad f = \dfrac{\alpha}{\varepsilon^4\beta^2}$ (note that for $p = 4$, f =const.), we have directly from Eq. (24) and Eq. (21):

$$\hat{A}_\varepsilon(t) = \frac{1}{\pi}\int_0^\infty \frac{y^{1/2}}{(f-y)^2 + y}e^{-isy}dy, \tag{35}$$

and the integral has been analyzed numerically in [7]. The decay law is non-exponential for finite f, while as $f \to \pm\infty$, one reaches the exponential and bound state behaviour, respectively.

We illustrate the two cases discussed above. In case 1 a plot of the leading term in $|A_\varepsilon(t)|^2$ is given in Fig. 1. In Fig. 2 we have illustrated case 2, for negative values of the parameter f. In Fig. 3 the same for positive values of f. In Fig. 4 we have taken $f = 24$. It is clear from this logarithmic plot that the decay law is exponential initially.

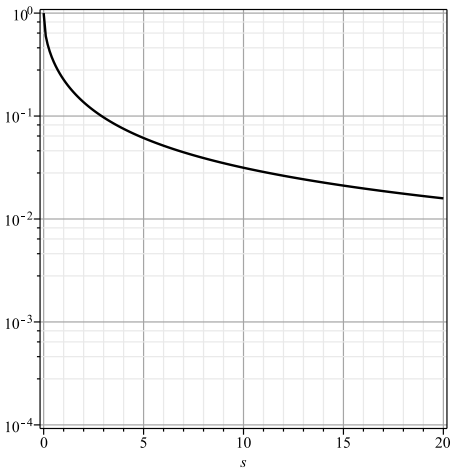

Fig. 1. Plot of the leading term in $|A_\varepsilon(t)|^2$ from Proposition 6.4. Vertical scale is logarithmic.

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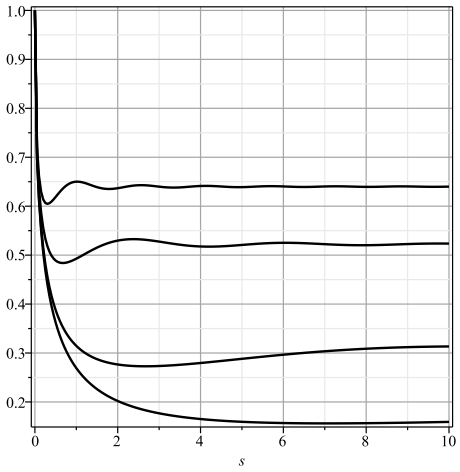

Fig. 2. Plot of the leading term in $|A_\varepsilon(t)|^2$ in case 2, $f = -6, -3, -1, -0.5$, from top to bottom. Vertical scale is linear.

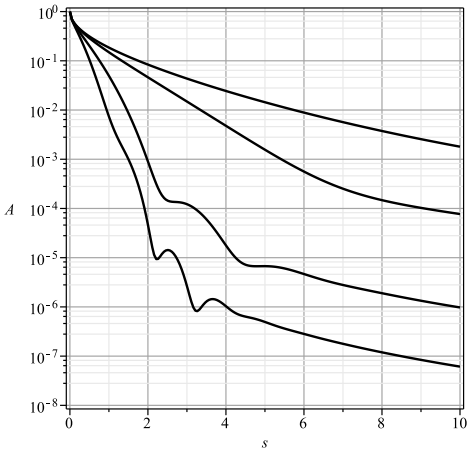

Fig. 3. Plot of the leading term in $|A_\varepsilon(t)|^2$ in case 2, $f = 0.5, 1, 3, 6$ from top to bottom. Vertical scale is logarithmic.

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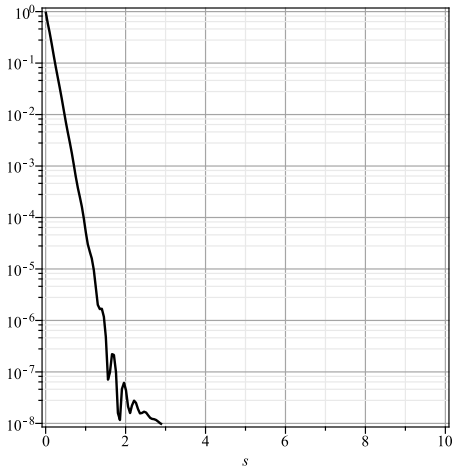

Fig. 4. Plot of the leading term in $|A_\varepsilon(t)|^2$ in case 2, $f = 24$. Vertical scale is logarithmic.

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LOCALIZATION FOR THE RANDOM DISPLACEMENT MODEL

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Dedicated to Ari Laptev on the occasion of his sixtieth birthday

This is a summary of recent work, jointly with J. Baker, F. Klopp and S. Nakamura, concerning the random displacement model resulting in a proof of localization near the edge of the deterministic spectrum. Localization is meant in both senses, pure point spectrum with exponentially decaying eigenfunctions as well as dynamical localization. The proof relies on a well established multiscale analysis and the main problem is to verify the necessary ingredients, such as a Lifshitz tail estimate and a Wegner estimate.

Keywords: Random Schrödinger operators.

1. Introduction

The random displacement model (RDM) is a natural way to model a solid with structural disorder. We assume that the Hamiltonian for a particle moving in such a disordered environment is given by

$$H_\omega = -\Delta + V_\omega \tag{1}$$

in $L^2(\mathbb{R}^d)$, $d \geq 1$, where the random potential has the form

$$V_\omega(x) = \sum_{i \in \mathbb{Z}^d} q(x - i - \omega_i). \tag{2}$$

Thus, the potential is a perturbation of the periodic potential $\sum_i q(x - i)$, i.e., the potential at each site is centered at the lattice point in $\mathbb{Z}^d$. The parameter $\omega = (\omega_i)_{i \in \mathbb{Z}^d}$ describes the displacements of the potential from the periodic configuration. The goal, broadly speaking, is to prove localization for H_ω for some suitable distributions of the displacements. This problem is markedly different from the more standard Anderson model in which the positions of the potentials are fixed but the coupling constants are random.

One avenue to prove localization has been opened by the pioneering paper of Fröhlich and Spencer [6], in which they introduced a multiscale technique for proving localization. These techniques have been improved and simplified by a number of authors and the exposition in [7] represents the latest development of this approach. There exists also another technique due to Aizenman and Molchanov [2] that has been extended to the continuum in [1], but we do not know how to apply this method to the problem at hand. The multiscale analysis starts with three basic ingredients. One is the determination of the edge of the almost sure spectrum of the Schrödinger operator. In a next step one proves a Lifshitz tail estimate, ensuring that, on average, there are very few eigenvalues near the edge for a fixed length scale and then using a Wegner estimate that ensures that there are, on average, very few eigenvalues in resonance as one boosts up the scale. Thus, one has to provide the three main ingredients, determining the edge of the almost sure spectrum, proving a Lifshitz tail, and finally, the most difficult one, proving a Wegner estimate. In the following we will relate some rough ideas that make the three ingredients palpable and refer the reader to various papers for details. In particular we will not say anything about the multiscale analysis. The reader may consult the original papers such as [7] and, for a very readable account with weaker results, the book of Stollmann [11]. Concerning the potential q we make the following assumptions.

Assumption 1: *The potential q has the same reflection symmetries as the lattice. It is C^∞ and compactly supported so that the open region*

$$G = \{a \in \mathbb{R}^d : \text{supp } q(\cdot - a)\} \subset \Lambda_1$$

is not empty. Here Λ_1 is the open unit cube centered at the origin. Note that, on account of the symmetry conditions on the potential, G is an open cube centered at the origin, $(-r, r)^d$. For technical reasons we require that this cube be large enough, namely that $r > \frac{1}{4}$. The last condition is the most peculiar and it is given in terms of the Neumann problem

$$\begin{cases} -\Delta u_0(x;a) + q(\cdot - a)u_0(x;a) = E_0(a)u_0(x;a) & x \in \Lambda_1 \\ \frac{\partial u_0(x;a)}{\partial n} = 0 & x \in \partial\Lambda_1. \end{cases}$$

Here, $E_0(a)$ is the smallest eigenvalue and $u_0(x;a)$ the corresponding eigenfunction which we can choose to be positive. We shall assume that the potential is such that $E_0(a)$ does not vanish identically for $a \in G$.

The last condition is certainly satisfied for sign definite potentials. It can be violated by choosing a positive function $\phi(x)$ which is constant near the boundary $\partial\Lambda_1$ and then define the potential $q(x)$ by setting

$$q(x-a) = \frac{\Delta\phi(x-a)}{\phi(x-a)} \ ,$$

as long as supp $q(\cdot - a) \subset \Lambda_1$. It is easy to see that the lowest eigenvalue $E_0(a)$ vanishes identically for $a \in G$. In case that the complement of the support of the potential is connected it is not very difficult to see the converse, namely that if the eigenvalue $E_0(a)$ vaninhes identically in G, then $u_0(x;a)$ must be constant in the

complement of the support of the potential. The following result was proven in [9] based on previous work in [3].

Theorem 1.1. *Under the above assumptions on the potential q, the function $E_0(a_1, a_2, \ldots, a_d)$ is in each variable a symmetric and strictly unimodal function. More precisely, for any $a_j, 1 \leq j \leq d$ and for all the other variables fixed, consider the function*

$$f_0(a_j) := E_0(a_1, \ldots, a_j, \ldots, a_d) \ .$$

Then f is a strictly decreasing function for $a_j > 0$ and strictly increasing for $a_j < 0$ in the sense that $f'(a_j) < 0$ for all $a_j \in (0, r]$ and $f'(a_j) > 0$ for all $a_j \in [-r, 0)$.

A first consequence of this theorem is that it can be used to determine the configuration of potentials that minimize $\inf(\sigma(H_\omega))$.

Corollary 1.1. *We have that*

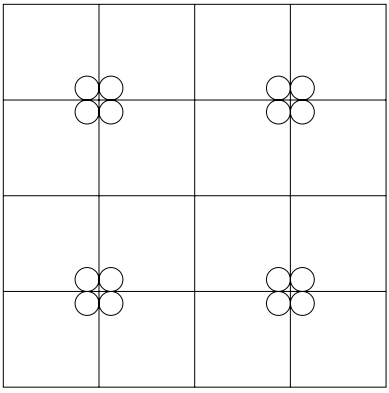
$$\inf_\omega \inf(\sigma(H_\omega)) = \inf(\sigma(H_{\overline{\omega}}),$$

where $\overline{\omega} = (\overline{\omega}_i)_{i \in \mathbb{Z}^d}$ and

$$\overline{\omega}_i = ((-1)^{i_1} r, (-1)^{i_2} r, \ldots, (-1)^{i_d} r),$$

where $i = (i_1, i_2, \ldots, i_d) \in \mathbb{Z}^d$.

The figure below (taken from [9]) shows the energy minimizing configuration for $d = 2$.



We are ready to state our assumptions on the randomness.

Assumption 2: *The variables ω_i are independent and identically distributed with the common distribution μ. We assume that*

$$\text{supp } \mu \subset [-r, r]^d$$

and the corners are in the support of μ. Moreover, we require that near the corners the measure has a density which is C^1. Otherwise, the measure can be arbitrary. We set $\mathbb{P} = \otimes_{\mathbb{Z}^d} \mu$.

The random operator H_ω is ergodic with respect to shifts in $\mathbb{Z}^d$, and, as a consequence of the general theory of ergodic operators, there exists a set Σ such that

$$\sigma(H_\omega) = \Sigma \text{ almost surely .}$$

A further consequence is that

$$E_0 := \inf \Sigma = \inf \sigma(H_{\overline{\omega}}).$$

Our main theorem, proved in [9], is:

Theorem 1.2. *Assume that $d \geq 2$, ω and q satisfy Assumptions 1 and 2. Then there exists $\delta > 0$ such that, almost surely, H_ω has pure point spectrum in $I = [E_0, E_0+\delta]$ 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*

$$\mathbb{E}\left(\sup_t \|\chi_x e^{-itH_\omega}\chi_I(H_\omega)\chi_y\|_2^2\right) \leq Ce^{-|x-y|^\zeta} \tag{3}$$

for all $x, y \in \mathbb{Z}^d$. Here χ_x denotes the characteristic functions of the unit cube centered at x and χ_I the characteristic function of the interval I.

2. Lifshitz tail estimates

For a non-negative integer L, let $\Lambda_{2L+1} = (-L - 1/2, L + 1/2)^d$ and $H_{\omega,L}$ the restriction of H_ω to Λ_L with Neumann boundary conditions. Also, let $\Lambda'_{2L+1} = \mathbb{Z}^d \cap \Lambda_{2L+1}$. We denote by $\mathbb{P}_L = \otimes_{i\in\Lambda'_{2L+1}}\mu(d\omega_i)$ and the integrated density of states is given

$$N(E) = \lim_{L\to\infty} \mathbb{E}_{\mathbb{P}_L}\left[\frac{\#\{\text{eigenvalues of } H_{L,\omega} < E\}}{(2L+1)^d}\right] .$$

On account of the ergodicity one can show that

$$N(E) = \lim_{L\to\infty}\left[\frac{\#\{\text{eigenvalues of } H_{L,\omega} < E\}}{(2L+1)^d}\right] \text{ almost surely.}$$

The following theorem was proved in [8] using results of [4].

Theorem 2.1. *Let $d \geq 2$. There exist $C < \infty$ and $\mu > 1$ such that, for all L,*

$$\mathbb{P}_L(H_{\omega,L} \text{ has an eigenvalue less than } E_0 + C/L^2) \leq L^d\mu^{-L}.$$

This estimate implies the following estimate on the integrated density of states

$$\lim_{E\downarrow E_0} \frac{\log|\log(N(E))|}{\log|E - E_0|} \leq -\frac{1}{2} . \tag{4}$$

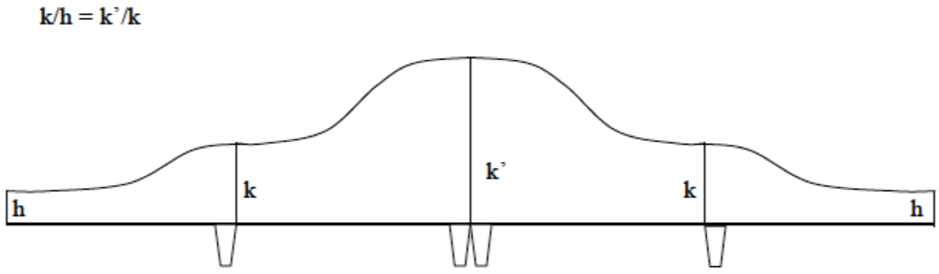
Estimate (4) is sometimes referred to as a weak Lifshitz tail (the stronger classical Lifshitz tail known from the Anderson model has right hand side $-d/2$). It says in essence that the probability that there are eigenvalues close to E_0 is very small. Note that it is crucial that the dimension $d \geq 2$. In one dimension, there are no Lifshitz tails. In fact one has the

Theorem 2.2. *Let H_ω be a one dimensional random displacement model. Then for μ the Bernoulli measure with equal weights in the endpoints r and $-r$,*

$$N(E) \geq \frac{C}{(\log(E - E_0))^2}$$

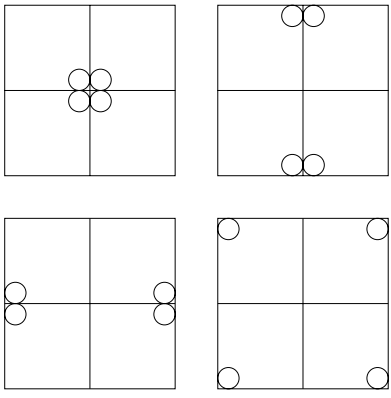
for some $C > 0$ and E close to E_0, i.e., no Lifshitz tails.

A proof of this theorem can be found in [4]. The reason for this rather different behavior is that the minimizing energy configuration is not unique. The figure below provides the intuition. It is a graph of the ground state wave function for an arrangement of the potentials in a Neumann problem. The potentials are arranged the 'wrong' way (not alternating between right and left), but nevertheless the Hamiltonian has the same ground state energy as the one with the 'correct' arrangement of the potentials. By scaling the wave function of unit cells, one can paste together the ground state wave function for any arrangement of the potentials without gaining energy, as long as the number of steps up is the same as the steps down (which allows for periodic extension).

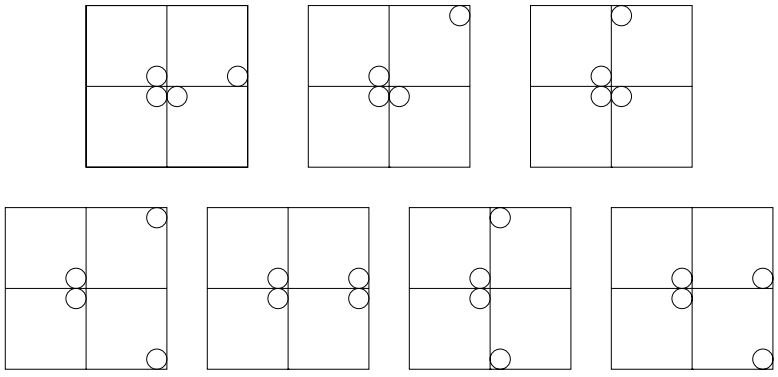


Despite this lack of Lifshitz tails, it has has been proved in [5] and also in [10], that there is localization in one dimension.

The situation is entirely different in dimension 2 and higher. Again, pictures explain the situation. The 'correct' arrangements of the potentials, i.e., those that minimize the lowest eigenvalue for the 2×2-Neumann problem, are shown in the following figure taken from [8].



For these four arrangements a number of 'wrong' arrangements are given by the figure



It was shown in [4] that these latter configurations have a strictly higher ground state energy than the ones in the previous figure. The proof of Lifshitz tails for the random displacement model proceeds now in two steps. First one proves the Lifshitz tail behavior for Bernoulli distributions with non-zero weights in the corners. This has been achieved in [8] and is by no means trivial. The idea is, roughly, to estimate that with overwhelming probability, there must be a 'wrong' configuration, i.e., a configuration from the second picture above, in each quasi-one-dimensional $2^{d-1}\times(2L+1)$ band for the Hamiltonian $H_{L,\omega}$. Using the fact that this configuration has a higher energy than the ones from picture (a) it is shown that the ground state energy is raised by an amount $\frac{\text{const.}}{L^2}$. Thus the probability is small that an eigenvalue of $H_{L,\omega}$ is larger than $E_0+\frac{C}{L^2}$ where C is some constant. In a further nontrivial step, using the energy estimate in Theorem 1.1 one can prove the Lifshitz tail estimate Theorem 2.1. That the right hand side in (4) is $-1/2$, and not $-d/2$, is related to the fact that one breaks up the problem into one-dimensional ones. One would expect that the correct behavior is $-d/2$, but this is an open problem. In any case it is immaterial for the proof of localization.

3. Wegner estimate

More involved is the proof of the Wegner estimate. The following theorem is proved in [9].

Theorem 3.1. *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 $L\in\mathbb{N}$,*

$$\mathbb{E}_{\mathbb{P}_L}(\operatorname{Tr}\chi_I(H_{\omega,L}))\le C_\alpha|I|^\alpha L^d.$$

The idea that such an estimate holds has to do with the fact that eigenvalues move when the potential is changed. This is the case in the Anderson model with a sign definite potential, where one can use first order perturbation theory to see that the eigenvalues move monotonically. This allows to conclude that the average density of the eigenvalues is small. For the random displacement model there is no monotonicity in the higher eigenvalues. One can expect, however, that the low lying

spectrum moves up as the potentials move away from the corners. If we introduce

$$\partial'_{c,\omega_i} H_\omega = \partial'_{c,\omega_i} q(\cdot - i - \omega_i) = -\eta(|c(\omega_i) - \omega_i|) \frac{c(\omega_i) - \omega_i}{|c(\omega_i) - \omega_i|} \cdot (\nabla q)(\cdot - i - \omega_i),$$

where η is a smooth cutoff function so that $\eta(|c(\omega_i) - \omega_i|)$ lives near the corner $c(\omega_i)$ nearest to the point ω_i then we have

Proposition 3.1. *There exist $\delta_1 > 0$ and $\delta_2 > 0$ such that*

$$-\sum_{i \in \Lambda'_{2L+1}} \langle \psi, (\partial'_{c,\omega_i} H_{\omega,L}) \psi \rangle \geq \delta_1 \|\psi\|^2$$

for all $L \in \mathbb{N}$, and $\psi \in H^1(\Lambda_{2L+1})$ with $\langle \psi, (H_{\omega,L} - E_0)\psi \rangle \leq \delta_2 \|\psi\|^2$.

Theorem 1.1 is again an important ingredient for this result. The details of the proof of this key estimate as well as the ensuing proof of Theorem 3.1 are quite involved and we refer the reader to the paper [9].

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CONTRIBUTED TALKS

LARGE TIME BEHAVIOR OF THE HEAT KERNEL OF TWO-DIMENSIONAL MAGNETIC SCHRÖDINGER OPERATORS AND ITS APPLICATIONS

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We study the heat semigroup generated by two-dimensional Schrödinger operators with compactly supported magnetic field. We show that if the field is radial, then the large time behavior of the associated heat kernel is determined by its total flux. We also discuss some applications to eigenvalue estimates for magnetic Schrödinger operators in two dimensions.

CALOGERO-SUTHERLAND TYPE SYSTEMS AND CONFORMAL FIELD THEORY

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I plan to give a general introduction to Calogero-Sutherland type systems. I also plan to present some of our own results, including the solution of the elliptic Calogero-Sutherland model and recent generalizations of this work.

Spectral theory

Session organizer:

Michael Loss

EXTREMAL FUNCTIONS IN SOME INTERPOLATION INEQUALITIES: SYMMETRY, SYMMETRY BREAKING AND ESTIMATES OF THE BEST CONSTANTS

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This contribution is devoted to a review of some recent results on existence, symmetry and symmetry breaking of optimal functions for Caffarelli-Kohn-Nirenberg (CKN) and weighted logarithmic Hardy (WLH) inequalities. These results have been obtained in a series of papers [1–5] in collaboration with M. del Pino, S. Filippas, M. Loss, G. Tarantello and A. Tertikas and are presented from a new viewpoint.

Keywords: Caffarelli-Kohn-Nirenberg inequality; Gagliardo-Nirenberg inequality; logarithmic Hardy inequality; logarithmic Sobolev inequality; extremal functions; radial symmetry; symmetry breaking; Emden-Fowler transformation; linearization; existence; compactness; optimal constants.

1. Two families of interpolation inequalities

Let $d \in \mathbb{N}^*$, $\theta \in [0,1]$, consider the set $\mathscr{D}$ of all smooth functions which are compactly supported in $\mathbb{R}^d \setminus \{0\}$ and define $\vartheta(d,p) := d\,\frac{p-2}{2\,p}$, $a_c := \frac{d-2}{2}$, $\Lambda(a) := (a-a_c)^2$ and $p(a,b) := \frac{2\,d}{d-2+2\,(b-a)}$. We shall also set $2^* := \frac{2\,d}{d-2}$ if $d \ge 3$ and $2^* := \infty$ if $d = 1$ or 2. For any $a < a_c$, we consider the two families of interpolation inequalities:

(CKN) *Caffarelli-Kohn-Nirenberg inequalities* [3, 4, 6] – Let $b \in (a+1/2, a+1]$ and $\theta \in (1/2,1]$ if $d = 1$, $b \in (a, a+1]$ if $d = 2$ and $b \in [a, a+1]$ if $d \ge 3$. Assume that $p = p(a,b)$, and $\theta \in [\vartheta(d,p),1]$ if $d \ge 2$. There exists a finite positive constant $\mathsf{C}_{\rm CKN}(\theta,p,a)$ such that, for any $u \in \mathscr{D}$,

$$\||x|^{-b}\,u\|^2_{\mathrm{L}^p(\mathbb{R}^d)} \le \mathsf{C}_{\rm CKN}(\theta,p,a)\,\||x|^{-a}\,\nabla u\|^{2\,\theta}_{\mathrm{L}^2(\mathbb{R}^d)}\,\||x|^{-(a+1)}\,u\|^{2\,(1-\theta)}_{\mathrm{L}^2(\mathbb{R}^d)}\,.$$

(WLH) *Weighted logarithmic Hardy inequalities* [3, 4] – Let $\gamma \ge d/4$ and $\gamma > 1/2$ if $d = 2$. There exists a positive constant $\mathsf{C}_{\rm WLH}(\gamma,a)$ such that, for any $u \in \mathscr{D}$, normalized by $\||x|^{-(a+1)}\,u\|_{\mathrm{L}^2(\mathbb{R}^d)} = 1$,

$$\int_{\mathbb{R}^d} \frac{|u|^2\,\log\left(|x|^{d-2-2\,a}\,|u|^2\right)}{|x|^{2\,(a+1)}}\,dx \le 2\,\gamma\,\log\Big[\mathsf{C}_{\rm WLH}(\gamma,a)\,\|\,|x|^{-a}\,\nabla u\|^2_{\mathrm{L}^2(\mathbb{R}^d)}\Big]\,.$$

According to [3, 4], (WLH) appears as a limiting case of (CKN) with $\theta = \gamma\,(p-2)$ as $p \to 2_+$. By a standard completion argument, these inequalities can be extended to

the set $\mathscr{D}_a^{1,2}(\mathbb{R}^d) := \{u \in \mathrm{L}^1_{\rm loc}(\mathbb{R}^d) : |x|^{-a}\,\nabla u \in \mathrm{L}^2(\mathbb{R}^d)$ *and* $|x|^{-(a+1)}\,u \in \mathrm{L}^2(\mathbb{R}^d)\}$. We shall assume that all constants in the inequalities are taken with their optimal values. For brevity, we shall call *extremals* the functions which realize equality in (CKN) or in (WLH).

Let $\mathsf{C}^*_{\rm CKN}(\theta,p,a)$ and $\mathsf{C}^*_{\rm WLH}(\gamma,a)$ denote the optimal constants when admissible functions are restricted to the radial ones. *Radial extremals* are explicit and the values of the constants, $\mathsf{C}^*_{\rm CKN}(\theta,p,a)$ and $\mathsf{C}^*_{\rm WLH}(\gamma,a)$, are known: see [3]. Moreover, we have

$$\begin{aligned}&\mathsf{C}_{\rm CKN}(\theta,p,a) \ge \mathsf{C}^*_{\rm CKN}(\theta,p,a) = \mathsf{C}^*_{\rm CKN}(\theta,p,a_c-1)\,\Lambda(a)^{\frac{p-2}{2p}-\theta}\,,\\ &\mathsf{C}_{\rm WLH}(\gamma,a) \ge \mathsf{C}^*_{\rm WLH}(\gamma,a) = \mathsf{C}^*_{\rm WLH}(\gamma,a_c-1)\,\Lambda(a)^{-1+\frac{1}{4\,\gamma}}\,.\end{aligned} \tag{1}$$

Radial symmetry for the extremals of (CKN) and (WLH) implies that $\mathsf{C}_{\rm CKN}(\theta,p,a) = \mathsf{C}^*_{\rm CKN}(\theta,p,a)$ and $\mathsf{C}_{\rm WLH}(\gamma,a) = \mathsf{C}^*_{\rm WLH}(\gamma,a)$, while *symmetry breaking* only means that inequalities in (1) are strict.

2. Existence of extremals

Theorem 2.1. *Equality in (CKN) is attained for any $p \in (2,2^*)$ and $\theta \in (\vartheta(p,d),1)$ or $\theta = \vartheta(p,d)$, $d \ge 2$, and $a \in (a_\star^{\rm CKN}, a_c)$, for some $a_\star^{\rm CKN} < a_c$. It is not attained if $p = 2$, or $a < 0$, $p = 2^*$, $\theta = 1$ and $d \ge 3$, or $d = 1$ and $\theta = \vartheta(p,1)$.*

Equality in (WLH) is attained if $\gamma \ge 1/4$ and $d = 1$, or $\gamma > 1/2$ if $d = 2$, or for $d \ge 3$ and either $\gamma > d/4$ or $\gamma = d/4$ and $a \in (a_\star^{\rm WLH}, a_c)$, where $a_\star^{\rm WLH} := a_c - \sqrt{\Lambda_\star^{\rm WLH}}$ and $\Lambda_\star^{\rm WLH} := (d-1)\,e\,(2^{d+1}\,\pi)^{-1/(d-1)}\,\Gamma(d/2)^{2/(d-1)}$.

These results have been obtained in [4]. Let us give some hints on how to prove such a result. Consider first Gross' logarithmic Sobolev inequality in Weissler's form (as in [7])

$$\int_{\mathbb{R}^d} |u|^2\,\log|u|^2\,dx \le \frac{d}{2}\,\log\Big(\mathsf{C}_{\rm LS}\,\|\nabla u\|^2_{\mathrm{L}^2(\mathbb{R}^d)}\Big) \quad \forall\, u \in \mathrm{H}^1(\mathbb{R}^d) \text{ s.t. } \|u\|_{\mathrm{L}^2(\mathbb{R}^d)} = 1\,.$$

The function $u(x) = (2\,\pi)^{-d/4}\,\exp(-|x|^2/4)$ is an extremal for such an inequality. By taking $u_n(x) := u(x + n\,\mathsf{e})$ for some $\mathsf{e} \in \mathbb{S}^{d-1}$ and any $n \in \mathbb{N}$ as test functions for (WLH), and letting $n \to +\infty$, we find that $\mathsf{C}_{\rm LS} \le \mathsf{C}_{\rm WLH}(d/4,a)$. If equality holds, this is a mechanism of loss of compactness for minimizing sequences. On the opposite, if $\mathsf{C}_{\rm LS} < \mathsf{C}_{\rm WLH}(d/4,a)$, which is the case if $a \in (a_\star^{\rm WLH}, a_c)$ where $a_\star^{\rm WLH} = a$ is given by the condition $\mathsf{C}_{\rm LS} = \mathsf{C}^*_{\rm WLH}(d/4,a)$, we can establish a compactness result which proves that equality is attained in (WLH) in the critical case $\gamma = d/4$.

A similar analysis for (CKN) shows that $\mathsf{C}_{\rm GN}(p) \le \mathsf{C}_{\rm CKN}(\theta,p,a)$ in the critical case $\theta = \vartheta(p,d)$, where $\mathsf{C}_{\rm GN}(p)$ is the optimal constant in the Gagliardo-Nirenberg-Sobolev interpolation inequalities

$$\|u\|^2_{\mathrm{L}^p(\mathbb{R}^d)} \le \mathsf{C}_{\rm GN}(p)\,\|\nabla u\|^{2\,\vartheta(p,d)}_{\mathrm{L}^2(\mathbb{R}^d)}\,\|u\|^{2\,(1-\vartheta(p,d))}_{\mathrm{L}^2(\mathbb{R}^d)} \quad \forall\, u \in \mathrm{H}^1(\mathbb{R}^d)$$

and $p \in (2,2^*)$ if $d = 2$ or $p \in (2,2^*]$ if $d \ge 3$. However, extremals are not known explicitly in such inequalities if $d \ge 2$, so we cannot get an explicit interval of existence in terms of a, even if we also know that compactness of minimizing sequences

for (CKN) holds when $\mathsf{C}_{\rm GN}(p) < \mathsf{C}_{\rm CKN}(\vartheta(p,d),p,a)$. This is the case if $a > a_\star^{\rm CKN}$ where $a = a_\star^{\rm CKN}$ is defined by the condition $\mathsf{C}_{\rm GN}(p) = \mathsf{C}^*_{\rm CKN}(\vartheta(p,d),p,a)$.

It is very convenient to reformulate (CKN) and (WLH) inequalities in cylindrical variables as in [8]. By means of the Emden-Fowler transformation

$$s = \log|x| \in \mathbb{R}\,, \quad \omega = x/|x| \in \mathbb{S}^{d-1}\,, \quad y = (s,\omega)\,, \quad v(y) = |x|^{a_c-a}\,u(x)\,,$$

(CKN) for u is equivalent to a Gagliardo-Nirenberg-Sobolev inequality on the cylinder $\mathscr{C} := \mathbb{R}\times\mathbb{S}^{d-1}$ for v, namely

$$\|v\|^2_{\mathrm{L}^p(\mathscr{C})} \le \mathsf{C}_{\rm CKN}(\theta,p,a)\left(\|\nabla v\|^2_{\mathrm{L}^2(\mathscr{C})} + \Lambda\,\|v\|^2_{\mathrm{L}^2(\mathscr{C})}\right)^\theta \|v\|^{2\,(1-\theta)}_{\mathrm{L}^2(\mathscr{C})} \quad \forall\, v\in \mathrm{H}^1(\mathscr{C})$$

with $\Lambda = \Lambda(a)$. Similarly, with $w(y) = |x|^{a_c-a}\,u(x)$, (WLH) is equivalent to

$$\int_{\mathscr{C}} |w|^2\,\log|w|^2\,dy \le 2\,\gamma\,\log\left[\mathsf{C}_{\rm WLH}(\gamma,a)\left(\|\nabla w\|^2_{\mathrm{L}^2(\mathscr{C})}+\Lambda\right)\right]$$

for any $w\in\mathrm{H}^1(\mathscr{C})$ such that $\|w\|_{\mathrm{L}^2(\mathscr{C})}=1$. Notice that radial symmetry for u means that v and w depend only on s.

Consider a sequence $(v_n)_n$ of functions in $\mathrm{H}^1(\mathscr{C})$, which minimizes the functional

$$\mathscr{E}^p_{\theta,\Lambda}[v] := \left(\|\nabla v\|^2_{\mathrm{L}^2(\mathscr{C})}+\Lambda\,\|v\|^2_{\mathrm{L}^2(\mathscr{C})}\right)^\theta \|v\|^{2\,(1-\theta)}_{\mathrm{L}^2(\mathscr{C})}$$

under the constraint $\|v_n\|_{\mathrm{L}^p(\mathscr{C})}=1$ for any $n\in\mathbb{N}$. As quickly explained below, if bounded, such a sequence is relatively compact and converges up to translations and the extraction of a subsequence towards a minimizer of $\mathscr{E}^p_{\theta,\Lambda}$.

Assume that $d\ge 3$, let $t := \|\nabla v\|^2_{\mathrm{L}^2(\mathscr{C})}/\|v\|^2_{\mathrm{L}^2(\mathscr{C})}$ and $\Lambda=\Lambda(a)$. If v is a minimizer of $\mathscr{E}^p_{\theta,\Lambda}[v]$ such that $\|v\|_{\mathrm{L}^p(\mathscr{C})}=1$, then we have

$$(t+\Lambda)^\theta = \mathscr{E}^p_{\theta,\Lambda}[v]\,\frac{\|v\|^2_{\mathrm{L}^p(\mathscr{C})}}{\|v\|^2_{\mathrm{L}^2(\mathscr{C})}} = \frac{\|v\|^2_{\mathrm{L}^p(\mathscr{C})}}{\mathsf{C}_{\rm CKN}(\theta,p,a)\,\|v\|^2_{\mathrm{L}^2(\mathscr{C})}} \le \frac{\mathsf{S}_d^{\vartheta(d,p)}}{\mathsf{C}_{\rm CKN}(\theta,p,a)}\,\left(t+a_c^2\right)^{\vartheta(d,p)}$$

where $\mathsf{S}_d = \mathsf{C}_{\rm CKN}(1,2^*,0)$ is the optimal Sobolev constant, while we know from (1) that $\lim_{a\to a_c}\mathsf{C}_{\rm CKN}(\theta,p,a)=\infty$ if $d\ge 2$. This provides a bound on t if $\theta>\vartheta(p,d)$. An estimate can be obtained also for v_n, for n large enough, and standard tools of the concentration-compactness method allow to conclude that, up to a subsequence, $(v_n)_n$ converges towards an extremal. A similar approach holds for (CKN) if $d=2$, or for (WLH).

The above variational approach also provides an existence result of extremals for (CKN) in the critical case $\theta=\vartheta(p,d)$, if $a\in(a_1,a_c)$ where $a_1 := a_c-\sqrt{\Lambda_1}$ and $\Lambda_1 = \min\{(\mathsf{C}^*_{\rm CKN}(\theta,p,a_c-1)^{1/\theta}/\,\mathsf{S}_d)^{d/(d-1)}, (a_c^2\,\mathsf{S}_d/\mathsf{C}^*_{\rm CKN}(\theta,p,a_c-1)^{1/\theta})^d$.

If symmetry is known, then there are (radially symmetric) extremals; see [3]. Anticipating on the results of the next section, we can state the following result which arises as a consequence of Schwarz' symmetrization method (see Theorem 3.2, below). The following result has been established in [5].

Proposition 2.1. *Let $d\ge 3$. Then (CKN) with $\theta=\vartheta(p,d)$ admits a radial extremal if $a\in[a_0,a_c)$ where $a_0 := a_c-\sqrt{\Lambda_0}$ and $\Lambda=\Lambda_0$ is defined by the condition $\Lambda^{(d-1)/d} = \vartheta(p,d)\,\mathsf{C}^*_{\rm CKN}(\theta,p,a_c-1)^{1/\vartheta(d,p)}/\,\mathsf{S}_d$.*

A similar estimate also holds if $\theta>\vartheta(d,p)$, with less explicit computations; see [5].

3. Symmetry and symmetry breaking

Define

$$\underline{a}(\theta,p) := a_c - \tfrac{2\sqrt{d-1}}{p+2}\sqrt{\tfrac{2\,p\,\theta}{p-2}-1}\,, \quad \tilde{a}(\gamma) := a_c - \tfrac{1}{2}\sqrt{(d-1)(4\,\gamma-1)}\,,$$
$$\Lambda_{\rm SB}(\gamma) := \tfrac{1}{8}\,(4\,\gamma-1)\,e\,\big(\tfrac{\pi^{4\,\gamma-d-1}}{16}\big)^{\frac{1}{4\,\gamma-1}}\,\big(\tfrac{d}{\gamma}\big)^{\frac{4\,\gamma}{4\,\gamma-1}}\,\Gamma\,\big(\tfrac{d}{2}\big)^{\frac{2}{4\,\gamma-1}}\,.$$

Theorem 3.1. *Let $d \ge 2$ and $p \in (2, 2^*)$. Symmetry breaking holds in (CKN) if either $a < \underline{a}(\theta,p)$ and $\theta \in [\vartheta(p,d), 1]$, or $a < a_\star^{\rm CKN}$ and $\theta = \vartheta(p,d)$.*

Assume that $\gamma > 1/2$ if $d = 2$ and $\gamma \ge d/4$ if $d \ge 3$. Symmetry breaking holds in (WLH) if $a < \max\{\tilde{a}(\gamma), a_c - \sqrt{\Lambda_{\rm SB}(\gamma)}\}$.

These results have been established in [3, 5]. When $\gamma = d/4$, $d \ge 3$, we observe that $\Lambda_\star^{\rm WLH} = \Lambda_{\rm SB}(d/4) < \Lambda(\tilde{a}(d/4))$ with the notations of Theorem 2.1 and there is symmetry breaking if $a \in (-\infty, a_\star^{\rm WLH})$, in the sense that $\mathsf{C}_{\rm WLH}(d/4,a) > \mathsf{C}^*_{\rm WLH}(d/4,a)$, although we do not know if extremals for (WLH) exist when $\gamma = d/4$.

Results of symmetry breaking for (CKN) with $a < \underline{a}(\theta,p)$ have been established first in [1, 8, 9] when $\theta = 1$ and later extended in [3] to $\theta < 1$. The main idea in case of (CKN) is consider the quadratic form associated to the second variation of $\mathscr{E}^p_{\theta,\Lambda}$ around a minimizer among functions depending on s only and observe that the linear operator $\mathscr{L}^p_{\theta,\Lambda}$ associated to the quadratic form has a negative eigenvalue if $a < \underline{a}$. Results in [3] for (WLH), $a < \tilde{a}(\gamma)$, are based on the same method.

For any $a < a_\star^{\rm CKN}$, we have $\mathsf{C}^*_{\rm CKN}(\vartheta(p,d),p,a) < \mathsf{C}_{\rm GN}(p) \le \mathsf{C}_{\rm CKN}(\vartheta(p,d),p,a)$, which proves symmetry breaking. Using well-chosen test functions, it has been proved in [5] that $\underline{a}(\vartheta(p,d),p) < a_\star^{\rm CKN}$ for $p-2>0$, small enough, thus also proving symmetry breaking for $a - \underline{a}(\vartheta(p,d),p) > 0$, small, and $\theta - \vartheta(p,d) > 0$, small.

Theorem 3.2. *For all $d \ge 2$, there exists according to [2, 5] a continuous function a^* defined on the set $\{(\theta,p) \in (0,1] \times (2,2^*) : \theta > \vartheta(p,d)\}$ such that $\lim_{p\to 2_+} a^*(\theta,p) = -\infty$ with the property that (CKN) has only radially symmetric extremals if $(a,p) \in (a^*(\theta,p), a_c) \times (2,2^*)$, and none of the extremals is radially symmetric if $(a,p) \in (-\infty, a^*(\theta,p)) \times (2,2^*)$.*

Similarly, for all $d \ge 2$, there exists according to [5] a continuous function $a^{**} : (d/4,\infty) \to (-\infty, a_c)$ such that, for any $\gamma > d/4$ and $a \in [a^{**}(\gamma), a_c)$, there is a radially symmetric extremal for (WLH), while for $a < a^{**}(\gamma)$ no extremal is radially symmetric.

According to [5] Schwarz' symmetrization allows to characterize a subdomain of $(0,a_c)\times(0,1) \ni (a,\theta)$ in which symmetry holds for extremals of (CKN), when $d \ge 3$. If $\theta = \vartheta(p,d)$ and $p > 2$, there are radially symmetric extremals if $a \in [a_0, a_c)$ where a_0 is given in Propositions 2.1.

Symmetry also holds if $a - a_c$ is small enough, for (CKN) as well as for (WLH), or when $p \to 2_+$ in (CKN), for any $d \ge 2$, as a consequence of the existence of the spectral gap of $\mathscr{L}^p_{\theta,\Lambda}$ when $a > \underline{a}(\theta,p)$.

For given θ and p, by [2, 5] there is a unique $a^* \in (-\infty, a_c)$ for which there is symmetry breaking in $(-\infty, a^*)$ and for which all extremals are radially symmetric when $a \in (a^*, a_c)$. This follows from the observation that, if $v_\sigma(s,\omega) := v(\sigma\, s, \omega)$ for

$\sigma > 0$, then $(\mathscr{E}^p_{\theta,\sigma^2\Lambda}[v_\sigma])^{1/\theta} - \sigma^{(2\,\theta-1+2/p)/\theta^2}\,(\mathscr{E}^p_{\theta,\Lambda}[v])^{1/\theta}$ is equal to 0 if v depends only on s, while it has the sign of $\sigma - 1$ otherwise.

From Theorem 3.1, we can infer that radial and non-radial extremals for (CKN) with $\theta > \vartheta(p,d)$ coexist on the threshold, in some cases.

Numerical results illustrating our results on existence and on symmetry / symmetry breaking have been collected in Fig. 1 below in the critical case for (CKN).

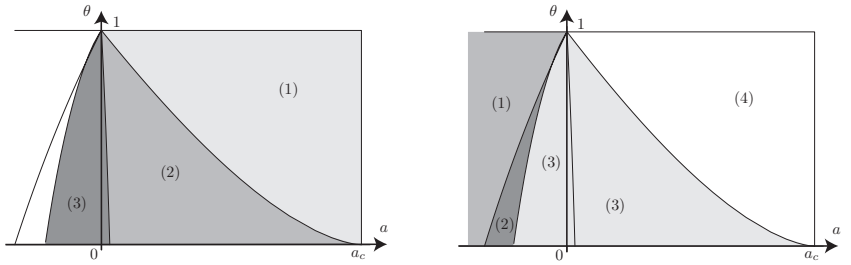

Fig. 1. Critical case for (CKN): $\theta = \vartheta(p,d)$. Here we assume that $d = 5$.
(a) The zones in which existence is known are (1) in which $a \geq a_0$, because extremals are achieved among radial functions, (1)+(2) using the *a priori* estimates: $a > a_1$, and (1)+(2)+(3) by comparison with the Gagliardo-Nirenberg inequality: $a > a_\star^{\rm CKN}$.
(b) The zone of symmetry breaking contains (1) by linearization around radial extremals: $a < \underline{a}(\theta,p)$, and (1)+(2) by comparison with the Gagliardo-Nirenberg inequality: $a < a_\star^{\rm CKN}$; in (3) it is not known whether symmetry holds or if there is symmetry breaking, while in (4) symmetry holds by Schwarz' symmetrization: $a_0 \leq a < a_c$.
Numerically, we observe that $\underline{a}$ and $a_\star^{\rm CKN}$ intersect for some $\theta \approx 0.85$.

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EFFECTIVE HAMILTONIANS FOR THIN DIRICHLET TUBES WITH VARYING CROSS-SECTION

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We show how to translate recent results on effective Hamiltonians for quantum systems constrained to a submanifold by a sharply peaked potential to quantum systems on thin Dirichlet tubes. While the structure of the problem and the form of the effective Hamiltonian stays the same, the difficulties in the proofs are different.

Keywords: Thin tubes; effective Hamiltonians; constraints; spectral asymptotics.

The question whether a Schrödinger Hamiltonian, which localizes states close to a submanifold of the configuration space by large forces, may be replaced by an effective operator on the submanifold is studied extensively and in various different settings in the literature (see e.g. [1–9]).

It is well-known that restricting the classical Hamiltonian system to the submanifold and then using Dirac's approach to quantizing constrained Hamiltonian systems [10] is too restricted. For there are lots of cases where the extrinsic curvature of the submanifold, which never shows up in Dirac's approach, plays a role. Therefore two other approaches have been investigated:

- *Soft constraints:* A rapidly increasing potential is used to localize solutions close to the submanifold (see [1, 2] and references therein).
- *Hard constraint:* the localization is achieved via Dirichlet boundary conditions on a thin tube centered around the submanifold (see the reviews [3, 4]).

If the potential or the tube's cross-section depend on the point on the submanifold, the constraint is called *varying*. First results for such constraints were given in [5–7].

Recently two of the authors have deduced effective Hamiltonians for the case of a varying soft constraint in arbitrary (co-)dimension (see [8, 9]). Here we explain how these results may also be obtained for the case of a varying hard constraint.

1. The setting

Let $(\mathscr{A}, G)$ be a Riemannian manifold of dimension $d + k$ and $\mathscr{C}$ a submanifold of dimension d without boundary, which is equipped with the induced metric $g = G|_{T\mathscr{C}}$. We assume that there is a non-self-intersecting tube $\mathscr{B}_\delta$ of radius $\delta > 0$

around $\mathscr{C}$.

If $\mathscr{C}$ is compact, such a tube $\mathscr{B}_\delta$ always exists and is compact itself. For the sake of a simple presentation we will focus on the latter case in the following and only shortly comment on the necessary adjustments in the case of a non-compact $\mathscr{C}$.

Since there is a canonical diffeomorphism Φ from B_δ into the normal bundle $\pi : N\mathscr{C} \to \mathscr{C}$, we can scale any subset of B_δ in the normal direction via

$$D_\varepsilon : N\mathscr{C} \to N\mathscr{C}\,, \quad (q, N) \mapsto (q, \varepsilon N)\,.$$

Let $\Omega \subset B_\delta$ be an open subset with smooth boundary such that the cross-sections

$$\Omega(q) := \Phi(\overline{\Omega}) \cap N_q\,\mathscr{C}$$

are all diffeomorphic, compact, and connected. Then $\pi : \Omega \to \mathscr{C}$ has the structure of a fiber bundle compatible with the one of $N\mathscr{C}$. We assume that this bundle has smooth local trivializations. In the case of a non-compact $\mathscr{C}$ one has to postulate the existence of a set of local trivializations whose derivatives satisfy global bounds in a suitable manner. The ε-thin tube Ω^ε is now defined via

$$\Omega^\varepsilon := \Phi^{-1} D_\varepsilon \Phi\, \Omega\,.$$

Our goal is to approximate the spectrum of and the unitary group generated by

$$H^\varepsilon := -\varepsilon^2 \Delta_G \quad \text{on} \quad L^2(\Omega^\varepsilon, \mu_G)$$

with Dirichlet boundary conditions by using an *effective Schrödinger operator* $H^\varepsilon_{\text{eff}}$ on $L^2(\mathscr{C})$. Here Δ_G is the Laplace–Beltrami operator associated with G and the factor ε^2 has been put in for convenience because otherwise the spectrum of H^ε would diverge in the limit $\varepsilon \to 0$. H^ε is obviously unitarily equivalent to the operator

$$-\varepsilon^2 \Delta_{\Phi_* G} \quad \text{on} \quad L^2(\Phi(\Omega^\varepsilon), \mu_{\Phi_* G})$$

with Dirichlet boundary conditions. We will identify the two operators in the following without making the diffeomorphism Φ explicit anymore.

2. Basic ideas

Consider the vector bundle $\mathscr{E}_{\text{f}} := \{(q, \varphi)\,|\,q \in \mathscr{C},\, \varphi \in C^\infty(\Omega(q))\}$ over $\mathscr{C}$, where the fibers $\Omega(q)$ of the bundle Ω are replaced with $C^\infty(\Omega(q))$ and the bundle structure of Ω is lifted by using the composition with the local trivializations of Ω as the new trivializations. Via the normal connection $\nabla^\perp$ on $N\mathscr{C}$, which is induced by G, every vector $\tau \in T_q\mathscr{C}$ tangent to $\mathscr{C}$ can be lifted into the tangent spaces $T_{q,n}\Omega$ of the corresponding fiber. The derivative of sections of $\mathscr{E}_{\text{f}}$ into the direction of the lift defines the so-called *horizontal connection* ∇^{h} on $\mathscr{E}_{\text{f}}$ (see [8]). The associated Laplacian Δ_{h} coincides with the Laplace–Beltrami operator Δ_g on $\mathscr{C}$ for functions that are constant on the fibers.

As in [8, 9] the basic idea is that after a measure transformation and rescaling the normal coordinates $n = N/\varepsilon$ the Hamiltonian H^ε may be split as

$$H^\varepsilon = -\varepsilon^2 \Delta_{\text{h}} - \Delta_n + \mathscr{O}(\varepsilon)\,.$$

This suggests to define for each $q \in \mathscr{C}$ the local *fiber Hamiltonian*

$$H_{\text{f}}(q) := -\Delta_n \quad \text{on} \quad L^2(\Omega(q), \mathrm{d}\lambda)$$

with Dirichlet boundary conditions. Here $\mathrm{d}\lambda$ is the Lebesgue measure induced from $N_q\mathscr{C} \simeq \mathbb{R}^k$. Since each fiber $\Omega(q)$ is compact, the spectrum of $H_{\mathrm{f}}(q)$ is discrete for all $q \in \mathscr{C}$. At some fixed q we number the eigenvalues by $J \in \mathbb{N}_0$. Due to the smooth dependence of $\Omega(q)$ on q this gives rise to continuous families of eigenvalues $E_J(q)$, so-called *energy bands*. In general, these bands may cross.

Definition 2.1. An energy band E_J is called *admissible*, if $E_J(q)$ is simple for all $q \in \mathscr{C}$ and the associated complex eigenspace bundle is trivializable, i.e., there is a global section φ_J of normalized eigenfunctions. In addition, if $\mathscr{C}$ is non-compact, E_J has to satisfy a gap condition as in [8].

As is well-known from the theory of elliptic operators, the lowest eigenvalue $E_0(q)$ on the connected domain $\Omega(q)$ is simple and $\varphi_0(q)$ can be chosen positive. So the lowest energy band E_0 is always admissible because the positivity of φ_0 ensures that it is a global section. For an admissible energy band E_J the subspace

$$\mathscr{P}_J := \left\{\psi(x)\varphi_J(x,n) \,|\, \psi \in L^2(\mathscr{C},g)\right\} \subset L^2(\Omega,G)$$

may be identified with $L^2(\mathscr{C},g)$ via the unitary operator

$$U_J : \mathscr{P}_J \to L^2(\mathscr{C},g)\,, \quad \psi(x)\varphi_J(x,n) \mapsto \psi(x).$$

$\mathscr{P}_J$ is approximately invariant under H^ε because the associated projector P_J satisfies

$$[P_J, H^\varepsilon] = [P_J, -\varepsilon^2\Delta_{\mathrm{h}}] + \mathscr{O}(\varepsilon) = \mathscr{O}(\varepsilon)$$

in $\mathscr{L}(D(H^\varepsilon),\mathscr{H})$. However, we are interested in the way the spectrum and the unitary group are affected by the geometry and the global structure of $\mathscr{C}$. These effects are of order ε^2. Therefore we have to improve on the invariance of the subspaces.

3. Results

Fix $E_{\max} < \infty$. Via adiabatic perturbation theory it is possible to construct a projector $P_J^\varepsilon = P_J + \varepsilon P_J^1 + \varepsilon^2 P_J^2$ and a unitary $U_J^\varepsilon : \mathscr{P}_J^\varepsilon \to L^2(\mathscr{C})$ such that

$$[P_J^\varepsilon, H^\varepsilon]\chi_{(-\infty,E_{\max}]}(H^\varepsilon) = \mathscr{O}(\varepsilon^3), \tag{1}$$

where $\chi_{(-\infty,E_{\max}]}$ is the characteristic function of $(-\infty,E_{\max}]$. The construction of P_J^ε is quite similar to the one in [8]. We comment on the differences below. Here we could in principle continue the construction to obtain a projector which is invariant up to errors of order ε^N for any $N \in \mathbb{N}$.

Now we reformulate the main result from [8] for the case of thin Dirichlet tubes. Here we use the index formalism including the convention that one sums over repeated indices. Moreover, we use latin indices $i,j,..$ running from 1 to d for coordinates on $\mathscr{C}$, greek indices $\alpha,\beta,\ldots$ running from $d+1$ to $d+k$ for the normal coordinates, and latin indices $a,b,..$ running from 1 to $d+k$ for coordinates on Ω.

Theorem 3.1. *Let E_J be an admissible energy band and $E_{\max} < \infty$. There are $C < \infty$ and $\varepsilon_0 > 0$ such that for all $\varepsilon < \varepsilon_0$ there exist a Riemannian metric g_J^ε on $\mathscr{C}$, an orthogonal projection P_J^ε, a unitary $U_J^\varepsilon : P_J^\varepsilon L^2(\Omega,\mu_G) \to L^2(\mathscr{C},\mu_{g_J})$ and*

$$H_J^\varepsilon := U_J^\varepsilon P_J^\varepsilon H^\varepsilon P_J^\varepsilon U_J^{\varepsilon *} \quad \textit{with domain} \quad U_J^\varepsilon D(H^\varepsilon),$$

which satisfy the following:

(a) ***Dynamics:*** *H_J^ε is self-adjoint on $L^2(\mathscr{C},\mu_{g_J})$ and*

$$\Big\| \Big(\mathrm{e}^{-\mathrm{i}H^\varepsilon t} - U_J^{\varepsilon *}\ \mathrm{e}^{-\mathrm{i}H_J^\varepsilon t}\ U_J^\varepsilon \Big)\ P_J^\varepsilon\ \chi_{(-\infty,E_{\max}]}(H^\varepsilon) \Big\| \leq C\,\varepsilon^3 |t|.$$

(b) ***Spectrum:*** *For all (E^ε) with $\limsup_\varepsilon E^\varepsilon < E_{\max}$ one has*

(i) $\quad H_J^\varepsilon\,\psi^\varepsilon = E^\varepsilon\,\psi^\varepsilon \quad\Rightarrow\quad \|(H^\varepsilon - E^\varepsilon)\,U_J^{\varepsilon *}\psi^\varepsilon\| \leq C\,\varepsilon^3\,\|U_J^{\varepsilon *}\psi^\varepsilon\|,$

(ii) $\quad H^\varepsilon\,\Psi^\varepsilon = E^\varepsilon\,\Psi^\varepsilon \quad\Rightarrow\quad \|(H_J^\varepsilon - E^\varepsilon)\,U_J^\varepsilon P_J^\varepsilon \Psi^\varepsilon\| \leq C\,\varepsilon^3\,\|\Psi^\varepsilon\|.$

For $\psi_1 = \chi_{(-\infty,E_{\max}]}(-\varepsilon^2\Delta_g + E_J)\psi_1$ the effective Hamiltonian H_J^ε is given by

$$\begin{aligned}\langle\psi_2|H_J^\varepsilon\psi_1\rangle_{\mathscr{C}} = \int_{\mathscr{C}} \Big(& g_J^{\varepsilon\,ij}\,\overline{p_{\varepsilon\,i}^J\psi_2}\,p_{\varepsilon\,j}^J\psi_1 \;+\; \overline{\psi_2}E_J\psi_1 \;-\; \varepsilon^2\,\overline{\psi_2}\,U_1^{\varepsilon\,*}R_{H_{\mathrm{f}}}(E_J)U_1^\varepsilon\,\psi_1 \\ & + \varepsilon^2\overline{\psi_2}\,(V_{\mathrm{geom}} + V_{\mathrm{BH}} + V_{\mathrm{amb}})\,\psi_1\Big) d\mu_{g_J^\varepsilon} \;+\; \mathscr{O}(\varepsilon^3),\end{aligned}$$

where

$$\begin{aligned} g_J^{\varepsilon\,ij} &= g^{ij} + \varepsilon\,2\mathrm{II}_\alpha^{ij}\langle\varphi_J|n^\alpha\varphi_J\rangle_{\Omega(q)} + \varepsilon^2\overline{\mathscr{R}}^{i\ j}_{\alpha\ \beta}\big\langle\varphi_J\big|n^\alpha n^\beta\varphi_J\big\rangle_{\Omega(q)} \\ &\quad + \varepsilon^2\mathscr{W}_{\alpha l}^i g^{lm}\mathscr{W}_{\beta m}^j\big\langle\varphi_J\big|3n^\alpha n^\beta\varphi_J\big\rangle_{\Omega(q)}, \\ p_{\varepsilon\,j}^J &= -\mathrm{i}\varepsilon\partial_j - \varepsilon\langle\varphi_J|\mathrm{i}\nabla_j^{\mathrm{h}}\varphi_J\rangle_{\Omega(q)} - \varepsilon^2\overline{\mathscr{R}}_{j\alpha\ \beta}^{\ \ \gamma}\langle\varphi_J|\tfrac{2}{3}n^\alpha n^\beta\mathrm{i}\partial_\gamma\varphi_J\rangle_{\Omega(q)} \\ &\quad + \varepsilon^2\mathscr{W}_\alpha^{ji}\big\langle\,\varphi_J\,\big|\,2\,\big(n^\alpha - \langle\varphi_J|n^\alpha\varphi_J\rangle\big)\mathrm{i}\nabla_i^{\mathrm{h}}\varphi_J\,\big\rangle_{\Omega(q)}, \\ R_{H_{\mathrm{f}}}(E_J) &= (1-P_J)\big(H_{\mathrm{f}} - E_J\big)^{-1}(1-P_J), \\ U_1^\varepsilon &= 2g^{ij}\overline{\nabla_i^{\mathrm{h}}\varphi_J}\varepsilon\partial_j + n^\alpha\varphi_J\mathscr{W}_\alpha^{ij}\varepsilon^2\partial_{ij}^2, \\ V_{\mathrm{geom}} &= -\tfrac{1}{4}\eta^\alpha\eta_\alpha + \tfrac{1}{2}\mathscr{R}^{ij}_{\ \ ij} - \tfrac{1}{6}\big(\overline{\mathscr{R}}^{ab}_{\ \ ab} + \overline{\mathscr{R}}^{aj}_{\ \ aj} + \overline{\mathscr{R}}^{ij}_{\ \ ij}\big), \\ V_{\mathrm{BH}} &= g^{ij}\big\langle\nabla_i^{\mathrm{h}}\varphi_J\big|(1-P_J)\nabla_j^{\mathrm{h}}\varphi_J\big\rangle_{\Omega(q)}, \\ V_{\mathrm{amb}} &= \overline{\mathscr{R}}^{\gamma\ \ \delta}_{\ \alpha\ \beta}\langle\partial_\gamma\varphi_J|\tfrac{1}{3}n^\alpha n^\beta\partial_\delta\varphi_J\rangle_{\Omega(q)}, \end{aligned}$$

with $\mathscr{W}$ the Weingarten mapping, η the mean curvature vector, $\mathscr{R}$ and $\overline{\mathscr{R}}$ the Riemann tensors of $\mathscr{C}$ and $\mathscr{A}$ (see [9] for definitions of all the geometric objects).

For a non-compact $\mathscr{C}$ additional bounds on the derivatives of φ_J as in [8] are required. There a detailed discussion of the effective Hamiltonian is provided, too.

As soon as (1) has been established, the proof of Theorem 3.1 goes exactly along the same lines as in [8]. The strategy to obtain (1) is also the same here, but the technical difficulties are different. The key facts that have to be derived are

$$\|[-\varepsilon^2\Delta_{\mathrm{h}}, P_J]\|_{\mathscr{L}(D(H_\varepsilon^{m+1}),D(H_\varepsilon^m))} = \mathscr{O}(\varepsilon), \tag{2}$$

$$\|[-\varepsilon^2\Delta_{\mathrm{h}}, R_{H_{\mathrm{f}}}(E_J)]\|_{\mathscr{L}(D(H_\varepsilon^{m+l}),D(H_\varepsilon^m))} = \mathscr{O}(\varepsilon) \tag{3}$$

for some $l \in \mathbb{N}$ and all $m \in \mathbb{N}_0$. In addition, in [8] we had to make sure that the derivatives of φ_J decay fast enough in the spatially infinite fibers and that their decay is not destroyed by application of energy cutoffs and resolvents, which is not necessary in the case considered here due to the boundary conditions. However,

the boundary poses new problems in the proof of (2) & (3). On the one hand, the volume of the fibers is varying so that ∇^{h} is only metric on sections which satisfy the Dirichlet condition. On the other hand, application of ∇^{h} destroys the Dirichlet condition. Therefore one cannot only stick to the differential operators but has to make use of the spectral representation, too.

Roughly speaking, (2) means to show that all the derivatives of φ_J are uniformly bounded, in particular at the boundary. This can be done by locally mapping Ω to the constant tube equipped with a suitable product metric and applying the procedures from [8]. Here the smoothness of the trivializations of Ω enters.

For (3) one makes use of the fact that the fibers are compact so that the resolvent may be written as $R_{H_{\mathrm{f}}}(E_J) = \sum_{I \neq J} P_I/(E_I - E_J)$. Then its derivatives may be controlled via some Weyl's law by choosing l large enough.

4. Discussion of the results

Due to Theorem 3.1 the spectrum of H^ε is given, up to errors of order ε^3, by the spectra of H_J^ε for $J \in \mathbb{N}_0$. With our approach it is possible to obtain not only the energies close to $\inf \sigma(H_J^\varepsilon)$ but also the excitations of order 1. In this energy regime the leading part $-\varepsilon^2\Delta_g + E_J$ is a semiclassical operator, whose dynamics explores distances of order 1 for times of order ε^{-1}. Therefore this is the relevant time scale, on which the global structure of an ε-independent $\mathscr{C}$ is seen. Theorem 3.1 allows to look at even much longer times.

The spectrum of $-\varepsilon^2\Delta_g + E_J$ is quite well-understood. We discuss here the role of the corrections in H_J^ε for constant E_J and an E_J with one non-degenerate minimum on a compact $\mathscr{C}$. By using standard results from semiclassical analysis this discussion could be extended also to several degenarate minima.

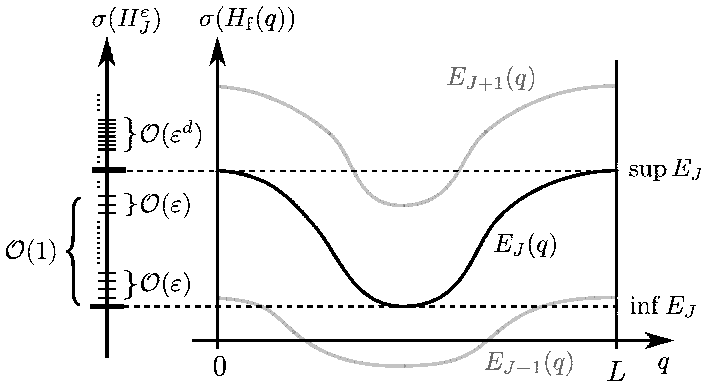
1) E_J is constant: In this case the level spacing of $-\varepsilon^2\Delta_g + E_J$ is of order ε^2 close to E_J. So the low eigenvalues strongly depend both on the corrections in p_ε^J and on the effective potentials V_{geom} and V_J (see [9] for an example with global effects). Since the kinetic energy is small for eigenvalues close to E_J, the corrections to g and the off-band coupling $U_1^{\varepsilon\,*} R_{H_{\mathrm{f}}}(E_J) U_1^\varepsilon$ do not matter here.

They only become relevant for energies of order 1 above E_J. Let $0 \leq \alpha < 2$. According to Weyl's law, the level spacing at energies of order ε^α above E_J is of order $\varepsilon^{\alpha(1-d/2)+d}$. For $d = 1, 2$ this is always bigger than the approximation error of order ε^3. For $d \geq 3$ the approximation error is only smaller for $\alpha > (2d-6)/(d-2)$. Note that the minimal α is always strictly smaller than 2. To fully resolve the spectrum for energies of order 1 one would have to go to order d in the construction of the super-adiabatic projector and the effective Hamiltonian. However, even in cases where the effective Hamiltonian is not precise enough to resolve the small level spacing, Theorem 3.1 still yields good control over the dynamics of states in this energy regime on the relevant time scales.

2) E_J has one non-degenerate minimum: Order 1 above $\sup E_J$ the level spacing of H_J^ε is again given by Weyl's law, i.e., only of order ε^d. So we are in the same situation as for energies of order 1 above a constant E_J. Close to $\sup E_J$ no general statements can be made about the level spacing. Order 1 below $\sup E_J$ the spectrum of H_J^ε is dominated by E_J resulting in a level spacing of order ε. Thus the effective

potentials, which are of order ε^2, may be ignored here. For energies of order 1 above $\inf E_J$, however, the ε-corrections to the kinetic energy become relevant because the eigenfunctions oscillate on a scale of order ε^{-1}.

We sketch the emerging picture for the case of a closed curve $\mathscr{C}$ of length L:



For energies above $\sup E_J$ the corresponding eigenfunctions are not localized but extended over the whole submanifold. Hence, global effects may occur here, too.

5. Conclusions and outlook

We have derived an effective Hamiltonian for the problem of hard constraints in quantum mechanics that covers all the interesting energy scales. Although the technical difficulties in the soft and the hard constraint approach differ, the results have a very similar structure. This is due to the fact that the wave function concentrates close to the submanifold. In the future, we will investigate the Laplacian on thin Riemannian fiber bundles using our adiabatic techniques. To do so we split up the metric into a horizontal and a vertical part and scale only the latter by ε:

$$G = G_{\rm h} + \varepsilon^2 G_{\rm v}\,.$$

This is related to the so-called adiabatic limit in global analysis (see e.g. [11]). In this setting there is no concentration inside the fibers. Therefore an expansion of the metric must be replaced by an averaging procedure. As a consequence, the effective Hamiltonian will have a somewhat different structure.

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OTHER TALKS

INVITED TALK

SPECTRAL MINIMAL PARTITIONS

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We give a survey about recent developments concerning spectral minimal partitions. This subject is related to spectral theory. In particular we will give a characterization for the case that there is equality in Courants nodal theorem. This is joint work with Bernard Helffer, Susanna Terracini and Virginie Bonnaillie-Noel.

CONTRIBUTED TALKS

HOMOGENIZATION OF THE WAVEGUIDES WITH FREQUENT ALTERNATION BOUNDARY CONDITIONS

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We consider Laplacian in a planar strip with Dirichlet boundary condition on the upper boundary and with frequent alternation boundary condition on the lower boundary. The alternation is introduced by the periodic partition of the boundary into small segments on which Dirichlet and Neumann conditions are imposed in turns. We show that under the certain condition the homogenized operator involves either Dirichlet or Neumann boundary condition on the lower boundary and prove the uniform resolvent convergence. The spectrum of the perturbed operator consists of its essential part only and has a band structure. We construct the leading terms of the asymptotic expansions for the first band

functions. We also construct the complete asymptotic expansion for the bottom of the spectrum.

ABSOLUTELY CONTINUOUS SPECTRUM FOR PERIODIC MAGNETIC FIELDS

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The spectral theory of Schrödinger operators with periodic magnetic fields (non-zero flux) still poses surprisingly many unsettled questions. We review the main methods and results pertaining to the measure theoretic nature of the spectrum (absolutely continuous vs. pure point) and present new results for AC spectrum.

RESONANT CYCLOTRON ACCELERATION OF PARTICLES BY A TIME PERIODIC SINGULAR FLUX TUBE

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We study the dynamics of a nonrelitivistic charged particle moving on a punctured plane under the influence of a homogeneous magnetic field and driven by a periodically time-dependent singular flux tube through the hole. We exhibit an effect of resonance of the flux and cyclotron frequencies in the framework of classical as well as quantum mechanics. In particular, we show that in both statements of the problem an infinite growth of the energy is possible.

ABSOLUTELY CONTINUOUS SPECTRUM FOR SUBSTITUTION TREES

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We study a class of rooted trees with a substitution type structure. These trees are not necessarily regular but exhibit a lot of symmetries. The spectrum of the corresponding graph Laplace operator is purely absolutely continuous and consists of finitely many intervals. We show stability of absolutely continuous spectrum under small random perturbations. Moreover for such trees which are not regular the absolutely continuous spec-

trum is stable under small deterministic perturbations by radially symmetric potentials. (This is joint work with Daniel Lenz and Simone Warzel.)

ADIABATIC SPECTRAL ASYMPTOTICS ON FOLIATED MANIFOLDS

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In this talk we are going to discuss some recent results concerning the asymptotic behavior of the eigenvalue distribution function of the Laplace operator on a compact Riemannian foliated manifold when the metric on the ambient manifold is blown up in directions normal to the leaves (in the adiabatic limit). In particular we will address the noncommutative Weyl formula and related problems on the distribution of integer points.

RESONANCES IN QUANTUM GRAPHS

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We consider a quantum graph with finite number of internal edges and some infinite leads equipped with Hamiltonian acting as negative second derivative. If the graph contains a loop of edges with lengths equal to integer multiples of l_0 and suitable coupling conditions are applied then eigenvalues $(n\pi/l_0)^2$ occur embedded in the continuous spectrum. We use Kuchment's flower-like model for describing these eigenvalues arose from correlations of lengths of the edges for a general graph. When changing the ratio of the lengths, the poles of the resolvent (formerly eigenvalues) may become resonances. In the general case we determine the total number of poles of the perturbed resolvent (with their multiplicities taken into account) in the neighbourhood of former eigenvalue. Furthermore, we derive a criterion for the asymptotics of resonances to be of a non-Weyl character. We construct examples of graphs with nontrivial coupling which do not preserve Weyl's law.

SPECTRAL PROPERTIES OF LEAKY STAR GRAPH

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A δ-perturbation supported by a family of straight lines on the plane intersecting at one point is studied. Several integral representations of the eigenvalue equation are obtained.

Estimates for the bottom of the spectrum are provided. Asymptotic expansions for the lowest eigenvalue as angles between lines tend to extremal values are calculated.

WEAK DISORDER IN THE KRONIG-PENNEY MODEL: STABILITY OF THE ABSOLUTELY CONTINUOUS SPECTRUM AND EIGENVALUES IN GAPS

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One-dimensional Schrödinger operator with δ-interactions on a discrete set X is considered. Conditions for the stability of the essential and the absolutely continuous spectra under perturbations of the set X are given. Using Schatten-von Neumann estimates of the resolvent difference of perturbed and unperturbed operator we compare their generalized discrete spectra. The results are applied to the investigation of eigenvalues in gaps for the Kronig-Penney model with a weak disorder.

SELF-ADJOINT EXTENSIONS OF THE AHARONOV-BOHM HAMILTONIAN ON RIEMANNIAN MANIFOLDS

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We consider the magnetic Schrödinger operator on a Riemannian manifold. We assume the magnetic field is given by the sum of a regular field and the Dirac δ measures supported on a discrete set. We give a complete characterization of the self-adjoint extensions of the minimal operator, in terms of the boundary conditions.

ON THE SINGULAR BEHAVIOUR OF SPECTRAL DENSITY FOR SCHRÖDINGER OPERATORS WITH WIGNER-VON NEUMANN PERTURBATION

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The analysis of the spectral density behaviour near singular points of the absolutely continuous spectrum of the Schrodinger operators with a periodic potential perturbed by a Wigner-von Neumann type potential to be presented.It is based on the asymptotic

methods and discrete linear system theory. The location of the singular points is subordinated by a sort of Bohr-Sommerfeld quantization condition.The talk is based on the common work with S. Simonov.

BOUNDARY TRIPLETS AND A RESULT OF JOST AND PAIS: AN ABSTRACT APPROACH

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In 1951 was published by R. Jost and A. Pais (Phys. Rev. 82, 840-851, 1951), a remarkable paper which relates the so-called Jost solution of the scattering problem for Schrödinger operators in 1D with a certain perturbation determinant. The result was generalized by F. Gesztesy, M. Mitrea and M. Zinchenko very recently to higher dimensions in a series of papers. We give an abstract version of this result in the framework of boundary triplets for symmetric operators. The main ingredients are the notions of perturbation determinant for extensions and of the abstract Weyl function both defined in this framework. The talk is based on a common work with M. Malamud from Donetsk (Ukraine).

ON THE DEGENERATE SPECTRAL GAPS OF THE ONE-DIMENSIONAL SCHRÖDINGER OPERATORS WITH PERIODIC POINT INTERACTIONS

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We discuss the spectrum of the one-dimensional Schrödinger operator which possesses three point interactions in the basic period cell and investigate its band structure. We suppose that each point interaction on a lattice is given by a rotation or is defined by the Dirac delta function. Under some particular assumption on a lattice, we discuss the coexistence problem. Namely, we determine whether or not the jth spectral gap is degenerate for a given natural number j.

SPECTRAL PROBLEMS AND QUANTUM FEATURES OF FLUID IN NANOTUBE

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Fluid flows through nanostructures are intensively studied now. Experiments show that these flows have many specific features, which cannot be explained in classical terms only. Particularly, flow through nanotube is extremely fast in comparison with its classical analog. We suggest a model based on the possibility of existence of molecular clusters (Frenkel crystallites) in the fluid [1]. There are some experimental evidences of such phenomenon. Under this assumption one needs to take into account quantum effects. Particularly, the boundary condition, which plays the crucial role for the flow in nanostructures, takes the form of sliding condition instead of the no-slip condition for the classical flow. The parameters of the boundary conditions are determined by solving of quantum scattering problem for the particle of the fluid by the wall potential. The character of this solution is related with the existence of bands in the spectrum corresponding to surface waves along the nanotube boundary. Main features of the flow are described in the framework of the model. For very narrow nanotubes another phenomena have an influence on the flow – possibility of existence of solitons in nanotube walls. These soliton solutions are similar to Davidov solitons in molecular chains. This model of flow is also described.

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EFFECTIVE HAMILTONIAN IN CURVED QUANTUM WAVEGUIDES AS A CONSEQUENCE OF STRONG RESOLVENT CONVERGENCE

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The Dirichlet Laplacian in a curved two-dimensional strip built along a plane curve is investigated in the limit when the uniform cross-section of the strip diminishes. We show that the Laplacian converges in a strong resolvent sense to the well known one-dimensional Schrödinger operator whose potential is expressed solely in terms of the curvature of the reference curve. In comparison with previous results we allow curves which are unbounded and whose curvature is not differentiable. This is a joint work with David Krejčiřík.

ON THE EIGENVALUE PROBLEM FOR A PARTICULAR CLASS OF JACOBI MATRICES

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A function F with simple and nice algebraic properties will be defined on a subset of the space of complex sequences. A relation between the function F and the eigenvalue problem for the Jacobi matrix of a special type will be illustrated. Especially, it will be shown the spectrum of infinite Jacobi matrix whose parallels to the diagonal are constant

and the diagonal depends linearly on the index coincides with zeros of the Bessel function of the first kind as function of its order.

WEYL LAW FOR LAPLACIANS WITH CONSTANT MAGNETIC FIELD ON NONCOMPACT HYPERBOLIC SURFACES WITH FINITE AREA

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We consider a magnetic Laplacian $H(A)$ on a noncompact hyperbolic surface M with finite area. A is a real one-form and the magnetic field dA is constant in each cusp. When the harmonic component of A satisfies some quantified condition, it turns out that the spectrum of $H(A)$ is discrete and that the eigenvalue counting function satisfies the classical Weyl formula, even when $dA = 0$. Moreover the order of the remainder term is the same as in the sharp asymptotic formula recently established by W. Müller in the context of automorphic forms.

ON THE TWO-DIMENSIONAL COULOMB-LIKE POTENTIAL WITH A CENTRAL POINT INTERACTION

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We provide an exact mathematical meaning to the formal differential expression $-\Delta_{x,y} - C/\sqrt{x^2+y^2}$, $C > 0$ as a quantum mechanical observable. The resulting one-parametric family of operators comprises not only the two-dimensional Coulomb-like Hamiltonian but also the Hamiltonians with the additional point interaction. Spectral properties of these Hamiltonians as well as their Green functions are investigated in detail. The problem is also reformulated into the momentum representation. This contribution is based on the joint work with Pavel Št'ovíček.

FRACTIONAL MOMENT METHOD FOR NON-MONOTONE MODELS

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The fractional moment method is a tool to show exponential decay of the averaged Green's function (in an appropriate sense) and thus Anderson localisation for many

classes of ergodic, random difference operators on a lattice. Typically the method heavily relies on the monotone dependence of the operator on the random parameters. For certain models it is possible to extend the method to non-monotone parameter dependence.

Many body quantum systems

Session organizer:

Marcel Griesemer

DIFFUSION IN HAMILTONIAN QUANTUM SYSTEMS

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We discuss an example of a quantum system in which one can establish long-time diffusive bahaviour rigorously.

1. Model

We are in interested in dissipative quantum systems described in the Hamiltonian framework. By 'dissipative systems', we mean that one part of the system is large and can effectively act as a heat bath or a thermostat to the rest of the composite system. We will in general call the part that acts as a thermostat the 'Environment' and denote it by the subscript E, whereas the rest of the total system is called 'Subsystem' and is denoted by the subscript S. Since dissipative behaviour in the long-time limit cannot occur in finite systems (because of Poincare recurrencies), we necessarily need to put at least the environment in infinite volume. The joint Hilbert space of system and environment is then

$$\mathscr{H} = \mathscr{H}_{\mathrm{S}} \otimes \mathscr{H}_{\mathrm{E}} \tag{1}$$

The environment is usually modelled by a bosonic quantum field, described by a Fock space built on $l^2(\mathbb{Z}^d)$;

$$\mathscr{H}_{\mathrm{E}} = \Gamma(l^2(\mathbb{Z}^d)) = \mathbb{C} \oplus l^2(\mathbb{Z}^d) \oplus l^2(\mathbb{Z}^d) \underset{\text{symm}}{\otimes} l^2(\mathbb{Z}^d) \oplus \dots \tag{2}$$

where $\underset{\text{symm}}{\otimes}$ denotes the symmetrized tensor product, and the spaces on the right are respectively the vacuum, one-particle space, two-particle space, etc. We assume the field to be free, or, in other words, we asssume its Hamiltonian to be quadratic in the creation-annihilation operators (satisfying the canonical commutation relations)

$$H_{\mathrm{E}} = \int_{\mathbb{T}^d} dq \omega(q) a_q^* a_q, \qquad \text{with } [a_q, a_{q'}^*] = \delta(q - q') \tag{3}$$

where $q \in \mathbb{T}^d$ is the (quasi-)momentum of one particle and $\omega(q)$ is its dispersion relation (energy). The 'particles' should be thought of as lattice vibrations, or phonons, with dispersion relation either $\omega(q) \propto |q|$ for small q (accoustical branch), or $\omega(q) \sim \sqrt{m_{\mathrm{ph}}^2 + |q|^2}$ for small q (optical branch). The initial state of the

environment is conveniently assumed to be the Gibbs state at a given inverse temperature β.

$$\rho_{\mathrm{E}}^{\beta} \approx \frac{1}{Z(\beta)} \mathrm{e}^{-\beta H_{\mathrm{E}}}, \qquad Z(\beta) = \mathrm{Tr} \mathrm{e}^{-\beta H_{\mathrm{E}}} \tag{4}$$

where we have put $\approx$ to indicate that in infinite volume, these concepts need to be interpreted carefully, (in particular $Z(\beta) = \infty$ if $\beta < \infty$), either by setting up the problem in finite volume, and taking the infinite-volume limit at the end of the construction, or by using the algebraic theory of infinite-volume states. In fact, if one uses the second option, than the Hilbert space $\mathscr{H}_{\mathrm{E}}$ has to be abandoned as it cannot accomodate a finite density of excitations. If one uses finite-volume approximations, no such complication arises and we assume this henceforth to the be case. Since $\rho_{\mathrm{E}}^{\beta}$ is Gaussian, it is completely characterized by its covariance or two-point function

$$\rho_{\mathrm{E}}^{\beta}(a_q^* a_{q'}) = \delta(q - q') \frac{1}{\mathrm{e}^{\beta\omega(q)} - 1}, \qquad \text{The Bose-Einstein distribution} \tag{5}$$

where the notation $\rho_{\mathrm{E}}^{\beta}(A)$ means ' the expectation value of the observable A in the state $\rho_{\mathrm{E}}^{\beta}$'. We now turn to the subsystem S. The archetypical example is of course a free particle, but for reasons to become clear soon, we prefer to give it more structure by endowing it with an internal degree of freedom that is called 'spin', for the sake of simplicity. Hence we have

$$\mathscr{H}_{\mathrm{S}} = l^2(\mathbb{Z}^d) \otimes \mathscr{H}_{spin}, \qquad \mathscr{H}_{spin} = \mathbb{C}^N, \qquad N < \infty \tag{6}$$

and the Hamiltonian of the particle is

$$H_{\mathrm{S}} = \frac{1}{M_{el}} \Delta \otimes 1 + 1 \otimes H_{spin} \tag{7}$$

where Δ is the discrete Laplacian, M_{el} is the mass of the particle ('el' for electron), and H_{spin} is some Hermitian $N \times N$ matrix.

The interaction between subsystem and environment is then assumed to be linear in creation and annihilation operators for simplicity (although a small quadractic interaction can be treated just as well)

$$H_{\mathrm{Int}} = \int_{\mathbb{T}^d} dq \phi(q) \mathrm{e}^{-\mathrm{i}qX} \otimes W \otimes a_q + \mathrm{h.c.} \tag{8}$$

where X is the position operator on $l^2(\mathbb{Z}^d)$, $\phi(\cdot)$ is the form-factor that is inserted to smear out the interaction between particle and field and W is a Hermitian $N \times N$ matrix that mediates the interaction between the spin degrees of freedom and the field. To avoid ultraviolet problems, one assumes that $\phi(q)$ is square-integrable at large q, and to reduce infrared problems, one chooses ϕ smooth at small q. This is seen most clearly on the level of the 'free correlation function' $\zeta(x,t)$, which arises naturally if one expands the evolution in powers of λH_{Int} and which has the following form

$$\zeta(x-x', t-t') = \rho_{\mathrm{E}}^{\beta}[\Phi(x,t)\Phi(x',t')], \qquad \Phi(x,t) = \int dq \phi(q) \mathrm{e}^{\mathrm{i}(xq+\omega(q)t)} a_q + \mathrm{h.c.} \tag{9}$$

The behavior of $\zeta(x,t)$ is (we assume here that ϕ is chosen sufficiently smooth) that $\sup_x |\zeta(x,t)| \leq C(1+|t|)^{-\frac{d-1}{2}}$ for accoustical phonons and $\sup_x |\zeta(x,t)| \leq C(1+|t|)^{-\frac{d}{2}}$ for optical phonons. One sees that correlations never decay very quickly, which is a general feature in momentum conserving models (this is also the reason for the occurence of anomalous transport in low dimensions).

The full Hamiltonian of our model is

$$H = H_{\mathrm{S}} + H_{\mathrm{E}} + \lambda H_{\mathrm{Int}}, \tag{10}$$

where we inserted a coupling constant $\lambda \in \mathbb{R}$. Let us start the dynamics in a state where the particle is localized at the origin, with density matrix $\rho_{\mathrm{S},0}$, and let the environment be in the themal state $\rho_{\mathrm{E}}^{\beta}$. Consider the time-evolved state

$$\rho_{\mathrm{SE},t} := \mathrm{e}^{-\mathrm{i}tH} \left(\rho_{\mathrm{S},0} \otimes \rho_{\mathrm{E}}^{\beta} \right) \mathrm{e}^{\mathrm{i}tH} \tag{11}$$

Since we are mainly interested in properties of the subsystem, it is natural to 'trace out' the degrees of freedom of the environment; i.e. we define the time-evolved *reduced* density matrix

$$\rho_{\mathrm{S},t} = \mathrm{Tr}_{\mathrm{E}} \rho_{\mathrm{SE},t} \tag{12}$$

Let us assume that the spin Hamiltonian H_{spin} has non-degenerate spectrum, such that the corresponding eigenvectors unambiguously span a basis in $\mathbb{C}^N$; labelled by $e \in \mathrm{sp}(H_{spin})$. Then $\rho_{\mathrm{S},t}$ is naturally expressed as a kernel $\rho_{\mathrm{S},t}(x,e;x',e')$ in the variables $x \in \mathbb{Z}^N, e \in \mathrm{sp}(H_{spin})$. The question that concerns us here is: "what happens to $\rho_{\mathrm{S},t}$ for large times t"? We could distinguish three cases, depending on the value of the particle mass M_{el}. By 'intermediate times', we mean times of order λ^{-2}.

mass M_{el}	long-time behaviour	intermediate times
$M_{el} = \infty$	thermalization of spin dgf.	Pauli master equation
$M_{el} \propto \lambda^{-2}$	diffusion, $D \sim \lambda^2$	Bloch-Boltzmann equation
$M_{el} \sim 1$	diffusion, $D \sim \lambda^{-2}$	Linear Boltzmann equation

The case $M_{el} = \infty$ (note that the well-known spin-boson model falls into this class) is broadly discussed in the literature and the long-time limit is under good control. We refer to [1, 2] for the original results and to [3] for a simple (yet more general) recent treatment. The long time limit in the case $M_{el} \sim 1$ is widely open, even though there are spectacular results for intermediate times, notably [4, 5]. Our work is concerned with the long-time control of the case $M_{el} \propto \lambda^{-2}$.

2. Result

To allow for a brief presentation, we merely consider the x-dependence of the reduced density matrix $\rho_{\mathrm{S},t}$ since we mainly want to exhibit diffusion, and hence we define the probability density

$$\nu_t(x) := \sum_{e \in \mathrm{sp} H_{spin}} \rho_{\mathrm{S},t}(x,e;x,e), \qquad \nu_t(x) \geq 0, \ \sum_x \nu_t(x) = \mathrm{Tr}\rho_{\mathrm{S},t} = 1 \tag{13}$$

Recall that by our choice of initial condition, at initial time $t = 0$, we have $\nu_0(x) = \delta_{x,0}$. We expect that there is a diffusion constant D such that

$$\nu_t(x) \sim (2\pi D t)^{-d/2} \mathrm{e}^{-\frac{x^2}{2Dt}}, \qquad t \nearrow \infty \tag{14}$$

One way to formalize this is by stating that the characteristic function of $\frac{x}{\sqrt{t}}$ converges to a Gaussian with variance D.

$$\sum_x \mathrm{e}^{\mathrm{i}q\frac{x}{\sqrt{t}}} \nu_t(x) \qquad \underset{t\nearrow\infty}{\to} \qquad \mathrm{e}^{-\frac{1}{2}Dq^2}, \qquad q \in \mathbb{R}^d \tag{15}$$

Our project consists of proving this claim for $M_{el} \sim \lambda^{-2}$ (recall that λ is also the coupling strength) with λ sufficiently small, but finite. A first result is in [6], it requires severe infrared assumptions and is restricted to 4 (or higher) dimensions. Recently, it has been generalized to 3 dimensions (work in progress with A. Kupiainen) for dispersion relations that vanish as $\omega(q) \propto |q|^2$ as $|q| \to 0$. More generally, the property that we require for our proofs to go through is that

$$\sup_x |\zeta(x,t)| \leq C(1+|t|)^{-(1+\alpha)}, \qquad \alpha > \frac{1}{4} \tag{16}$$

In particular, we have no clue how to handle the case $\omega(q) \propto |q|$ in 3D since there the correlation function is not integrable ($\propto |t|^{-1}$).

The diffusion constant $D = D_\lambda$ that we obtain is of the form $D_\lambda = \tilde{D}_\lambda + o(\lambda^2)$ where $\tilde{D}_\lambda \propto \lambda^2$ is the diffusion constant predicted by weak coupling theory. It is the diffusion constant associated to a Bloch-Boltzmann equation that describes the particle for intermediate times. We remark that some assumptions were omitted in this presentation. In particular, one is not allowed to eliminate the spin degrees of freedom from the setup by, for example, choosing $H_{spin} = 0$ or $[H_{spin}, W] = 0$. This restriction is a consequence of the fact that we choose the mass M_{el} to be large.

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GROUND STATE PROPERTIES IN NON-RELATIVISTIC QED

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We discuss recent results concerning the ground state of non-relativistic quantum electrodynamics as a function of a magnetic coupling constant or the fine structure constant, obtained by the authors in [12–14].

1. Introduction

We consider a system of finitely many non-relativistic quantum mechanical electrons bound to a static nucleus. The electrons are minimally coupled to the quantized electromagnetic field, and we denote the coupling constant by g. We impose an ultraviolet cutoff on the electromagnetic vector potential appearing in the covariant derivatives.

Models of this type are known as non-relativistic quantum electrodynamics (qed). They provide a reasonable description of microscopic low energy phenomena involving electrons, nuclei, and photons. A systematic mathematical investigation of these models started in the mid 90s with the work of V. Bach, J. Fröhlich, and I.M. Sigal [3–5]. They showed existence of ground states. Furthermore, they showed that excited bound states of the unperturbed system become unstable and turn into resonances when the electrons are coupled to the radiation field. To prove this result they introduced an operator theoretic renormalization analysis. Later, the existence of ground states was shown in more generality by M. Griesemer, E.H. Lieb, and M. Loss, see [8, 15].

In [13] we showed that the ground state of an atom with spinless electrons is an analytic function of the coupling constant g. That result is explained in Section 2, and it provides an algorithm to determine the ground state to arbitrary precision. To obtain the result we used the operator theoretic renormalization analysis of [3] and that renormalization preserves anlyticity [9].

In Section 3, we consider expansions in the fine structure constant α. We consider a scaling where the ultraviolet cutoff is of the order of the binding energy of the unperturbed atom. In this scaling lifetimes of excited states of atoms were calculated

which agree with experiment [11]. V. Bach, J. Fröhlich, and A. Pizzo [1, 2] showed that there exists an asymptotic expansion of the ground state and the ground state energy with α dependent coefficients. In [13] this result was extended and it was shown that these expansions are convergent. Furthermore, it was shown in [14] that the ground state energy as well as the ground state are k-times continuously differentiable functions of α respectively $\alpha^{1/2}$ on some nonempty k-dependent interval $[0, c_k)$. This result implies that there are no logarithmic terms in this scaling limit. This resolves an open issue raised in [2], since for other scalings of the ultraviolet cutoff logarithmic terms do occur, [6, 7, 10].

2. Model and analyticity of the ground state

We introduce the bosonic Fock space over the one photon Hilbert space $\mathfrak{h} := L^2(\mathbb{R}^3 \times \mathbb{Z}_2)$ and set

$$\mathscr{F} := \mathbb{C} \oplus \bigoplus_{n=1}^{\infty} S_n(\mathfrak{h}^{\otimes^n}),$$

where S_n denotes the orthogonal projection onto the subspace of totally symmetric tensors in $\mathfrak{h}^{\otimes^n}$. By $a^*(k,\lambda)$ and $a(k,\lambda)$, with $(k,\lambda) \in \mathbb{R}^3 \times \mathbb{Z}_2$, we denote the so called creation and annihilation operator. They satisfy the following commutation relations, which are to be understood in the sense of distributions,

$$[a(k,\lambda), a^*(k',\lambda')] = \delta_{\lambda\lambda'}\delta(k-k'), \qquad [a^{\#}(k,\lambda), a^{\#}(k',\lambda')] = 0\,,$$

where $a^{\#}$ stands for a or a^*. The operator $a(k,\lambda)$ annihilates the vacuum $(1,0,...) \in \mathscr{F}$. We define the operator of the free field energy by

$$H_f := \sum_{\lambda=1,2} \int a^*(k,\lambda)|k|a(k,\lambda)d^3k.$$

For $\lambda = 1,2$ we introduce the so called polarization vectors $\varepsilon(\cdot,\lambda) : S^2 := \{k \in \mathbb{R}^3 | |k| = 1\} \to \mathbb{R}^3$ to be maps such that for each $k \in S^2$ the vectors $\varepsilon(k,1), \varepsilon(k,2), k$ form an orthonormal basis of $\mathbb{R}^3$. For $x \in \mathbb{R}^3$ we define the field operator

$$A_\Lambda(x) := \sum_{\lambda=1,2} \int_{|k|<\Lambda} \frac{d^3k}{\sqrt{2|k|}} \left[e^{-ik\cdot x}\varepsilon(\widehat{k},\lambda)a^*(k,\lambda) + e^{ik\cdot x}\varepsilon(\widehat{k},\lambda)a(k,\lambda) \right] , \qquad (1)$$

where $0 < \Lambda$ is a finite ultraviolet cutoff and $\widehat{k} := k/|k|$. The Hilbert space is $\mathscr{H} := \mathscr{H}_{\text{at}} \otimes \mathscr{F}$, where

$$\mathscr{H}_{\text{at}} := \bigwedge^N L^2(\mathbb{R}^3)$$

is the Hilbert space describing N spin-less electrons. We study the following operator in $\mathscr{H}$

$$H_g := \sum_{j=1}^{N} (p_j + gA_\Lambda(x_j))^2 + V + H_f, \qquad (2)$$

where $x_j \in \mathbb{R}^3$ denotes the coordinate of the j-th electron, $p_j = -i\partial_{x_j}$, and V denotes the potential. For the result concerning analyticity in the coupling constant g on a disk $D_r := \{z \in \mathbb{C} | |z| < r\}$, we need the following hypothesis. It contains assumptions about the atomic Hamiltonian $H_{\rm at} := \sum_{j=1}^N p_j^2 + V$ acting in $\mathscr{H}_{\rm at}$.

Hypothesis (H) The potential V satisfies the following properties:

(i) V is invariant under permutations and rotations.
(ii) V is infinitesimally operator bounded with respect to $\sum_{j=1}^N p_j^2$.
(iii) $E_{\rm at} := \inf \sigma(H_{\rm at})$ is a non-degenerate isolated eigenvalue of $H_{\rm at}$.

All assumptions of Hypothesis (H) are satisfied for the hydrogen atom. Part (i) is satisfied for atoms, but not for molecules. We note that (iii) is a restrictive assumption.

Theorem 2.1. *Suppose (H). Then there exists a positive constant g_0 such that for all $g \in D_{g_0}$ the operator H_g has a non-degenerate eigenvalue $E(g)$ with eigenvector $\psi(g)$ and eigen-projection $P(g)$ satisfying the following properties.*

(i) For $g \in \mathbb{R} \cap D_{g_0}$, $E(g) = \inf\sigma(H_g)$.
(ii) $g \mapsto E(g)$ and $g \mapsto \psi(g)$ are analytic on D_{g_0}.
(iii) $g \mapsto P(g)$ is analytic on D_{g_0} and $P(g)^* = P(\overline{g})$.

Concerning the proof of the theorem, we note that the ground state energy is embedded in continuous spectrum. In such a situation analytic perturbation theory is typically not applicable and other methods have to be employed. In [13] Theorem 2.1 is proven using a variant of the operator theoretic renormalization analysis. Using the rotation invariance assumption of Hypothesis (H) one can prove that marginal terms in the renormalization analysis are absent. This implies that the renormalization analysis converges. Theorem 2.1 can then be shown using that renormalization preserves analyticity [9, 12].

Theorem 2.1 implies that the ground state and the ground state energy admit convergent power series expansions in g. The coefficients of these expansions can be calculated by means of analytic perturbation theory. To this end, one introduces an infrared cutoff which renders all expansion coefficients finite. In [13] it was shown using a continuity argument, that the individual expansion coefficients converge as the infrared cutoff is removed. This is not obvious; the expansion coefficients obtained by regular perturbation theory, [16], can involve cancellations of infrared divergent terms [12].

3. Expansions in the fine structure constant

In this section, we consider the ground state and the ground state energy of a hydrogen atom as a function of the fine structure constant α. We assume that the ultraviolet cutoff is of the order of the binding energy of the unperturbed atom. In suitable units the corresponding Hamiltonian is

$$H_{\alpha,\Lambda} := (p + \alpha^{3/2} A_\Lambda(\alpha x))^2 - \frac{1}{|x|} + H_f.$$

By a scaling transformation we can relate this operator to the operator

$$\widetilde{H}_{\alpha,\Lambda} := (p + \sqrt{\alpha}A_\Lambda(x))^2 - \frac{\alpha}{|x|} + H_f$$

using the following unitary equivalence $\widetilde{H}_{\alpha,\alpha^2\Lambda} \cong \alpha^2 H_{\alpha,\Lambda}$. We are interested in the behavior of the ground state and the ground state energy of $H_{\alpha,\Lambda}$ as $\alpha \downarrow 0$ while Λ remains constant. The ground state and the ground state energy are smooth in the sense of the following theorem [14].

Theorem 3.1. *Suppose (H) and let $\Lambda > 0$. There exists a positive α_0 such that for $\alpha \in [0, \alpha_0)$ the operator $H_{\alpha,\Lambda}$ has a ground state $\psi(\alpha^{1/2})$ with ground state energy $E(\alpha)$ such that we have the convergent expansions on $[0, \alpha_0)$*

$$E(\alpha) = \sum_{n=0}^{\infty} E_\alpha^{(2n)} \alpha^{3n}, \qquad \psi(\alpha^{1/2}) = \sum_{n=0}^{\infty} \psi_\alpha^{(n)} \alpha^{3n/2}. \tag{3}$$

The coefficients $E_\alpha^{(n)}$ and $\psi_\alpha^{(n)}$ are as functions of α in $C^\infty([0,\infty))$ and $C^\infty([0,\infty); \mathscr{H})$, respectively. For every $k \in \mathbb{N}_0$ there exists a positive $\alpha_0^{(k)}$ such that $\psi(\cdot)$ and $E(\cdot)$ are k-times continuously differentiable on $[0, \alpha_0^{(k)})$.

By the differentiability property of Theorem 3.1 and Taylor's theorem one can write the ground state and the ground state energy in terms of an asymptotic series with constant coefficients in the sense of [17]. To prove Theorem 3.1, we consider the Hamiltonian

$$H(g, \beta, \Lambda) := (p + gA_\Lambda(\beta x))^2 - \frac{1}{|x|} + H_f.$$

Using the identity $H(\alpha^{3/2}, \alpha, \Lambda) = H_{\alpha,\Lambda}$, Theorem 3.1 will follow as an application of Theorem 3.2, below. A corollary of that theorem is that the ground state of $H(g, \beta, \Lambda)$ is analytic in g with coefficients which are C^∞ functions of β. To state the theorem precisely, let X be a Banach space and let $C_B^k(\mathbb{R}; X)$ denote the space of X-valued functions having bounded, continuous derivatives up to order k normed by $\|f\|_{C_B^k(\mathbb{R};X)} := \max_{0 \le s \le k} \sup_{x \in \mathbb{R}} \|D_x^s f(x)\|_X$.

Theorem 3.2. *Suppose (H), let $k \in \mathbb{N}_0$, and $\Lambda > 0$. Then there exists a positive g_0 such that for all $(g, \beta) \in D_{g_0} \times \mathbb{R}$ the operator $H(g, \beta, \Lambda)$ has an eigenvalue $E_\beta(g)$ with eigenvector $\psi_\beta(g)$ and eigen-projection $P_\beta(g)$ satisfying the following properties.*

(i) For $g \in \mathbb{R} \cap D_{g_0}$ we have $E_\beta(g) = \inf\sigma(H_{g,\beta})$, and for all $g \in D_{g_0}$ we have $P_\beta(g)^* = P_\beta(\overline{g})$.

(ii) $g \mapsto E_{(\cdot)}(g)$, $g \mapsto \psi_{(\cdot)}(g)$, and $g \mapsto P_{(\cdot)}(g)$ are analytic functions on D_{g_0} with values in $C_B^k(\mathbb{R})$, $C_B^k(\mathbb{R}; \mathscr{H})$, and $C_B^k(\mathbb{R}; \mathscr{B}(\mathscr{H}))$, respectively.

In [14] Theorem 3.2 is shown using an operator theoretic renormalization analysis, which involves controlling arbitrarily high derivatives with respect to β.

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NON-ADIABATIC TRANSITIONS IN A SIMPLE BORN-OPPENHEIMER SCATTERING SYSTEM

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We study non-adiabatic scattering transitions in the Born-Oppenheimer limit for a molecular Schrödinger operator in which the nuclei have one degree of freedom and the electron Hamiltonian is a 2×2 matrix.

Keywords: Born-Oppenheimer approximation; non-adiabatic transitions; molecular quantum mechanics.

1. Introduction

We describe non–adiabatic transitions in a simple Born–Oppenheimer scattering system. The detailed proofs are long and technical. They can be found in Ref. 4. These transitions are difficult to study because they are exponentially small and cannot be determined by perturbation theory.

We study scattering theory for the equation

$$i\,\epsilon^2\,\frac{\partial\psi}{\partial t} \;=\; -\,\frac{\epsilon^4}{2}\,\frac{\partial^2\psi}{\partial x^2} \;+\; h(x)\,\psi \tag{1}$$

in the Born–Oppenheimer limit $\epsilon \to 0$. Here we assume $h(x)$ is a 2×2 matrix that depends parametrically on x and has an analytic continuation to a sufficiently wide strip about the real axis. We also assume $h(x)$ approaches limits $h(\pm\infty)$ sufficiently rapidly, as $\operatorname{Re} x \to \pm\infty$, uniformly in the strip. We further assume that the eigenvalues of $h(x)$ are never equal for real x. A typical example is

$$h(x) \;=\; \begin{pmatrix} \tanh(x) & 1 \\ 1 & -\tanh(x) \end{pmatrix}.$$

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To describe solutions to equation (1), we introduce 1–dimensional semiclassical wave packets for the nuclei

$$\varphi_k(A,\, B,\, \epsilon^2,\, a,\, \eta,\, x) = \pi^{-1/4}\, \epsilon^{-1/2}\, 2^{-k/2}\, (k!)^{-1/2}\, \overline{A}^{k/2}/A^{(k+1)/2}\, H_k((x-a)/(|A|\,\epsilon)) \times \exp\left(-\frac{B\,(x-a)^2}{2\,A\,\epsilon^2} \;+\; i\,\eta\,(x-a)/\epsilon^2\right).$$

We always impose the condition that $\mathrm{Re}\,\overline{A}\,B \;=\; 1$. Under this condition, $\{\,\varphi_k(A,\, B,\, \epsilon^2,\, a,\, \eta,\, \cdot)\,\}$ is an orthonormal basis of $L^2(\mathbb{R})$ for fixed A, B, ϵ, a, and η when $k = 0,\, 1,\, 2,\, \cdots$. A detailed discussion of these wave packets may be found in Ref. 2.

For each k, there is a solution to equation (1) of the form

$$\psi(x,\, t) \;=\; e^{iS(t)/\epsilon^2}\, \varphi_k(A(t),\, B(t),\, \epsilon^2,\, a(t),\, \eta(t),\, x)\; \Phi_1(x) \;+\; O(\epsilon),$$

where $\Phi_1(x)$ is an eigenvector of $h(x)$ that depends smoothly on x and has phase chosen to obey the adiabatic connection. (If $h(x)$ is real symmetric for real x then $\Phi_1(x)$ can be chosen real for all real x.) The quantities $A(t)$, $B(t)$, $a(t)$, $\eta(t)$, and $S(t)$ are determined by the classical phase space flow with the eigenvalue $E_1(x)$ corresponding to $\Phi_1(x)$ being used as an effective potential. [1] This result can be improved by optimally truncating the associated perturbation expansion. [3] We obtain

$$\psi(x,\, t) \;=\; e^{iS(t)/\epsilon^2} \sum_{n=0}^{N(\epsilon)} \epsilon^n\; \psi_n(x,\, t,\, \epsilon) \;+\; O\left(\exp\left(-\Gamma/\epsilon^2\right)\right). \tag{2}$$

Here $\Gamma > 0$, and the $\psi_n(x,\, t,\, \epsilon)$ have the form

$$\psi_n(x,\, t,\, \epsilon) = \sum_{j=0}^{3n+3+k} c_{j,k}(t,\, \epsilon)\, \varphi_j(A(t),\, B(t),\, \epsilon^2,\, a(t),\, \eta(t),\, x)\; \Phi_1(x) + \sum_{j=0}^{3n+3+k} d_{j,k}(t,\, \epsilon)\, \varphi_j(A(t),\, B(t),\, \epsilon^2,\, a(t),\, \eta(t),\, x)\; \Phi_2(x),$$

where $\{\Phi_1(x),\, \Phi_2(x)\}$ is the basis of eigenvectors for $h(x)$.

2. Non–Adiabatic Transitions

The approximate solution (2) is concentrated near a single classical orbit with position $a(t)$ determined by classical mechanics with the effective potential $E_1(x)$. Our main goal is to compute the leading order correction to this solution that obeys the classical mechanics governed by the second electronic potential energy surface $E_2(x)$.

We further assume that the two levels $E_1(x)$ and $E_2(x)$ have a single avoided crossing with a sufficiently small, but positive minimum gap between them. We assume that this avoided crossing is associated with a crossing for some complex value of x inside the strip of analyticity of $h(x)$.

By inserting energy cut offs, we assume that we are studying states whose energy lies strictly above the maxima of both electronic levels $E_1(\cdot)$ and $E_2(\cdot)$. Of course we also assume that the classical energy

$$\frac{\eta(t)^2}{2} \;+\; E_1(a(t))$$

satisfies this condition. Then one can find the leading order non-adiabatic contribution that is in the error term in formula (2). [4]

There are several surprises. First, the leading order transition probability is strictly greater than what one would obtain by naïvely applying the Landau–Zener formula to the Schrödinger equation

$$i\,\epsilon^2\,\frac{\partial \phi}{\partial t} \;=\; h(a(t))\,\phi. \tag{3}$$

Since the nuclei are localized near $a(t)$, and the Landau–Zener formula correctly describes the non–adiabatic transtions for solutions to (3), one might expect this to yield the correct leading order result for (1), but it is wrong. Second, one might expect classical energy conservation to predict the momentum of the nuclei after a non–adiabatic transtion has occurred. This, too, is simply the wrong leading order result. The true average nuclear momentum after the transition is strictly greater than this prediction. Third, for a fixed value of k, when the incoming state is asymptotic in the remote past to

$$e^{iS(t)/\epsilon^2}\,\varphi_k(A(t),\,B(t),\,\epsilon^2,\,a(t),\,\eta(t),\,x)\;\Phi_1(x),$$

then for sufficiently small ϵ, the leading order non–adiabatic contribution in the remote future is asymptotic to

$$C_1\;\exp(-\,C_2/\epsilon^2)\;\epsilon^{-k}\;e^{i\widetilde{S}(t)/\epsilon^2}\,\varphi_0(\widetilde{A}(t),\,\widetilde{B}(t),\,\epsilon^2,\,\widetilde{a}(t),\,\widetilde{\eta}(t),\,x)\;\Phi_2(x),$$

with $C_1 \neq 0$ and $C_2 > 0$. Here, $\widetilde{A}(t)$, $\widetilde{B}(t)$, $\widetilde{a}(t)$, $\widetilde{\eta}(t)$, and $\widetilde{S}(t)$ are determined by the classical phase space flow for the potential energy $E_2(x)$. We should comment that under our hypotheses on the energy, $\eta(t)$ never changes sign. The particular $\widetilde{\eta}(t)$ that arises also must have constant sign, and the sign is the same as that of $\eta(t)$. Any transitions that change direction are exponentially smaller in $1/\epsilon^2$ because of our assumption that the minimum gap between E_1 and E_2 is sufficiently small.

So, for a wide variety of incoming states, the leading order outgoing non–adiabatic term is always a complex Gaussian.

3. Comments about the Proof

We prove our main result by first studying the generalized eigenfunctions of the full Hamiltonian. These are solutions to the equation

$$-\,\frac{\epsilon^4}{2}\,\frac{\partial^2 \psi}{\partial x^2} \;+\; h(x)\,\psi \;=\; \mathscr{E}\;\psi.$$

For each $\mathscr{E}$ above the maxima of $E_j(\cdot)$, there are four independent solutions to this equation. One is incoming from the left and associated with E_1; one is incoming from the right and associated with E_1. The other two are similarly incoming from the left

and right and associated with E_2. For small ϵ we perform a WKB analysis of these solutions, and since we are interested in the transitions, we extend this analysis to complex values of x so that we can integrate the full Schrödinger equation around the crossing point of E_1 and E_2 in the complex plane.

We decompose our wave packets as superpositions of these generalized eigenfunctions. From the complex WKB analysis, we can compute the leading order non–adiabatic scattering component of each generalized eigenfunction. Computing the non–adiabatic transition wave packet then becomes an exercise in finding the asymptotics of an integral that arises from the superposition. This is quite tedious, but can be done quite explicitly. [4]

One thus gets the correct leading order transition component of the wave function. One also can understand why the naïve approach is wrong.

In the naïve approach, one computes the average momentum of the nuclei as they go through the transition. One then uses this in the Landau–Zener calculation. However, the higher momentum components of the wave function are much more likely to make a transition than the slower components. To get the correct results, one must compute the transition probability for each component and then average over the components. This yields a higher total transition probability than what one gets by averaging first. It also explains why the simple energy conservation calculation yields the wrong momentum prediction. The faster parts of the wave function are more likely to make a transition.

Finally, when using a φ_k as the incoming wave packet with $k > 0$, one can see why the non–adiabatic transition component is a Gaussian if ϵ is sufficiently small. The extra shift in momentum associated with the faster parts of the wave function being more likely to make a transition just affects the Gaussian factor in the formula for the φ_k in momentum space. (When one Fourier transforms from position space to momentum space, $\varphi_k(A,\, B,\, \epsilon^2,\, a,\, \eta,\, x)$ becomes $(-i)^k\, e^{-i\eta a/\epsilon^2}\, \varphi_k(B,\, A,\, \epsilon^2,\, \eta,\, -a,\, p)$.) The Hermite polynomial factor $H_k((p-\eta)/(|B|\,\epsilon))$ does not get shifted. The momentum space wave packet is largest near the point where the Gaussian is centered, and near this shifted point, the Hermite polynomial is approximately equal to its highest order term, which is a constant times $((p-\eta)/(|B|\,\epsilon))^k$. This times the shifted Gaussian is approximately another constant times ϵ^{-k} times another Gaussian.

Thus, all of the results that are surprising arise from the rapid increase of the transition probability as a function of the momentum when one examines the generalized wave functions.

4. Generalizations

Similar results hold for $m \times m$ matrices $h(x)$ whose spectra display suitable avoided crossings. Incoming states, given as superpositions of generalized eigenvectors, can also be accommodated, provided the corresponding energy density is sharply peaked around some value above that of the relevant electronic energy levels. [4]

These ideas have been further generalized in Ref. 5 to tackle the semiclassical study of waves driven by systems of autonomous PDEs in $1 + 1$ space-time dimen-

sions in a scattering regime. Consider operators of the form

$$\mathscr{R}(x,\, i\epsilon\partial/\partial t,\, i\epsilon\partial/\partial x) \;=\; \sum_{\substack{0\le l\le m\\ 0\le n\le r}} A_{ln}(x)\,(i\epsilon\partial/\partial x)^l\,(i\epsilon\partial/\partial t)^n$$

where $A_{ln}(x)$ are $d\times d$ matrices, analytic in x in some strip, which tend rapidly enough to limits as $\mathrm{Re}\, x\to\pm\infty$, uniformly in the strip.

The main assumptions are made on the modes on the system, which are the roots $\{k_j(x,\, E)\}_{j=1,\cdots,md}$ of the dispertion relation $\det\mathscr{R}(x,\, E,\, k)=0$. We assume they are real valued in some energy window, do not to cross as x varies in $\mathbb{R}$, and display some avoided crossing. Under these assumptions, the generalized eigenvectors, $\psi_\epsilon(x,\, E)\in\mathbb{C}^d$, solutions to $\mathscr{R}(x,\, E,\, i\epsilon\partial/\partial x)\,\psi_\epsilon(x,\, E)=0$, can be expanded in a basis of polarization vectors associated with the different modes. Superpositions of generalized eigenvectors yield exact solutions to the evolution equation in $L^2(\mathbb{R})$

$$\mathscr{R}(x,\, i\epsilon\partial/\partial t,\, i\epsilon\partial/\partial x)\,\Psi_\epsilon(x,\, t) \;=\; 0.$$

By selecting solutions which live on a specific mode in the remote past with a group velocity that makes them go through an avoided crossing, it is possible to compute the asymptotics as $\epsilon\to 0$ of the exponentially small part of the solution which makes a transition to the closest mode, for large but finite values of x and t.

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CONTRIBUTED TALKS

ON THE GROUND STATE ENERGY FOR MASSLESS NELSON MODEL

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I will present new results obtained in joint work with D. Hasler, on the ground state energy of Nelson's model in the massless case.

ON THE IONIZATION ENERGY OF THE SEMIRELATIVISTIC PAULI-FIERZ MODEL

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We consider the semi-relativistic Pauli-Fierz model which is defined by the relativistic kinetic energy $\sqrt{[\sigma \cdot (\mathbf{p} + e\mathbf{A}(\hat{\mathbf{x}}))]^2 + M^2} - M$, instead of the non-relativistic one $[\sigma \cdot (\mathbf{p} + e\mathbf{A}(\hat{\mathbf{x}}))]^2/2M$, in the Pauli-Fierz Hamiltonian. We show that the ionization energy of the semi-relativistic Pauli-Fierz model is strictly positive for all values of a coupling constant and particle mass $M \geq 0$. The total Hamiltonian contains the nuclear potential $V(\mathbf{x})$, and it is assumed that the semi-relativistic Schrödinger operator $\sqrt{\mathbf{p}^2 + M^2} - M + V(\mathbf{x})$ has a negative energy ground state.

COMPLETELY LOCAL INTERPRETATION OF MANY-BODY QUANTUM PHENOMENA

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The purpose of this talk is to come up with a framework that "converts" existing concepts from configuration space to ordinary one. This is done by modeling our universe as a big "computer" that simulates configuration space. If that "computer" exists in ordinary space and is ran by "classical" laws, our theory becomes "local", "deterministic" and "classical" by default. This concept will first be applied to a version of quantum field theory in which elementary particles have size (that is, a theory that does not yet exists). After that, we will do the same with Pilot Wave model of discrete jumps, due to Dürr et al.

ROTATING ULTRACOLD DIPOLAR GASES

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The basic physics of rotating ultracold dilute trapped atomic gases, with emphasis on Bose-Einstein condensation is briefly reviewed. The solution to the nonlinear Schrodinger equation in the rotating frame is presented. The effect of dipole-dipole interaction on an off-axis straight vortex in a rotating ultracold gas is studied and vortex nucleation with many observable consequences is discussed.

Quantum chaos

Session organizer:

Tomaz Prosen

RELATIONSHIP BETWEEN CHAOS AND THERMALIZATION IN ONE-DIMENSIONAL QUANTUM MANY-BODY SYSTEMS

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We consider an isolated one-dimensional quantum system of many interacting hard-core bosons and analyze the conditions under which it thermalizes. Thermalization occurs when the eigenstates of the system become chaotic. Chaotic eigenstates may appear in the middle of the spectrum of systems with few-body interactions, but not at the edges, and they are observed even when the systems becomes gapped and/or different symmetry sectors are mixed.

Keywords: Quantum chaos; quantum many-body systems; thermalization; eigenstate thermalization hypothesis.

1. Introduction

The current interest in the problem of thermalization in isolated quantum systems and its relationship with quantum chaos has in part been motivated by recent experiments in optical lattices. Optical lattices are crystals of light, where ultracold atoms play the role of electrons in solid crystals. They are very isolated and highly controllable, which allows for the study of condensed matter models not easily accessible with real solid state systems [1]. The observation of the Tonks-Girardeau gas in one-dimension (1D) [2, 3], for example, was one of a sequence of striking experiments with optical lattices. In this regime, the repulsive interaction between the bosons is so strong that, in real space, they resemble non-interacting fermions and are referred to as hard-core bosons (HCBs). In terms of thermalization in 1D, an inspiring experiment was performed by the group at Penn State [4]. They prepared a Bose-Einstein-condensate in a superposition of positive and negative momentum and then released it. The atoms were seen to move back and forth and collide thousands of times without ever thermalizing, that is, the momentum distribution never reached a thermal equilibrium shape. On the other hand, in 3D the system was seen to thermalize in less than three average collisions per atom. They argued that the absence of thermalization in 1D was due to the proximity of the system to

the integrable point.

But what do we exactly mean by thermalization in *isolated* quantum many-body systems? Consider a quantum system described by eigenvalues E_α and eigenvectors $|\psi_\alpha\rangle$. The time evolution of a generic observable $\hat{O}(t)$ is given by $\langle\hat{O}(t)\rangle \equiv \langle\Psi(t)|\hat{O}|\Psi(t)\rangle = \sum_{\alpha\beta} C^*_\alpha C_\beta e^{i(E_\alpha - E_\beta)t} O_{\alpha\beta}$, where the components $C_{\alpha,\beta}$ depend on the initial state $|\Psi(0)\rangle = \sum_\alpha C_\alpha |\psi_\alpha\rangle$ and $O_{\alpha\beta}$ are the matrix elements of $\hat{O}$ in the energy eigenbasis. The question we are after is whether the infinite time average for a generic nondegenerate system, $\overline{\langle\hat{O}(t)\rangle}$, (conveniently denoted by result of the diagonal ensemble, $O_{\rm diag}$ [5–7]) agrees or not with the universal predictions from a microcanonical ensemble $O_{\rm mic}$, that is, whether the equality below holds,

$$\overline{\langle\hat{O}(t)\rangle} \equiv O_{\rm diag} = \sum_\alpha |C_\alpha|^2 O_{\alpha\alpha} \overset{?}{=} O_{\rm mic} = \frac{1}{\mathscr{N}_{E,\Delta E}} \sum_{\substack{\alpha \\ |E-E_\alpha|<\Delta E}} O_{\alpha\alpha}.$$

Above $\mathscr{N}_{E,\Delta E}$ is the number of energy eigenstates with energy in the window $[E - \Delta E, E + \Delta E]$ and $O_{\alpha\alpha}$ are the eigenstate expectation values (EEVs).

Already in the 90's, Deutsch [8] and Srednicki [9] argued that this equality should hold when the expectation values of few-body observables do not fluctuate for eigenstates close in energy, which became known as the Eigenstate Thermalization Hypothesis (ETH). ETH was shown to be valid when the system is fully chaotic and its eigenstates are random vectors; expectation values of observables obtained with different random vectors close in energy should be very similar. Thus, the structure of the eigenstates plays a fundamental role in the studies of thermalization [10, 11]. However, only for random matrices can all the eigenstates be chaotic. Real systems are not described by random matrices [12, 13]. They have few-body interactions, usually only two-body interactions, and are then described by banded matrices. Contrary to random matrices, where the density of states is semicircular, the level density of banded matrices is Gaussian, which leads to chaotic (but not necessarily fully chaotic) eigenstates only away from the edges of the spectrum. Therefore, thermalization may only happen away from the edges of the spectrum [14–16].

Next, we briefly examine numerical results obtained in Refs. [15, 16], which show the strong relationship between the onset of quantum chaos and thermalization.

2. Numerical results and conclusions

We consider a 1D HCB model with nearest-neighbor (NN) hopping t and interaction V, and next-nearest-neighbor (NNN) interaction V'. The Hamiltonian is given by

$$\hat{H}_b = \sum_{i=1}^{L} \left[-t \left(\hat{b}_i^\dagger \hat{b}_{i+1} + \text{H.c.} \right) + V \left(\hat{n}_i - \frac{1}{2} \right) \left(\hat{n}_{i+1} - \frac{1}{2} \right) + V' \left(\hat{n}_i - \frac{1}{2} \right) \left(\hat{n}_{i+2} - \frac{1}{2} \right) \right], \tag{1}$$

where L is the size of the chain, $\hat{b}_i$ ($\hat{b}_i^\dagger$) is the bosonic annihilation (creation) operator on site i and $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ is the boson local density operator. We set $\hbar = 1$, $t = 1$, and take advantage of the translational symmetry of Hamiltonian (1) to independently diagonalize each block with total momentum k. In the particular case of $k = 0, L/2$, parity is also conserved and, at half-filling, particle-hole symmetry is present.

The system shows two transitions: from integrability to chaos, as V' increases from zero, and away from chaoticity and towards the atomic limit for larger values of V'. In addition, it opens a gap above a critical point [17]. In contrast, the model is gapless in the thermodynamic limit when NNN hopping is also included. This case was considered in Ref. [14], where differences in behavior associated with particle statistics were analyzed. It was shown that the transition to chaos in fermionic systems requires integrability breaking terms larger than in the bosonic case and that with respect to eigenstate structures, larger fluctuations are verified for fermions.

At 1/3 filling, we set $V = 6$ and vary V' ($0 \leq V' \leq 9$). In the thermodynamic limit, a gap opens for $V' \geq V'_c = 3$. In Fig. 1 (A), the level spacing distribution $P(s)$ is parametrized by β, which is used to fit the Brody distribution [12], $P_B(s) = (\beta+1)bs^{\beta}\exp\left(-bs^{\beta+1}\right)$, where $b = \left[\Gamma\left(\frac{\beta+2}{\beta+1}\right)\right]^{\beta+1}$. Two transitions are seen: from integrable [$\beta \to 0$, $P(s)$ is Poissonian] to chaotic [$\beta \to 1$, $P(s)$ is Wigner-Dyson] as V' increases from $V' = 0$, and a departure from chaoticity for large values of V'. A strong dependence of the results on the system size is also observed. For larger systems, (i) smaller values of V' lead to the first integrable-chaos transition and (ii) larger values of V', beyond the gapless-gapped transition point, are required for the second transition [15].

↪ *Item (i) suggests that in the thermodynamic limit an infinitesimally small integrability breaking term suffices for the onset of chaos.*

↪ *Item (ii) indicates that chaos emerges even in the gapped phase.*

The inverse participation ratio (IPR) measures the level of delocalization of the eigenstates [18]. For an eigenstate $|\psi_\alpha\rangle$ of (1) written in the basis vectors $|\phi_j\rangle$ as $|\psi_\alpha\rangle = \sum_{j=1}^{D_k} c_\alpha^j |\phi_j\rangle$, we have $\mathrm{IPR}_\alpha \equiv (\sum_{j=1}^{D_k} |c_\alpha^j|^4)^{-1}$. The choice of basis for the analysis of the structure of the eigenstates depends on the questions we want to address [11]. In Fig. 1 (B), we investigate IPR in two bases: the mean-field (mf) basis ($\mathrm{IPR}_{\mathrm{mf}}$) and the k-basis (IPR_k). In the first case, $|\phi_j\rangle$'s are the eigenstates of the integrable Hamiltonian ($V' = 0$); this choice separates regular from chaotic behavior. In the second case, $|\phi_j\rangle$'s are the total momentum basis vectors. The values of IPRs for eigenstates close in energy fluctuate significantly as one moves away from the chaotic limit, namely, as $V' \to 0$, where the system localizes in the mf-basis, and for $V' \gg V'_c$, where the system localizes in the k-basis. Thus, ETH is

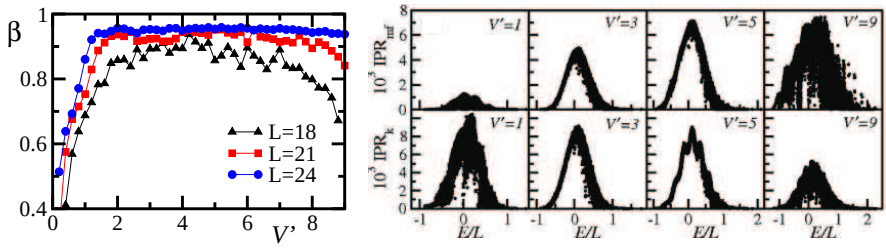


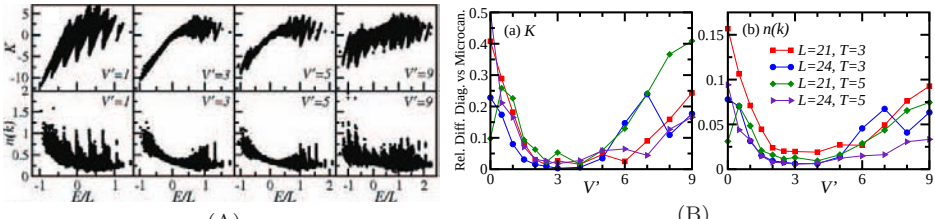
Fig. 1. (A) Parameter β of the Brody distribution used to fit the average of the level spacing distributions over all sectors with $k = 1, \ldots, \lfloor (L-1)/2 \rfloor$. (B) Inverse participation ratio in the mean-field (top) and momentum (bottom) basis vs energy per site; $L = 24$, $k = 2$, $D_k = 30\,624$.

not expected to hold in these regions. On the contrary, for intermediate values of V' (including $V' \gtrsim V'_c$), $\mathrm{IPR}_{\mathrm{mf}}$ and IPR_k become smooth functions of energy [15].
↪ *We thus anticipate compliance with the ETH even after the opening of the gap.*
↪ *Notice, however, that chaotic/delocalized eigenstates appear away from the edges of the spectrum, since model (1) has only two-body interactions.*

Figure 2 (A) shows the EEVs of the kinetic energy, $\hat{K} = \sum_i -t\left(\hat{b}_i^\dagger \hat{b}_{i+1} + \mathrm{H.c.}\right)$, and the momentum distribution function, $\hat{n}(k) = \frac{1}{L}\sum_{i,j} e^{-k(i-j)}\hat{b}_i^\dagger \hat{b}_j$, for all eigenstates of the Hamiltonian and for different values of V'. For small values of V' ($V' < 2$ for $L = 24$), there are large fluctuations of the EEVs of both observables over the entire spectrum. As V' increases and one departs from integrability, these fluctuations reduce in the center of the spectrum and ETH becomes valid [15]. Increasing V' even further increases the fluctuations of the EEVs once again as the eigenstates begin to localize in k-space.
↪ *The uniformization of the eigenvectors in the chaotic regime is reflected in the EEVs and guarantees the validity of ETH in the middle of the spectrum.*

The static properties shown in Figs. 1 and 2 help us to anticipate the results for the dynamics. It now remains to confirm whether the predictions are indeed correct. The procedure involves two steps. First, we verify that the observables relax to the values predicted by the diagonal ensemble, as shown in Ref. [15]. Second we check whether these results agree with the predictions of the microcanonical ensemble. If they do, then we say that thermalization has occurred.
↪ *Figure 2 (B) shows that the microcanonical ensemble predicts the outcome of the relaxation dynamics with high accuracy for the intermediate values of V' where ETH was shown to be valid.* It also depicts that the predictions of the microcanonical ensemble become more accurate with increasing system size, and that the agreement remains good for larger values of V' as the system size increases [15].

At 1/2 filling, it was demonstrated in Ref. [16] that the mixing of the remaining symmetries in each k-sector, parity and particle-hole, obscures the effects of level



(A) (B)

Fig. 2. (A) EEVs of K (top) and $n(k)$ (bottom) vs energy per site for the full spectrum (which include all momentum sectors); $L = 24$. (B) Relative differences between the predictions of the microcanonical and diagonal ensembles for (a) K and (b) $n(k)$ vs V'. The diagonal ensembles correspond to the quenches from nine initial states selected from the eigenstates of the Hamiltonian with $V'_{ini} = 0, 1, ..., 9$ (excluding the V' used to compute the relative difference). The nine states were chosen such that the energies are the same in all cases and correspond to a fixed value of the temperature T obtained from $E = \frac{1}{Z}\mathrm{Tr}\left\{\hat{H}e^{-\hat{H}/k_BT}\right\}$, where $Z = \mathrm{Tr}\left\{e^{-\hat{H}/k_BT}\right\}$ is the partition function, and $k_B = 1$.

repulsion and the transition to a Wigner-Dyson distribution is not verified even when the system is known to become chaotic. On the other hand, the two transitions, from integrability to chaos as V' increases from zero and from chaos to localization in k-space as $V' \to \infty$, are clearly captured by IPR and similar delocalization measures, even when eigenstates from different subspaces are considered. The same is verified for EEVs.
$\hookrightarrow$ *Measures of the complexity of the eigenvectors and EEVs are reliable quantities to identifying the chaotic region, especially when unknown symmetries are present.*
$\hookrightarrow$ *The existence of chaotic eigenstates when different symmetry sectors are mixed indicate that thermalization should still be valid in these situations.*

It remains to further investigate whether the presence of states close in energy (due to the mixing of symmetries) may affect the relaxation time. In terms of fluctuations after relaxation, we have shown that in the chaotic regime the off-diagonal elements of the few-body observables of interest are very small and so the fluctuations are also expected to be small [16].

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QUANTIZED OPEN CHAOTIC SYSTEMS

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Two different "wave chaotic" systems, involving complex eigenvalues or resonances, can be analyzed using common semiclassical methods. In particular, one obtains fractal Weyl upper bounds for the density of resonances/eigenvalues near the real axis, and a classical dynamical criterion for a spectral gap.

Keywords: Semiclassical limit; chaotic dynamics; quantum scattering; damped waves.

1. Introduction

These notes present a sketch of semiclassical methods which can be used to describe the spectral properties (and as a consequence, the long time properties) of a certain class of 1-particle quantum chaotic systems. Here are two examples:

- damped waves $\psi(x,t)$ on a compact riemannian manifold X of negative sectional curvature. The dynamics is described by the damped wave equation
$$\big(\partial_t^2 - \Delta_X + 2b(x)\partial_t\big)\psi(x,t) = 0\,, \tag{1}$$
and the *damping function* $b(x) \geq 0$ is assumed to be smooth.
- quantum scattering on $\mathbb{R}^d$, described by the Schrödinger equation
$$i\hbar\partial_t\psi(x,t) = P(\hbar)\psi(x,t)\,, \quad P(\hbar) = -\frac{\hbar^2\Delta}{2} + V(x)\,, \tag{2}$$
where the potential $V(x)$ has compact support and consists of 3 peaks centered on an equilateral triangle; $\hbar$ is Planck's constant.

These two systems seem very different. The configuration spaces are respectively compact and of infinite volume, the wave equation does not depend on $\hbar$; the damped wave equation can be rewritten in terms of a contracting semigroup, while the propagator $e^{-itP(\hbar)/\hbar}$ is unitary.

In the damped wave situation, Eq. (1) can be diagonalized by a discrete set of metastable modes $e^{-ik_jt}\psi_j(x)$, where $\psi_j(x) \in L^2(X)$ satisfies the generalized eigenvalue equation
$$\big(\Delta + k_j^2 + 2i\,b(x)\,k_j\big)\psi_j(x) = 0\,. \tag{3}$$

The eigenvalues k_j are complex, and lie in the strip $-2\max(b) \leq \Im k_j \leq 0$. We are interested in the distribution of these eigenvalues in the *high-frequency limit* $\Re k_j \to \infty$.

In the scattering situation (2), the Hamiltonian $P(\hbar)$ is selfadjoint on $L^2(\mathbb{R})$, with absolutely continuous spectrum on $\mathbb{R}_+$. However, the Green's function $(P(\hbar) - z)^{-1}(x, y)$, well-defined for $\Im z > 0$, admits a meromorphic continuation through $\mathbb{R}_+$ to the lower half-plane, with discrete poles $\{z_j(\hbar)\}$ of finite multiplicities (the *resonances* of $P(\hbar)$). We will investigate the distribution of these resonances, in the vicinity of a fixed energy $E > 0$, in the *semiclassical limit* $\hbar \to 0$. To each resonance is associated a metastable state $\psi_j(x)$, which is not in L^2 but formally decays with time as $e^{-itz_j(\hbar)/\hbar}\psi_j(x)$.

The *lifetime* of a metastable state is given by the *imaginary part* of the eigenvalue, $\tau_j = \frac{1}{2|\Im k_j|}$, resp. $\tau_j = \frac{\hbar}{2|\Im z_j(\hbar)|}$.

Here are some common features of the two systems. In §2.1 we show that the high-frequency limit $\Re k_j \to \infty$ is similar with the semiclassical limit $\hbar \to 0$. It is then relevant to study the corresponding *classical dynamics*: in the damped wave situation, it is the geodesic flow on X, while in the scattering case it is the Hamiltonian flow generated by the Hamiltonian $p(x, \xi) = \frac{|\xi|^2}{2} + V(x)$, in some energy interval $[E - \delta, E + \delta]$. Our assumptions on X or $V(x)$ imply that these classical flows are both "strongly chaotic".

In both cases, the long time properties of our quantum system involves a spectrum of complex "eigenvalues" associated with metastable states. Our main aim is to understand the distribution of the lifetimes τ_j in the semiclassical/high energy limit, especially the ones which are not infinitesimally small when $\hbar \to 0$: we will thus focus on resonances such that $|\Im z_j(\hbar)| = \mathcal{O}(\hbar)$.

2. Transformation to nonselfadjoint spectral problems

Each of these two quantum systems can be recast into a spectral problem for an associated nonselfadjoint differential operator on L^2, with discrete spectrum near the real axis.

2.1. *Damped quantum mechanics*

Following [1], let us start from the damped wave system. The generalized eigenvalue equation (3) for $\Re k_j \gg 1$ can be rewritten using an effective "Planck's constant" $\hbar \approx (\Re k_j)^{-1}$, and replacing k_j by the "energy" $z_j = \frac{(\hbar k_j)^2}{2} = 1/2 + \mathcal{O}(\hbar)$:

$$P_{dw}(\hbar)\psi_j = z_j\psi_j + \mathcal{O}(\hbar^2), \qquad P_{dw}(\hbar) = -\frac{\hbar^2\Delta}{2} - i\hbar b(x)\,. \tag{4}$$

The principal symbol of the operator $P_{dw}(\hbar)$, $p_0(x, \xi) = |\xi|^2/2$, is real and generates the geodesic flow on X. The skew-adjointness of $P_{dw}(\hbar)$ only appears in the subprincipal symbol $-i\hbar b(x)$: the latter does not influence the classical dynamics, but is responsible for the decay of probability along the flow. Indeed, for ψ_0 a wavepacket microlocalized on $\rho_0 = (x_0, \xi_0) \in T^*X$, its evolution $\psi(t) = e^{-itP_{dw}(\hbar)/\hbar}\psi_0$ will be another wavepacket microlocalized at $\rho_t = (x_t, \xi_t) = \Phi^t(\rho_0)$, with total probability

reduced by a finite factor

$$\frac{\|\psi(t)\|^2}{\|\psi_0\|^2} \approx \exp\Big(-2\int_0^t b(x_s)\,ds\Big)\,. \tag{5}$$

In the limit $\hbar \to 0$, one can speak of a *damped classical dynamics*: each point ρ_t evolves according to the geodesic flow, and carries a weight which gets reduced by the above factor along the flow.

The horizontal spectral density of $P_{dw}(\hbar)$ is given by Weyl's law, which (to lowest order) does not depend on the damping [1]: for any $c > 0$,

$$\sharp\{\mathrm{Spec}(P_{dw}(\hbar)) \cap ([1/2 - c\hbar, 1/2 + c\hbar] + i\mathbb{R})\} = \hbar^{-d+1}\big(c\,C_X + \mathscr{O}(1)\big)\,, \tag{6}$$

where $C_X > 0$ only depends on X. On the other hand, we will see that the distribution of the imaginary parts $\Im z_j(\hbar)$ strongly depends on the *interplay* between the geodesic flow and the damping $b(x)$.

2.2. *Complex scaled scattering Hamiltonian and open dynamics*

The scattering operator $P(\hbar)$ in (2) can be transformed to a nonselfadjoint one through the complex scaling method [2]. One deforms the configuration space $\mathbb{R}^d$ into a complex contour $\Gamma_\theta = \{x + i\theta f(x)\}$, where $f(x) = 0$ for x in a ball $B(0,R)$ containing the support of $V(x)$ (the "interaction region"), while $f(x) = x$ for $|x| \geq 2R$. We take an angle $\theta = M\hbar\log(1/\hbar)$, $M > 0$ fixed. This leads to a "scaled" operator $P_\theta(\hbar)$, which is no more selfadjoint: in the sector $-2\theta < \arg(z) \leq 0$ it admits discrete eigenvalues, which correspond to the resonances of $P(\hbar)$.

Our quest for resonances has turned into the spectral study of $P_\theta(\hbar)$. This operator admits the symbol

$$p_\theta(x,\xi) = p(x,\xi) - i\theta\langle \xi, df(x)^t\xi\rangle + \mathscr{O}(\theta^2)|\xi|^2\,, \qquad p(x,\xi) = \frac{|\xi|^2}{2} + V(x)\,.$$

The operator $P_\theta(\hbar)$ presents similarities with (4): its principal symbol $p(x,\xi)$ is real and generates the Hamiltonian flow on $p^{-1}(E)$, while its imaginary part is of higher order $\hbar\log(1/\hbar)$, and generates a damping outside $B(0,R)$. One difference with P_{dw} lies in the strength of this damping: for an initial wavepacket localized on a point $\rho_0 \in p^{-1}(E)$, the full probability after time t will be reduced by a factor $\hbar^{2M\int_0^t \langle \xi_s, df(x_s)^t\xi_s\rangle ds}$: the probability is semiclassically strongly suppressed as soon as the trajectory enters the zone where $\langle \xi, df(x)^t\xi\rangle > 0$ (this "absorbing zone" contains the exterior of $B(0,2R)$).

Classically, this corresponds to an "open dynamics": the point ρ_t evolves according to the Hamiltonian flow, but it gets "absorbed", or "killed" as soon as it enters the absorbing zone.

Trapped set

For any energy $E > 0$, the forward (resp. backward) trapped set K_E^- (resp. K_E^+) is defined as the set of initial points which remain bounded for all positive (resp. negative) times:

$$K_E^\mp = \{\rho_0 = (x_0,\xi_0) \in p^{-1}(E),\ |x_t| \leq R,\ \forall t \gtrless 0\}\,,$$

while the trapped set is made of their intersection $K_E = K_E^- \cap K_E^+$. Notice that K_E is a compact flow-invariant set. The above remark shows that any wavepacket localized on a point $\rho_0 \notin K_E^-$ will be absorbed after a finite time, namely the time it takes to enter the absorbing zone. On the other hand, a point $\rho \in K_E^-$ will converge to the trapped set K_E as $t \to \infty$. This argument shows that, in some sense, long time quantum mechanics (at energy $\approx E$) takes place on K_E.

3. Fractal Weyl laws

The above argument can be made precise when estimating the number of resonances of $P(\hbar)$ near E. In the case we are interested in, K_E is a hyperbolic repeller (that is, there is no fixed point on K_E, and all trajectories are hyperbolic), this number is bounded above by a *fractal Weyl law* directly related with the geometry of K_E [4].

Theorem 3.1. *Assume that the trapped set K_E at some energy $E > 0$ is a hyperbolic repeller, and write its Minkowski dimension $\dim_M(K_E) = 1 + 2\nu$. Then for any $c, \alpha > 0$, one has in the semiclassical limit*

$$\sharp\{\mathrm{Res}(P(\hbar)) \cap ([E - c\hbar, E + c\hbar] - i\hbar[0, \alpha])\} = \mathscr{O}(\hbar^{-\nu-0}) . \tag{7}$$

This theorem is proved by conjugating $P_\theta(\hbar)$ by a suitable "weight" $G(\hbar)$, so that the symbol $p_{\theta,G}$ of the conjugated operator $e^{-G(\hbar)} P_\theta e^{G(\hbar)}$ satisfies $\Im p_{\theta,G} < -2C\hbar$ outside the $\sqrt{\hbar}$-neighbourhood of K_E. Estimating the volume of this neighbourhood, and some involved pseudodifferential calculus on $p_{\theta,G}$, lead to the above upper bound.

A similar argument can be used to study the distribution of decay rates $\Im z_j/\hbar$ for the operator (4). For any time $T > 0$, one can construct a weight $G_T(\hbar)$, such that the conjugate operator $P_{dw,G_T}(\hbar) = e^{-G_T(\hbar)} P_{dw}(\hbar) e^{G_T(\hbar)}$ admits the symbol

$$p_{dw,G_T}(x, \xi) = \frac{|\xi|^2}{2} - i\hbar b_T(x, \xi) + \mathscr{O}(\hbar^2) , \tag{8}$$

where the subprincipal symbol $b_T(\rho) = T^{-1} \int_{-T/2}^{T/2} b(x_t)\, dt$ is the average of the damping along the flow. The geometric assumption of negative curvature implies that the geodesic flow on X is *Anosov*, in particular it is ergodic. This implies that, on the energy shell $p^{-1}(1/2)$, the time average $b_T(\rho)$ converges almost everywhere to the microcanonical average $\bar{b} = \mathrm{Vol}(X)^{-1} \int_X b(x) dx$ when $T \to \infty$. From there one can deduce that most of the eigenvalues $\Re z_i(\hbar) \in [1/2, c\hbar, 1/2 + c\hbar]$ concentrate near the "typical line" $\Im z = -\hbar\bar{b}$ [1].

Using finer properties of the Anosov geodesic flow, one can estimate the number of eigenvalues away from this "typical line" [3]. To state the result, we need to introduce the extremal ergodic averages of the damping, $b_- = \lim_{T\to\infty} \min_{p^{-1}(1/2)} b_T$, and similarly for b_+.

Theorem 3.2. *Assume X is a compact surface of negative curvature. Then, there exists a function $H : \mathbb{R} \to \mathbb{R}$, strictly concave on $[b_-, b_+]$ and equal to $-\infty$ outside, with maximum $H(\bar{b}) = d - 1$, such that for any $c > 0$ and any $\alpha \in [0, \bar{b}]$,*

$$\sharp\{\mathrm{Spec}(P_{dw}(\hbar)) \cap ([1/2 - c\hbar, 1/2 + c\hbar] - i\hbar[0, \alpha])\} = \mathscr{O}(\hbar^{-H(\alpha)-0}) . \tag{9}$$

A similar estimate holds for the range $\Im z \geq \hbar\alpha$, $\alpha > \bar{b}$.

Comparing this "fractal Weyl upper bound" with the Weyl law (6) confirms that most resonances are on the typical line. The above theorem is obtained by studying the *large deviations* of the value distribution of b_T in the limit $T \to \infty$: roughly speaking, for $\alpha < \bar{b}$, the volume of the points $\rho \in p^{-1}(1/2)$ such that $b_T(\rho) \leq \alpha$ decays like $e^{T(H(\alpha)-(d-1))}$. This volume estimate is then used to get (9).

In both situations, the upper bounds on counting resonances/eigenvalues were obtained by deforming the operator P_θ (resp. P_{dw}) by an appropriate microlocal weight, and studying the imaginary part of the resulting operator by phase space volume arguments, where the classical dynamics plays a prominent rôle.

3.1. *Spectral gaps*

We now present a complementary type of spectral information, which can be obtained by a similar method for these two systems. Namely, we want to understand if the lifetimes $\tau_j(\hbar)$ can be arbitrarily large in the semiclassical limit; or on the opposite, if there exists a *gap* of size $\propto \hbar$ between the real axis and the eigenvalues/resonances. The presence of such a gap has important consequences on the long time properties of the system.

Let us start with the scattering problem. The gap question can be rephrased as: "Are the metastable states able to concentrate on K_E when $\hbar \to 0$?" The answer will result from a *competition* between, one one side, the fast dispersion of wavepackets due to the hyperbolic classical flow, on the other side the "thickness" of the trapped set allowing the state to reconstruct itself through constructive interferences.

A dynamical quantity reflecting this competition is of statistical nature, it is a *topological pressure* associated with the flow on K_E:

$$\mathscr{P}(-\varphi_u/2) = \lim_{T\to\infty} \frac{1}{T} \log \sum_{\gamma : T_\gamma \leq T} \exp\Big(- \int_0^{T_\gamma} \varphi_u(\rho_t)/2 \, dt \Big) .$$

Each γ is a periodic orbit in K_E with period T_γ, and $\varphi_u(\rho)$ is the unstable Jacobian of the flow. The above mentioned competition lies in the fact that each exponential weight gets very small when $T_\gamma \to \infty$, while the number of terms grows exponentially.

The following gap criterion was first obtained [5] for the case of hard obstacles, and then generalized in [6] to smooth potentials.

Theorem 3.3. *Assume the trapped set K_E is a hyperbolic repeller. If the pressure $\mathscr{P}(-\varphi_u/2) < 0$, then for any $c > 0$ and any small enough $\hbar$, the strip $[E - c\hbar, E + c\hbar] + i\hbar[\mathscr{P}(-\varphi_u/2) + 0, 0]$ does not contain any resonance of $P(\hbar)$.*

In dimension $d = 2$, the condition $\mathscr{P}(-\varphi_u/2) < 0$ is equivalent with a purely geometric statement, namely the fact that the Hausdorff dimension $\dim_H(K_E) < 2$ (notice that $\dim_H p^{-1}(E) = 3$).

In the case of damped waves, the gap question is nontrivial if $b_- = 0$, that is, if there exists a flow-invariant subset of $p^{-1}(1/2)$ with no damping. A result similar to the one above was obtained in [7]. In this case, the local decay of probability is due to both hyperbolic dispersion and damping.

Theorem 3.4. *Assume that X has negative curvature, and that the topological pressure $\mathscr{P}(-\varphi_u/2 - b) < 0$. Then, for any $c > 0$, and $\hbar > 0$ small enough, the strip $[1/2 - c\hbar, 1/2 + c\hbar] + i\hbar[\mathscr{P}(-b - \varphi_u/2) + 0, 0]$ does not contain eigenvalues of $P_{dw}(\hbar)$.*

4. Open questions

Most of the above results are upper or lower bounds. The natural question is: "Are these bounds sharp?" The fractal Weyl bound (7) is conjectured to be sharp for $\alpha > 0$ large enough, a fact which has been tested numerically on a number of examples, but could be proved only for a very specific toy model [8]. On the opposite, the bounds (9) for eigenmodes of the damped wave equation are not expected to be sharp for all values of α. The size of the gap itself is believed to be larger than the topological pressure bound we gave above. Such an "extra gap" was proved for the 3-disk scattering, using advanced estimates on classical mixing [9].

Acknowledgments

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OTHER TALKS

INVITED TALK

CLASSICAL ORBIT CORRELATIONS: THE KEY FOR UNDERSTANDING UNIVERSALITY IN QUANTUM CHAOTIC SYSTEMS

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A chaotic classical system is characterized by apparently random, ergodic phase space flow. However, a closer inspection shows that (periodic) orbits in chaotic systems are not independent but appear in bundles exhibiting strong classical correlations. While hidden in classical dynamics, these correlations are revealed through constructive interference in the corresponding quantum system.

I will introduce an advanced semiclassical path integral approach to demonstrate that such correlations are responsible for the universal behavior exhibited by quantum systems with a chaotic classical limit. Thereby I will provide a microscopic understanding of random matrix theory predictions for this universal behavior. This is relevant for spectral statistics but moreover in particular for chaotic scattering and for transport processes. I will address recent applications of this semiclassical theory to quantum transport of electrons on mesoscopic scales [1].

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CONTRIBUTED TALKS

MANY-PARTICLE SYSTEMS ON QUANTUM GRAPHS WITH SINGULAR INTERACTIONS

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Single quantum particles on graphs have proven to provide interesting models of complex quantum systems; their spectral properties have been studied in great detail. In this talk we discuss extensions to quantum many-particle systems on graphs with singular

interactions. We focus on two-particle interactions that are either localised at the vertices, or are of Dirac-delta type on the edges. In both cases the interactions are realised in terms of self-adjoint extensions of suitable Laplacians in two variables. These extensions can be characterised in terms of boundary conditions, and given particular boundary conditions the type of interactions can be identified. (This talk is based on joint work with Joachim Kerner.)

PARAMETER-DEPENDENT SPECTRAL STATISTICS OF QUANTUM GRAPHS

OLEH HUL

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Parameter-dependent spectral statistics of totally connected quantum graphs are studied. We consider two different types of spectra of quantum graphs. The first one is the spectrum of the Laplacian on a metric graph, and the second one is the spectrum (eigenphases) of the scattering matrix of a quantum graph. We found out that in both cases the parameter-dependent spectral statistics are very similar to each other.

INTEGRABLE THEORY OF QUANTUM TRANSPORT IN CHAOTIC CAVITIES

EUGENE KANZIEPER

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In this talk, I will show that the paradigmatic problem of conductance fluctuations in chaotic cavities with broken time-reversal symmetry is completely integrable in the universal transport regime. This observation will be utilised to prove that the cumulant generating function of the Landauer conductance in the cavities probed via ballistic point contacts is given by the fifth Painlevé transcendent. If time permits, a closely related integrable theory of the noise power fluctuations in the crossover regime between thermal and shot noise will also be outlined.

Quantum field theory

Session organizer:

Dirk Kreimer

INVITED TALKS

RENORMALIZATION AND RESOLUTION OF SINGULARITIES

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I will describe the combinatorial features of perturbative renormalization of Feynman integrals using resolutions of singularities in the sense of algebraic geometry, for example the Fulton-MacPherson compactification of configuration spaces. I will also sketch the relation to the Connes-Kreimer Hopf algebras and to other recent advances in the area. This is based on joint work with R. Brunetti and D. Kreimer.

RENORMALISATION HOPF ALGEBRAS FOR GAUGE THEORIES AND BRST SYMMETRIES

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The structure of the Connes–Kreimer renormalization Hopf algebra is studied for Yang-Mills gauge theories, with particular emphasis on the BRST-formalism. A coaction of the renormalization Hopf algebra is defined on the coupling constants and the fields. In this context, BRST-invariance of the action implies the existence of certain Hopf ideals in the renormalization Hopf algebra, encoding the (physical) Slavnov-Taylor identities for the coupling constants.

CONTRIBUTED TALKS

TOPOLOGICAL CHARGES FOR FINITE ENERGY FIELDS IN A SIGMA MODEL

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In the (2+1)-dimensional classical $O(3)$ sigma-model, all finite energy fields have integer topological charges regardless of their asymptotic behavior at infinity. Topological charge is conserved for the fields with finite Euclidean action, without further assumptions on the field equations or asymptotics. The fields with continuous first derivatives as well as fields in Sobolev-like spaces analogical to $W^{1,2}$ are considered.

PARAMETER-DEPENDENT SPECTRAL STATISTICS OF QUANTUM GRAPHS

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A novel deformation procedure has recently been proposed by Grosse and Lechner as a tool for construction of interacting quantum field theories with observables localized in spacelike wedges. In this talk this procedure is applied to two-dimensional theories of massless particles. The behavior of the scattering matrix under the deformation is obtained explicitly. It is shown that the deformation procedure not only introduces interaction but also preserves the property of asymptotic completeness. In particular, the deformations of chiral conformal quantum field theories give rise to interacting, wedge-local models which are asymptotically complete.

EXACT SOLUTION OF A $2+1$ DIMENSIONAL INTERACTING FERMION MODEL

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We present a quantum field theory model describing interacting fermions in 2+1 dimensions that can be solved exactly using bosonization (to our knowledge, this model was first proposed by Mattis). This model gives an effective description of spinless fermions on a square lattice with local hopping and density-density interactions if, close to half

filling, the system develops a partial energy gap. We present arguments that, after appropriate renormalizations, all short- and long distance cutoffs in this model can be removed. Based on common work with Jonas de Woul.

GROUND STATE OF SUPERSYMMETRIC MATRIX MODELS

DOUGLAS LUNDHOLM

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We review recent progress concerning the problem of determining existence, uniqueness, and structure of zero-energy ground states in supersymmetric matrix models, which arise from a quantum mechanical description of relativistic membranes, reduced Yang-Mills gauge theory, and of nonperturbative features of string theory, respectively M-theory. One of the recent approaches involves introducing a weighted Hilbert space, and counting the number of negative eigenvalues of a certain perturbation of the associated matrix-valued Schrödinger operator.

FACTORIZATION METHOD AND SPECIAL ORTHOGONAL FUNCTIONS

HOSSEIN MOTAVALLI

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We present a general construction for ladder operators for the special orthogonal functions based on Nikiforov-Uvarov mathematical formalism. A list of creation and annihilation operators are provided for the well known special functions. Furthermore, we establish the dynamic group associated with these operators.

INFRARED ASPECTS OF A MODEL OF QFT ON A STATIC SPACE TIME

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We consider the Nelson model with variable coefficients, which can be seen as a model describing a particle interacting with a scalar field on a static space time. We consider the problem of the existence of the ground state, showing that it depends on the decay rate of the coefficients at infinity. We also show that it is possible to remove the ultraviolet cutoff, as it is in the flat case (joint work with C.Gérard, F.Hiroshima, A.Suzuki).

ASYMPTOTIC COMPLETENESS BELOW THE TWO-BOSON THRESHOLD OF THE TRANSLATION INVARIANT NELSON AND POLARON MODELS

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We present some recent results on a class of models including the massive translation invariant Nelson model and the Polaron model of H. Fröhlich. The results are valid for arbitrary values of the coupling constant, and include absence of singular continuous spectrum below the two-boson threshold as well as a partial asymptotic completeness result, valid for the model restricted to the associated subspace. As a by-product, we get a so-called geometric asymptotic completeness result, which holds for the full model. The talk is based on joint work with Jacob Schach Møller.

KREIN SPACES IN DE SITTER QUANTUM THEORIES

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Experimental evidences and theoretical motivations lead to consider the curved space-time relativity based on the de Sitter group $SO(1,4)$ or $Sp(2,2)$ as an appealing substitute to the flat space-time Poincare relativity. Quantum elementary systems are then associated to unitary irreducible representations of that simple Lie group. At the lowest limit of the discrete series lies a remarkable family of scalar representations involving Krein structures and related indecomposable representation cohomology which deserves to be thoroughly studied in view of quantization of the corresponding carrier fields. The purpose of this presentation is to indicate possible extensions of an exemplary case, namely the so-called de Sitterian massless minimally coupled field. This is a joint work with J.-P.Gazeau and A. Youssef.

Quantum information

Session organizer:

Julia Kempe

INVITED TALKS

THE QUANTUM AND CLASSICAL EMBEDDING PROBLEMS

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The embedding problem is a long-standing open problem in probability theory, dating at least as far back as 1937. The problem is to characterise of the stochastic maps that can be generated by a continuous-time Markov process. A very similar question can be asked in the quantum setting, where the problem becomes one of characterising the completely-positive maps that can be generated by a master equation.

From the literature, these may appear to be very abstract mathematical problems. Far from it! The embedding problem (and its quantum generalisation) is closely related to a very practical task in experimental physics. Imagine that you have gathered a large amount of measurement data for some physical system, whose behaviour you would like to understand. The embedding problem is essentially the problem of using that experimental data to reconstruct the dynamical equations of the system.

In recent work, we [1,2] finally layed both the classical and quantum embedding problems to rest, by proving that they are NP-hard. I will explain the embedding problems and their relation to physics, outline their recent resolution, and discuss their implications.

T.S. Cubitt, J. Eisert, M.M. Wolf, `arXiv: 0908.2128 [math-ph]`
T.S. Cubitt, J. Eisert, M.M. Wolf, `arXiv: 1005.0005 [quant-ph]`

HOLOGRAPHIC QUANTUM STATES

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In this talk I'll describe how continuous matrix product states of quantum field theories can be described in terms of the dissipative non-equilibrium dynamics of a lower-dimensional auxiliary boundary field theory. This equivalence illustrates an intimate connection between the theory of continuous quantum measurement and quantum field theory and gives an explicit construction of the boundary field theory allowing the extension of real-space renormalization group methods to arbitrary dimensional quantum field theories without the introduction of a lattice parameter.

MIXING TIMES OF QUANTUM MARKOV PROCESSES

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We will talk about mixing times of quantum stochastic processes, and discuss applications to quantum spin systems, quantum field theories and the construction of novel quantum algorithms.

CONTRIBUTED TALKS

PERFECT STATE TRANSFER WITHIN NETWORKS OF ARBITRARY TOPOLOGY

THOMAS BROUGHAM

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The task of constructing a quantum computer has many technical challenges associated with it. One such example is transferring the state of a quantum system between different components of a quantum computer [1]. A common approach to this problem is the use of a quantum wire, i.e. a chain or network of coupled quantum systems where the interactions are such that the quantum state is transferred through the wire. Many different realizations of such perfect state transfer (PST), using quantum wires, have been proposed [2-4]. The approach that is often taken to the problem of PST is to construct a Hamiltonian and show that this allows the state to be perfectly transferred. An alternative approach has been proposed that enables a broad class of Hamiltonians to be constructed [5]. This approach does not make any assumptions about the coupling or the topology of the network. Instead, a class of Hamiltonians that lead to a particular permutation are derived. This work was developed for the task of transferring a state between two points in a network. We will show how one can use the formalism outlined in [5] to control quantum information in a more general manner. For example, we may wish to transfer a state to several different nodes within a network, at different times. This would enable us to generalize the problem of PST to networks with a nontrivial logical bus topology. The formalism can also be used to find Hamiltonians that enable PST when we have multiple interacting excitations.

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CONTROLLABILITY OF QUANTUM WALKS ON GRAPHS

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In recent years, quantum walks on graphs have emerged as one of the most useful protocols to design quantum algorithms. The study of the controllability of these systems refer to the analysis of the set of states the system can be in. In this talk, I will consider discrete time quantum walks on graphs with coin. These systems consist of two coupled quantum systems: a walker system whose states are in correspondence with the nodes of the underlying graph and a coin system whose states indicate the directions for the motion on the graph. The evolution consists of two operations at each step: a coin tossing operation which is a unitary operation on the space of the coin only and a conditional shift operation which changes the state of the walker system according to the current value of the coin. The talk deals with the case where the coin operation can be changed at every time step and presents a study of the set of possible evolutions and states. The first result discussed says that the set of available unitary transformations is a Lie group whose Lie algebra can be described explicitly in every case. The system is called completely controllable if the set of available evolutions is the full unitary group. I give both Lie algebraic and combinatorial tests to check complete controllability. In particular, the combinatorial tests are based on the construction of an auxiliary graph whose connectedness is equivalent to the controllability of the given system. This test avoids Lie algebraic calculations which typically involve commutators of very large matrices. I prove that controllability only depends on the underlying graph and not on the specific quantum walk considered on it. It is in particular always verified for complete graphs and product graphs of controllable systems. In view of this dynamical and control theoretic analysis, in the second part of the talk, I take a different look at two issues of current interest in quantum information: quantum algorithms and approximation of continuous dynamics by discrete time quantum walks. A quantum algorithm is a sequence of unitary operations to transfer the state of a quantum system from an initial value to a desired final value. As such, it can be seen as a control algorithm. I provide general constructive algorithms to transfer between two arbitrary states for a quantum walk. These consist of appropriate sequences of coin tossing operations and conditional shifts. I give an upper bound on the number of steps needed for an arbitrary transfer which depends on the features of the underlying graph. Furthermore, I discuss the interplay of these results with two types of algorithms of current interest in quantum information: search algorithms on a graph and algorithms to generate certain outputs with a prescribed probability distribution which are at the heart of classical randomized algorithms. As for the approximation of continuous time dynamics by discrete time quantum walks, the controllability analysis leads to the study of a special Lie algebra of skew-Hermitian operators on the full space for the coin and walker systems. The continuous time evolutions corresponding to Hamiltonians in this Lie algebra (modulo multiplication by the imaginary unit) can be reproduced using the discrete time quantum walk. This can be achieved both exactly and approximately with various constructive methods. I illustrate this using an example: a quantum walk on a 2-dimensional periodic lattice. Of particular interest are dynamics that correspond to continuous time quantum walks on the same graph. The described results give a general method to obtain the continuous time quantum walk as a limit of the discrete time quantum walk and, in that, answer an open question in quantum information theory. Moreover they offer tools to compare the performance of the discrete and continuous quantum walks in several cases. [In collaboration with Dr. F. Albertini at the University of Padova, Italy]

PHASE TRANSITIONS AND METASTABILITY IN THE DISTRIBUTION OF THE BIPARTITE ENTANGLEMENT OF A LARGE QUANTUM SYSTEM

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We study the distribution of the Schmidt coefficients of the reduced density matrix of a quantum system in a pure state. By applying general methods of statistical mechanics, we introduce a fictitious temperature and a partition function and translate the problem in terms of the distribution of the eigenvalues of random matrices.We investigate the appearance of two phase transitions, one at a positive temperature, associated with very entangled states, and one at a negative temperature, signaling the appearance of a significant factorization in the many-body wave function. We also focus on the presence of metastable states (related to two-dimensional quantum gravity) and study the finite size corrections to the saddle point solution.

CLASSICAL STATISTICAL MECHANICS APPROACH TO MULTIPARTICLE ENTANGLEMENT

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We characterize the multipartite entanglement of a system of n qubits in terms of the distribution function of the bipartite purity over balanced bipartitions. We search for maximally multipartite entangled states, whose average purity is minimal, and recast this optimization problem into a problem of statistical mechanics, by introducing a cost function, a fictitious temperature and a partition function. By investigating the high-temperature expansion, we obtain the first three moments of the distribution [1]. On the other hand, when many bipartitions are considered, the requirement that purity be minimal for all bipartitions can engender conflicts and frustration arises. This unearths an interesting link between frustration and multipartite entanglement [2].

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OPTIMAL PARAMETRIZATIONS OF ADIABATIC PATHS

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The parametrization of adiabatic paths is optimal when tunneling is minimized. Hamiltonian evolutions do not have unique optimizers. However, dephasing Lindblad evolutions do. The optimizers are simply characterized by an Euler-Lagrange equation and have a constant tunneling rate along the path irrespective of the gap. Application to quantum

search algorithms recovers the Grover result for appropriate scaling of the dephasing. Dephasing rates that beat Grover imply hidden resources in Lindblad operators.

ENTANGLEMENT AND FUNCTIONS OF NILPOTENT VARIABLES

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Within supersymmetric theories fermions are described with use of the grassmannian variables - anticommuting, hence, nilpotent. Recently proposed formalism based on nilpotent, but commuting variables, turns out to be suitable to describe qubit systems. Separability of multiqubit states can be examined in terms of factorability of functions of such nilpotent variables. Relevant functional determinants are naturally linked to the invariants known from the Classical Invariant Theory, and used for characterization of multiqubit pure state entanglement. I will present the "nilpotent" analog of the Schroedinger representation and formalism for description multiqubit systems and entanglement. It turns out that some of interesting multiqubit entangled states proposed in quantum optics context, are represented by elementary functions of nilpotent variables.

SINGLE PHOTON QUANTUM WALK WITH ADJUSTABLE COIN OPERATIONS

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We present a robust implementation of a coined quantum walk over 14 steps using only passive optical elements. At the core of our realization is a fiber optical network loop which allowed to keep the amount of required resources constant as the walker's position Hilbert space is increased. We have observed a non-Gaussian distribution of the walker's final position, thus characterizing a faster spread of the photon wave packet in comparison to the classical random walk. The walk is realized for many different coin settings and initial states, necessary for future implementation of quantum-walk-based search algorithms.

ASYMPTOTIC DYNAMICS OF QUANTUM SYSTEMS UNDER RANDOM UNITARY EVOLUTION

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We investigate the asymptotic dynamics of quantum systems resulting from large numbers of iterations of randomly applied unitary quantum operations. Despite the fact that

in general the evolution superoperator of such random unitary operations cannot be diagonalized it is shown that the resulting iterated asymptotic dynamics is described by a diagonalizable superoperator. As a consequence it turns out that tipically the resulting iterated asymptotic dynamics is governed by a low dimensional attractor space which is determined completely by the unitary transformations involved and which is independent of the probability distributions with which these unitary transformations are selected. Based on this general approach analytical results are presented for the asymptotic dynamics of large qubit networks whose nodes are coupled by randomly applied unitary operations. These networks appear to be a good tool for studying phenomena like decoherence, thermalization or quantum homogenization.

QUANTUM LÉVY WALKS

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Quantum walks form an interesting paradigm for quantum computing, which has been appreciated mainly for the faster spreading than classical random walks allow. On the other hand, in the classical theory one can meet so-called Levy random walks, which, by relaxing the condition on the locality of the steps, also have interesting spreading and hitting properties. Recently, Lévy walks have been shown to be optimal for searching for sparse samples in 2D, and they have been observed to be used for this purpose in real natural processes. In this talk, we propose a novel concept of Quantum Lévy Walks, obtained by combining of the two above enhancements of a random walk. We define a quantum Lévy walk on an infinite line and on a circle and discuss their basic properties. We briefly address the potential uses of this theory.

MOLECULAR SOLUTION FOR THE SUBSET-SUM PROBLEM ON DNA-BASED QUANTUM COMPUTING

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Molecular computation was proposed by Feynman in 1961 and it was showed that computing devices based on quantum theory are able to finish computations faster than the standard Turing machines. In 1994, Adleman succeeded to solve an instance of the Hamiltonian path problem in a test tube, just by handling DNA strands. Lipton investigated a special case of more general methods that could solve NP-complete problems using DNA experiments. Deutsch presented a general model of quantum computation i.e., the quantum Turing machine. Molecular solution for the subset-sum problem on DNA-based supercomputing has been offered by Chang in 2003. It has been proved, the subset-sum problem is the NP-complete problem (Cormen et al., 2003; Garey and Johnson, 1979; Cook, 1971; Karp, 1972).

Here, a finite set $S = \{s_1, \ldots, s_q\}$ is defined for solving subset-sum problem using DNA-based algorithm and it is supposed that every elements in S are positive integer. Now the aim is finding possible subsets S_i as a subset of S such that the sum of all elements in S_i be exactly equal to b, where b is a positive integer and can implement

by Hadamard gates, NOT gates, CNOT gates, CCNOT gates, Grover's operators, and quantum measurements on a quantum computer. In order to achieve this, first we use q number Hadamard gates to construct 2^q possible subsets of a q-element set S, then we apply NOT gates, CCNOT gates and Grover's operators to construct solution space. It is demonstrated, the DNA-based quantum algorithm of an n-qubit parallel adder and a DNA based quantum algorithm of an n-qubit parallel comparator can implement using quantum gates and Grover's operators to formally verify our designed molecular solutions for the subset-sum problem. For this propose, we introduce some quantum registers again and compute solutions spaces, in each step by using 19-CCNOT gates , and NOT gates. Last algorithm is parallel comparator for comparing the sum of elements for subsets of a finite set with any given positive integer by using quantum gates and Grover's operators.

OPTIMAL REPLICATION OF VON NEUMANN MEASUREMENTS

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Suitable mathematical representation of objects emerging in quantum mechanics is crucial for solving most of the optimization problems. Introduction of Process Positive Operator Valued Measures (PPOVM) and Quantum Combs allowed to solve several problems in which the most general (thought) experiments involving N uses of a tested quantum channel (completely positive trace preserving maps) have to be optimized. In this contribution, we apply quantum combs to optimize quantum circuits achieving transformations of measurements. More precisely, such a circuit has to work as one big POVM after N measurements are inserted into the open slots of the circuit. The aim of the circuit is to create M replicas of the inserted measurements, which are assumed to be unknown POVMs of the Von Neuman type (i.e. non-degenerate projective measurements). We show that for arbitrary figure of merit the presence of measurements in the circuit allow us to restrict the optimization to a subclass of quantum combs, which are called diagonal. Using diagonal quantum combs we solve the following tasks: N→ 1, 1→2 Learning of a qudit POVM (N=1,2,3) and 1→2 Cloning of a qudit POVM. The goal of N→M Learning of a POVM is to use the unknown measurement N times, store what was learned about it in a quantum memory and later retrieve M uses of the original measurement on a state that is not available in the learning phase. In contrast in N→M Cloning of a POVM the state to be measured is available from the very beginning, but we have to mimic M>N uses of the unknown measurement by using it just N times. We compare the performance of the optimal 1→2 Learning with 1→2 Cloning of a POVM. Similarly, to the analogous tasks for unitary channels the performance of cloning is much better than that of learning. We discovered that the uses of the unknown measurements in the optimal circuit cannot be parallelized for 3→1 Learning of a qudit POVM. Thus, N→1 Learning of a qudit POVM represents a task, where the optimal strategy is necessarily sequential. This feature of non-parallelizability is present also in Grover algorithm, where the calls to the oracle cannot be parallelized as was shown by Zalka. Indirectly, our findings can help to understand how to search for optimal quantum circuits i.e. optimal quantum algorithms with oracle callings, which cannot be parallelized.

QUANTUM WALKS WITH TWO PARTICLES

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We study the motion of two non-interacting particles performing a quantum walk on a line. We focus on the spatial correlations and the meeting problem. Influence of entanglement and indistinguishability of the particles are analyzed. Applications to experimental realizations of two-dimensional quantum walks are briefly discussed.

DECAY OF COHERENT STATES FOR DAMPED HARMONIC OSCILLATOR

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In this study, we discuss the effect of damping on the coherent states of the harmonic oscillator. The damping is represented by an exponentially increasing mass in time.

UNCERTAINTY RELATIONS AND ENTANGLEMENT IN FERMION SYSTEMS

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The entanglement-related features of systems of identical fermions are relevant to the study of diverse physical systems and also have implications for the development of quantum information technology. However, the concept of entanglement in fermion systems differs from the corresponding concept in systems consisting of distinguishable subsystems. In particular, the development of criteria for entanglement detection for mixed quantum states is much more difficult in the case of fermion systems and remains a largely unexplored problem. The aim of the present contribution is to investigate the violation of uncertainty relations as a signature of entanglement for both pure and mixed states of two identical fermions. In the case of fermions with a four dimensional single particle Hilbert space we obtain several different types of uncertainty-related entanglement criteria based on local uncertainty relations, on the sum of variances of projectors and on various entropic measures. Within the latter approach we consider either entropic uncertainty relations involving a single observable or relations based upon the sum of entropies associated with more than one observable. We extend the projector based entanglement criterion to the case of two-fermion and three-fermion systems with a six dimensional single particle Hilbert space.

Physics of social systems

Session organizer:

Petr Šeba

MORPHOLOGY OF THE LAND PARCEL MOSAIC: THE KEY TO UNDERSTAND THE URBANIZATION PROCESS

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In this paper we report recent results concerning urbanization process inferred from the analysis of the morphology of the land parcel mosaic. The morphological analysis is based on the parcel size distribution, $f(a)$, and provides a criterion enabling unambiguous classification of each piece of land as (i) city core, (ii) suburbs, and (iii) rural area. Properties of the distribution $f(a)$ exhibit regularities and are robust with respect to geographical, historical, and economical conditions accompanying development of a given area. The urbanization process can be described in terms of the changes of the morphology of the patterns of land fragmentation. A simple model based on a two-dimensional bond percolation is employed to mimic the process of the formation of the city. We argue that the city emerges from a collection of separated settlements in a process that resembles a structural phase transition.

Keywords: Land fragmentation pattern; scaling laws; urbanization; land parcel; percolation.

1. Introduction

Many structures both natural and artificial such as cities, arise as a result of continuous complex processes. These processes transform the environment and leave behind a characteristic spatial structure a kind of their morphological fingerprint. In some cases it is possible to infer the nature of the process from the observed final structure. The best known examples of such morphological analysis concern spatial two-dimensional processes [1]. In this paper we discuss processes of land fragmentation that accompany the urbanization process. Here, the morphological fingerprint

is the mosaic formed by the land parcels.

Urban systems have been found to conform to universal scaling laws describing city growth and spatial organization. The best known is the Zipf's law [2]. According to this law, the distribution of cities population obeys a power-law with the exponent $n = 2$. The Zipf law has been confirmed in a number of studies [3–5]. The distribution of the fraction of cities of a given area follows the power-law with $n = 1.85$ [6, 7]. There is much empirical evidence [8, 9] that the large-scale urban structure displays fractal morphology. It has been shown in Ref. 10 that the spatial arrangement of cities on a plane can be successfully modeled using the classical theory of liquids. Recently, the diffusion-limited aggregation model has been employed [6, 7, 11, 12] to simulate the growth of urban systems in a large scale, and successfully reproduced both the fractal morphology and the population power laws. The scaling laws of cities have also been reproduced in discrete [13] and continuous [14] stochastic models. Recent studies [15] on human agglomeration suggest the existence of an universal mechanism governing the population growth at different scales. On a smaller scale, the urban morphology has been studied [16–20] by investigating the structure of the street network. It has been found empirically [20] and reproduced in theoretical model [19] that the distribution of the areas of the cells created by streets obeys a power law with the exponent $n = 1.9$ [20].

The morphological analysis of the urban system on the *smallest* scale – on the level of the land parcels – has been done for the first time in Refs. 21, 22. Distribution of areas of parcels owned by natural persons in the Czech Republic was analyzed recently in Ref. 23. Studies presented in Refs. 21, 22 revealed that the morphology of the parcel pattern exhibits striking regularities. Each piece of land – irrespectively of its geographical location – represents well-defined morphological type that is distinct for a highly urbanized core of a city, rural area, and for suburban area. These regularities indicate that some universal mechanism underlies the process of land fragmentation by humans. In the following, we discuss the structure of the urban systems and the urbanization mechanism inferred from the morphological analysis performed in the works cited.

2. Morphological structure of an urban system

The analysis presented in Refs. 21, 22 was based on the Geographic Information System (GIS) parcel data in the ESRI Shapefile format. The land parcel is the basic spatial unit in a land survey system (a cadaster) and is assigned with a unique parcel number. Physically, the parcel is defined with its boundaries, and forms a polygon. Spatial position of the parcel was determined by the location of its centroid calculated as the geometric center of mass of the polygon. In the works cited [21, 22] the GIS data contained all types of land parcels, such as developed and undeveloped areas, green and industrial areas, public utilities, except for streets and roads. The areas analyzed were located in different geographical regions, including lowland, mountain, and seaside terrains. The morphology of the urban and suburban areas was investigated for 29 cities located in Australia (20), USA (8), and one European (Polish) city. Populations of the cities varied from about one thousand to about two million inhabitants.

To investigate the morphology of the land fragmentation pattern, the distri-

bution functions, $f(a)$, of the parcel areas, a, were studied. In the case of cities and suburbs the distribution was analyzed within the subsequent concentric rings around the "center of the city". It was located in the geometric center of the Central Business District (CBD). For cities possessing multiple CBDs, the main CBD – also referred to as downtown – was chosen. Similar analysis was performed for rural areas. In this case, the distribution function $f(a)$ was investigated in rings surrounding a point located away from any human settlements.

Our studies revealed that the parcel patterns displays only three, universal, well-defined morphological types. Each type is unambiguously determined from the shape of the distribution function, $f(a)$, of the parcel sizes. With respect to the morphology of the parcel pattern, one can classify each piece of land as (i) highly urbanized core of a city, (ii) suburban area, or (iii) rural area. The morphology of the rural area corresponds to a scale-free structure and is characterized by a reverse power law distribution of the parcel areas with the exponent $n = 1.1$. In suburbs, the area distribution follows the log-normal distribution. In the city core, $f(a)$ has an unimodal shape with a peak[a] located at around 10^3 m^2 and algebraically decaying tail, $f(a) \sim a^{-2}$.

The structure of a "regular" urban system that expands outwards on undeveloped land is shown in Fig. 1a. As seen, the core occupies a relatively small part of the whole urban system and is enclosed in a circle centered in the middle of CBD. The radius of the core ranges from about 0.5 km for small towns to about 10 km for the largest cities. The core represents the oldest part of the city with the highest urban density and consists of commercial and residential zones as well as green areas. In "regular" systems the core is surrounded by a wide ring of less urbanized suburbs that gradually undergo into rural area. Interestingly, the features of the morphology of the parcel pattern are universal and do not depend on the topography or geographical location of land. That is, the urban system exhibits the same sandwich-like structure with the suburbs located between the city core and rural areas. In a "reverse" system that is expanding inwards the core is located at the outer boundaries of the system. Such structure is observed, for example, in the urban system developed in the Hawaiian Islands shown in Fig. 1b. In this case, the core is the most outer part of the system and forms, approximately, a thin ring along the cost of the island. The rural area is a circle located in the center, and is surrounded by a ring of suburbs.

In the following, we describe in more detail the structure of the three morphological types of land. Also, we discuss fragmentation processes that lead to the each type of the land parcel mosaic, which can be deduced based on the morphological analysis.

2.1. *Rural Area*

The parcel size distributions were investigated in ten rural regions located in deserts in USA and Australia. The American regions were located in California and Hawaii Islands. The Australian regions were located in the state Queensland. Some of them

[a]Some cities exhibit two closely located peaks in the distribution function. For example, the city of Raleigh (USA) shown in Fig. 4.

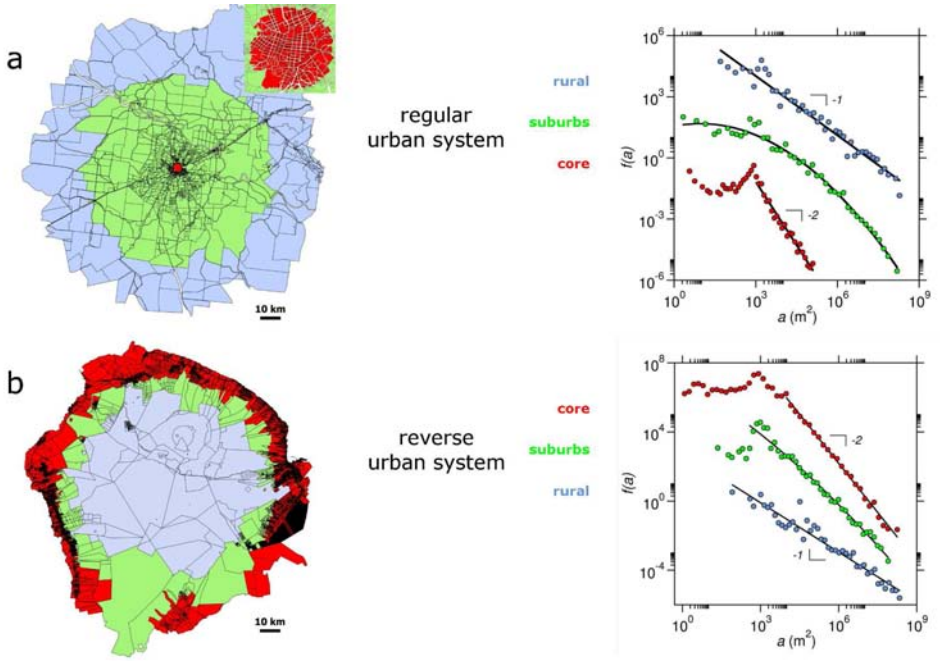

Fig. 1. (a) Example of regular urban system: the city of Charters Towers (Queensland, Australia) and its surroundings. The black lines are boundaries of the parcels. The colors of the parcels correspond to the three different morphological types: (1) the core (red), (2) suburban area (green), and (3) rural area (blue). Insert: Details of the city core. The parcel areas distributions, $f(a)$, for the three zones are plotted in the log-log scale. The core is characterized by the distribution function exhibiting the power law tail with the exponent $n = -2$; In rural area $f(a)$ follows the power-law with $n \approx -1$; In suburban area $f(a)$ is described by the log-normal distribution. (b) Reverse urban system developed in Hawaii Island (Kauai). Rural area occupies a circle located in the center of the island and is surrounded by the ring of suburbs. The core corresponds to the most outer ring. For the sake of clarity, in (a) and (b) all data sets have been mutually shifted in the vertical direction by multiplying the distribution functions by arbitrary numerical factors.

are marked on the map shown in Fig. 2a. It was found that all distribution functions follow an power-law dependence with the exponent $n = 1.1$. Examples of the distribution functions for rural areas are plotted in Fig. 1 and Fig. 2b. The fact that $f(a)$ obey a power law suggests that people, in their activities that spontaneously contribute to land fragmentation, follow some scale-invariant process [4, 5, 24]. To discuss a mechanism that underlies the invariance in the distributions of the parcel sizes, we invoke recent results on human population ecology. Namely, the distribution of the areas occupied by the world's nations was found [25] to obey the inverse power law with the exponent $n = 0.93$. Interestingly, note that the distribution of the areas occupied by colonies of the *E. coli* bacteria was also found [25] to follow the reverse power law function with the exponent $n = 0.89$. Both the values of the exponents are close to that of parcel sizes in rural areas, $n = 1.1$, reported in Ref. 21. The process of land occupation that leads to the observed area distribution of nations can be modeled within the framework of random partitioning of the

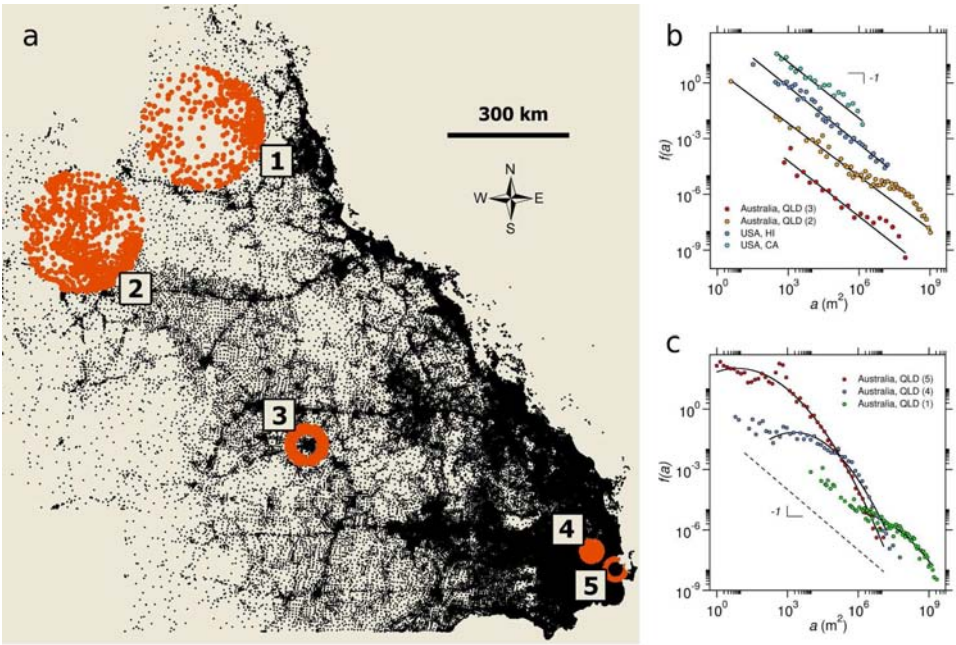

Fig. 2. (a) Map of Queensland, Australia. The dots represent centroids of the parcels. The centroids of the parcels in the regions analyzed are marked in orange. The regions are labeled with the numbers 1, ..., 5 in the map, and referred to as QLD(1), ..., QLD(5), respectively. The core of the city of Brisbane is located inside the ring "5". (b) Examples of $f(a)$ in rural areas: Results for QDL(2) and QLD(3) and two rural areas in USA located in California (CA), and Hawaiian Islands (HI) are plotted. (c) $f(a)$ for the regions QLD(1), QLD(4), and QLD(5) representing different stages of urbanization. The data sets have been mutually shifted in the vertical direction by multiplying the distribution functions by arbitrary numerical factors.

plane [25, 26]. In this process, the plane is successively subdivided by straight lines that are randomly oriented and positioned. Each line divides are available into two parts: the smaller part is selected and the larger one is further subdivided. The described above tesselation mechanism is referred to as the *fence off* process, and results in an inverse power law distribution of the areas with the exponent $n \approx 1$. The fact that both the exponents – that of nations and that of land parcel sizes – are close to unity suggests that human activity that leads to the fragmentation of land in rural areas into parcels as well as the area distribution of nations around the globe is governed by common stochastic spatial process – the *fence off* tesselation. Importantly, this mechanism is determined solely by the geometrical properties of the partitioning of the plane, and, as such, does not depend neither on socio-political context nor geographical location of the area.

2.2. *Suburban Area*

In Fig. 2c the distribution functions for three regions located in Queensland, Australia are plotted. The three regions, QLD(1), QLD(4), and QLD(5), represent dif-

ferent stages of urbanization. The degree of urbanization of land decreases with the distance from the CBD of Brisbane. Region QLD(1) is the least urbanized (rural) area; Region QLD(4) comprises features of both rural and suburban areas; Region QLD(5), forming a ring around Brisbane, is a well-developed suburban area and displays the log-normal parcel areas distribution. The value of the average parcel size increases with the distance from Brisbane. The plots presented in Fig. 2 illustrate that the urbanization process is accompanied by the transformation of the power law distribution characteristic of rural area (QLD(1)) into the log-normal distribution observed in suburban areas (QLD(5)) surrounding the city of Brisbane. Also, it follows from Figs. 2b and 2c, that when the land undergoes urbanization, the initial large scale patterns of fragmentation structure, represented by the parabolic bulge at the end of the distribution functions for QLD(1), QLD(2), and QLD(3), grow at the expense of smaller parcels. Eventually, the parcel size distribution function takes the log-normal shape.

The analysis of the morphology of parcel pattern helps one to understand the possible mechanism of the land inclusion and fragmentation associated with the sprawl of urban systems on rural areas. When a city grows its area is successively enlarged through the incorporation of available rural land. The newly included area undergoes urbanization. In the process, large parcels are successively sub-divided into smaller and smaller fragments. Eventually, this fragmentation process transforms the distribution function $f(a) \sim a^{-1}$ characteristic of rural areas into the log-normal one. Since the sprawl process gives rise to the log-normal distribution of the parcel sizes, one expects that the inclusion and the transformation of the rural area into the suburban one is governed by a geometric Brownian motion (GBM). GBM is a stochastic multiplicative process [14, 23, 27] where in which the logarithm of randomly varying quantity, x, performs a Brownian motion. It leads to the log-normal distribution of the variable x. GBM accounts for both splits and merges of a parcel - two basic transformations that a parcel undergoes during the urbanization process. For this reason GBM is a natural candidate for the process that transformers the rural morphology into the suburban one.

2.3. *City Core*

The formation of the city is accompanied by fast land development processes, in which the parcels get built up. The parcel pattern of the built up areas changes very slowly with time. For this reason the city core represents a 'frozen' morphology that was established at the time when it was formed. Thus, the morphology of the core – the oldest part of the urban system – contains the information about the mechanism leading to the formation of the city. Below, we present such a mechanism that was deduced from the structure of the parcel mosaic, which is based on a 2D bond percolation model [28]. Within this model, city emerges at the percolation threshold when neighboring urban settlements get connected by a common street network.

As it was found [21, 22], the morphology of the city exhibits scaling behavior for the parcel area distribution for the parcel areas, $a > 10^3\mathrm{m}^2$ The scaling follows from the self-similar, hierarchical spatial structure of the urban system [8]. The self-similarity holds in a statistical sense and reflects an important feature of the processes of the city formation – successive merging of neighboring urban set-

tlements into bigger and bigger systems. In this respect, the formation of urban system resembles the geometric phase transition in the percolation model. Close to the percolation threshold, the percolating system displays both the self-similar morphology and the scaling of the cluster areas distribution. The percolation theory predicts [28–30] that at the critical point the number of clusters of size a normalized per lattice follows the reverse power law with the exponent $n = 187/91 \approx 2.055$. Moreover, the morphological analysis showed [22] that the parcels are distributed homogeneously within the core and do not exhibit any spatial arrangement. This fact indicates that the urbanization process occurs simultaneously in the whole area. The two experimental findings – the universal scaling with the exponent $n = 2$ and the homogeneity of the core – suggests that a 2D bond percolation model is a suitable tool to mimic the morphology of the urban system. The street network emerges when the number of bonds increases and the system approaches the percolation threshold. Then, patches of regular "street grid" appear. The percolation model is not capable to reproduce the exact structure of the street network. However, it captures the basic *statistical* properties of the tessellation morphology.

The model presented in Ref. 22 assumes that the following two generic processes underlie the land fragmentation into parcels: The parcels are created (1) by the streets when they connect to form a cell (a loop). (2) along the existing street. The second process lead either to the fragmentation of an existing cell or – if the street is not a part of the loop – to the inclusion of a portion of suburban land. These processes can occur simultaneously, the second one dominates however at the late stages of the city formation. The two processes result in the partitioning of the plane into the first generation (FG) and the second generation (SG) parcels, respectively. They are presented schematically in Fig. 3a. In the simulations the street network was represented on a 2D square grid as a collection of segments (streets) of equal length linking two neighboring nodes. The connection between the nodes was open with the probability p or closed with the probability $1-p$. An example of the pattern resulting from the division of the plane into the FG parcels for $p = 0.45$ is shown in Fig. 3b. Evolution of the urban system for different values of p is shown in Fig. 3c. The black color corresponds to the FG parcels. As seen, when p approaches the percolation threshold, $p = 0.5$, separate settlements merge rapidly to form a city. The distribution of the areas of the FG parcels obeys the inverse power law with the exponent $n = 2$.

The fragmentation of the plane is completed after performing the division into the FG parcels and, subsequently, the SG parcels. An example of the distribution of the areas of the SG parcels obtained in the simulations at the percolation threshold is shown in Fig. 4. For comparison, $f(a)$ for four selected cities are also plotted. As seen, the shape of $f(a)$ obtained in the model reproduces – up to the scaling factor – faithfully those observed in the cities. The fragmentation of the plane into the FG parcels gives rise to the power law exhibited by the parcel areas distribution function that is universal for all cites. The fragmentation into the SG parcels occurs in a small length scale and is specific for a given city. It determines both the position and the shape of the peak in the distribution function. That is, the SG parcels represent the length scale that reflects intrinsic (system-dependent) properties of the city.

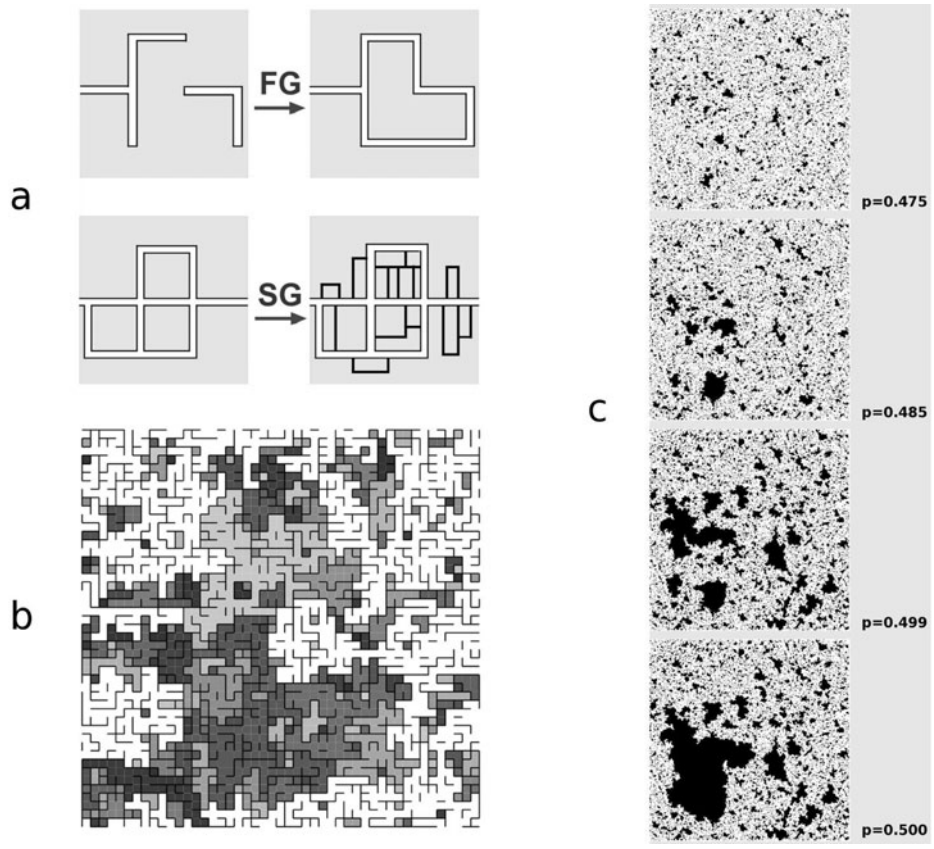

Fig. 3. (a) Schematic representation of the two generic processes that lead to the formation of the parcel: Top: The street network develops to form loops. The cells encircled by the loops are the FG parcels. Bottom: The SG parcels are cut out from the existing FG parcels. (b) An example of simulation of land division into the FG parcels carried out square lattice of the size 50×50 and for the probability $p = 0.55$. Each FG parcel is marked in different color. (c) Simulation of the urbanization process on the lattice of the size 500×500. Results obtained for four values of p are shown. The FG parcels, created due to the growth of the street network, are marked in black. The FG parcels form clusters (settlements), of the size increasing with the value of p. When p approaches the percolation threshold, $p = 0.5$, separate settlements merge rapidly to form a city.

3. Summary

To summarize, morphological analysis of the land parcel mosaic that is based on the parcel area distribution enables unambiguous classification of land as (i) the city core, (ii) suburbs, or (iii) rural area. This property of the land morphology is universal as it does not depend on the geographical location of the area analyzed. It follows that a common, generic mechanism underlies the urbanization processes. The nature of this mechanism is reflected in the way people divide their land and can be inferred from the morphology of the fragmentation pattern. That is, the land parcel pattern is a kind of spatial fingerprint of the urbanization process.

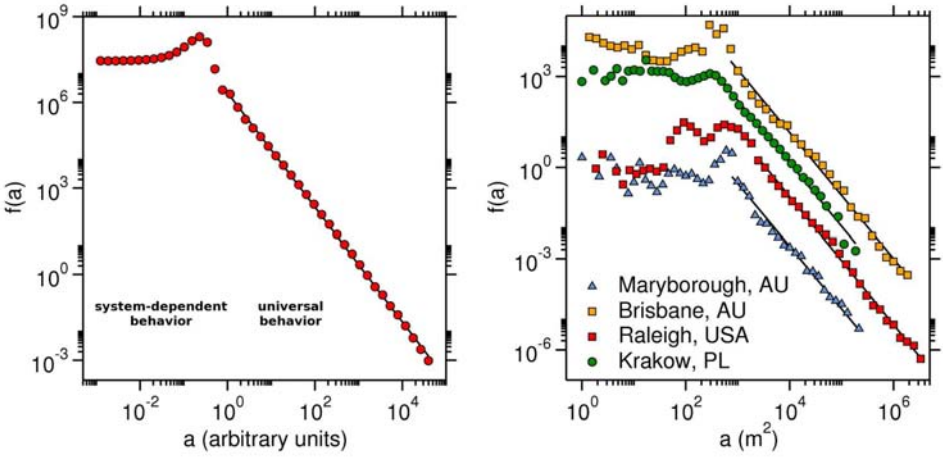

Fig. 4. The distribution of the SG parcels obtained in the simulations for the lattice size 2048 × 2048 for $p = 0.5$ (left plot). $f(a)$ displays the power-law tail with the exponent $n = -2$. For comparison, in the right plot the $f(a)$ obtained for four selected cities are shown. For the sake of clarity, the distributions have been shifted mutually in vertical direction.

Based on the properties of the parcel area distribution function, a simple stochastic scale-invariant process that leads to the fragmentation pattern observed in rural areas was inferred. The analysis of the morphology of parcel pattern helped to understand the possible mechanism of the land inclusion and fragmentation associated with the sprawl of urban systems on rural areas. The results indicate that large parcels are successively sub-divided into smaller and smaller fragments through stochastic multiplicative process that leads to the log-normal distribution of the parcel areas. The mechanism of the city formation was also proposed, that is based on a two-dimensional bond percolation. Within this model, a city is formed from the collection of settlements when the density of urban street network reaches some critical value corresponding to the percolation threshold. Within this approach, the evolution of the urban system is assumed to proceed spontaneously without any external control or design, and to bring the system to the point where it changes its structure and transforms from the collection of settlements into a new structure – the city.

To end, note that the studies presented here were based on the data originating mainly from USA and Australia, which have similar histories of colonization in terms of the mechanisms by which land was subdivided over time. We found, however, that the same features are exhibited by the city of Cracow, which is an medieval city established in the middle of 13th century, located in Poland. The fact that the city of Cracow exhibits the same distribution of the parcel sizes as relatively young Australian and American cities is remarkable. It strongly supports the hypothesis that there exists a robust mechanism which people follow around the globe in the urbanization process, and which can be studied by the tools provided by statistical physics.

Acknowledgments

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RELIABILITY ISSUES IN THE MICROSCOPIC MODELING OF PEDESTRIAN MOVEMENT

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Microscopic models of pedestrian movement have been developed since 1985 [1] mainly to gain insight into the mechanisms behind known pattern of movement or jamming, and were soon used to predict evacuation time and critical areas during evacuation of large buildings and pedestrian facilities. While microscopic models are in principle capable of detailed and accurate predictions, they are not verified in the sense that given a situation (building geometry, occupation, and type of occupants), they are proven to give a nearly correct description of the evacuation procedure. Overhead video recording and its automatic analysis is capable of giving correct trajectories of persons even in high density situations, and so a more detailed verification will be possible in the future, hopefully leading to much improved reliability of the models. The paper discusses how a verification process could be organized, both for a specific simulation and a model in general, and indicates pitfalls and problems in the use of simulations to calculate required safe evacuation times.

Keywords: Pedestrian flow; evacuation simulation; overhead video tracking; Voronoi diagram.

1. Introduction

Traditionally, pedestrian safety was handled by prescriptive regulations stating e.g. how wide doors, staircases etc. had to be for what number of persons in a facility or macroscopic models [2]. This approach worked reasonably well, but it does often restrict design or organization more than necessary, and for complicated buildings it is not satisfactory. Since the advent of microscopic modeling in 1985 [1], these models have been used to estimate required safe egress time for buildings and the planning of pedestrian facilities in general. This raises the question of reliability: Is the model capable of calculating the correct movement and to what detail, and are the parameters known well enough that they can be applied in routine practice of civil engineering. Microscopic modeling allows much higher flexibility in facility design than standard codes, and could be used to design facilities that are more convenient to use and cheaper to build without loss of safety.

In a test case, the different software tools all could predict evacuation times of a high rise building accurately enough [3] and give further useful information. However, the proper use requires expertise that is not always present, and all the models

tested had noticeable weaknesses for specific situations and were not correct down to the degree of detail they provide. A well defined verification procedure for specific simulations and software in general would certainly help making buildings and mass events safer and improve our knowledge on pedestrian motion along with the simulation software. The RiMEA-Project [4] aims at defining such a procedure for Germany, Austria and Switzerland, but at present the tests agreed upon are far from being comprehensive.
An additional motivation to investigate the verification of a microscopic egress simulation comes from the Hermes project [5]. This adds a new dimension to the use of microscopic models by applying such a model not in the planning of the facility but in a decision support system for heads of operation in an actual evacuation, using information from person counting to define occupancy, from sensors to know available egress routes, and from security staff. It gives a fifteen minute prediction of the egress to allow to react on problems arising before they get out of hand. The time scale here is a few minutes, which rules out any expert checking of the results of the simulation. It is therefore necessary to prove beforehand that it is wise (or at least not the road to disaster) to base decisions directly on numbers and pictures provided by the simulation. Therefore much effort has already gone into the verification of the model in use and further effort will go into verifying the software.

2. Verification strategies

The first question about a verification process is what to expect from a simulation. We assume the routing to be given. All microscopic models produce trajectories of persons. These depend on the specific behavioral parameters of the persons involved, for which at best statistical values are known in reality, so these trajectories are not meant to be predictions. What is supposed to be correct, at least in the sense that it gives approximately the proper distribution, are macroscopic and mesoscopic values:

- Times for 95% and 100% clearance of the building
- Flow rates at doors and passages as functions of time
- Occupation of rooms as functions of time
- Identification of bottlenecks in the egress
- Queue length, queue densities, and passing times for the bottlenecks

The scale decreases and the difficulty increases down the list. As the reliability of simulations increases, further requirements will come, but the above list encompasses the most pressing needs.
There are two principle problems with the verification of microscopic models of pedestrian movement. The first is that persons differ widely in their mobility behavior, and any one person will show a different behavior at different situations. The models can accommodate this by randomizing the behavior related parameters, but a deviation between a simulated and an observed motion of the size of the variation between experiments is not by itself a fault. The second is that evacuation experiments for large buildings are expensive and therefore very rare, and the methods of observing pedestrian motion have until very recently been quite unsatisfactory. Evacuation drills are performed routinely in some countries for all public buildings, but usually only the total evacuation time is reported, so this is little help. This

situation has been improving since the advent of digital video, but lack of reliable data will be a problem for some time to come. Useful reports on some evacuations are in [6], where the egress over time is reported for all outer doors. Together, these problems have led to the widespread reliance on human intuition: A simulation is visualized and shown to an expert. If he thinks it looks o.k., it is accepted. Of course, this procedure leaves something to be desired, but expert judgment will be required in many instances for some times to come.
What is a more scientific procedure feasible at the present time is a mesoscopic approach. The motion of persons through a building towards an exit can be broken down into a sequence of elementary blocks that are only weakly interacting, like leaving a room through a door, walking down a staircase, walking along a corridor, and so on. If each situation is handled correctly by the simulation, and if the outcome of the simulation is stable against small variations in the process, then the total simulation will give a reasonable result. Getting the experimental data for all the building blocks is a formidable task by itself, and for testing the simulation against reality, new concepts have to be developed. Even if this is all done, the question of stability of the situation remains a problem. We will address this below.

3. Getting data from experiments

Evacuation drills and experiments of entire buildings are without doubt of great importance, but are hardly ever monitored to give a full set of data. Mesoscopic experiments in specially chosen geometries that allow good data aquisition are an important data source. These can be equipped with person counters and video technique to give a complete picture of the individual movements and interactions.

3.1. *Data aquisition and analysis*

The best data possible for the comparison with simulations is a complete set of individual tracks with accuracy better than 10cm. For small groups of persons, this can be achieved with either wireless tracking with tags or with video recordings; for large groups with high density the only reasonable way is currently digital overhead video with suitable post processing [7]. For the correction of perspective, stereo video is optimal, but on level ground, other methods of correction of perspective are available, too, and mono pictures usually allow higher resolution. Large video coverage without occultation requires a placement of the camera high above the heads, which can be done only in special environments. Sideways video, as it common in CCTV surveillance and feasible almost everywhere, allows tracking only for very low densities that are of little interest for the modeling. At higher densities, the line of sight is obstructed too often. The correction of perspective is always a severe problem in sideways video.
One problem is that while all tracks produced by simulation are approximately center of mass movements, overhead video tracks the head movement which shows much more swaying and sudden jerks. Video based trajectories have to be smoothed for analysis or for comparison with simulated trajectories. An adequate smoothing method based on detecting step and interpolating mid-step points has been developed in [8], it works well as long as the walking speed is not too low (above

0.2m/s). On slower speeds the step detection is not reliable any more, but the method still does some useful smoothing. The smoothed trajectories are the basis for the production of mesoscopic data: average velocities, densities, and fluxes. The

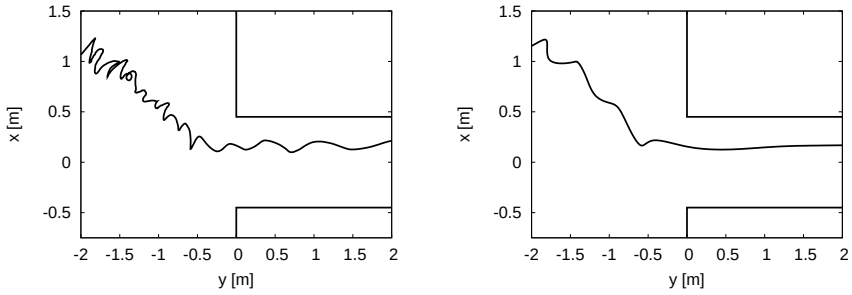

Fig. 1. Raw and smoothed trajectories of one person passing a bottleneck with jamming

usual measurement of velocities is by difference quotients over about 1s. The derivative of the smoothed trajectory allows a high resolution in time and is less affected by the swaying and jerking of heads [8]. Density is usually measured by counting heads within an area; fluxes are by counting heads passing a line. For useful sizes of area, this results in discrete values with large scatter. Defining an extended density distribution for every person gives better values for the density in a small area or the flux e.g. through a door in a small time interval. An appropriate personal density distribution is given by computing a Voronoi diagram for the persons (the Voronoi diagram describes to every person the area closer to him than to any other person, his Voronoi cell), crop the individual Voronoi cells at walls and at some limiting distance, and define the local density inside each such cell as the inverse cell area. With this, the density and the flux at a point in time and space become reasonable quantities (Fig. 2).

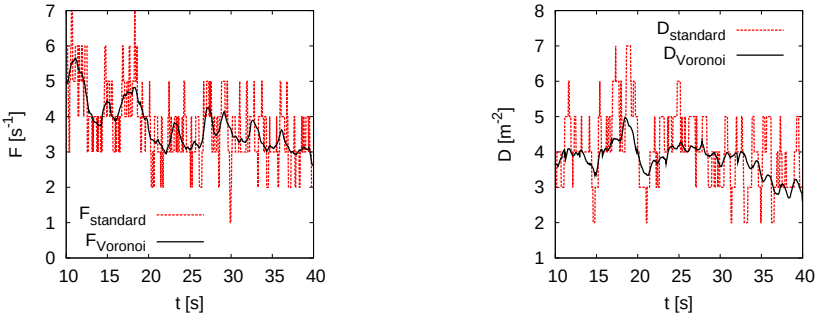

Fig. 2. Flux F and density D by standard and Voronoi method

3.2. *Trajectory based verification*

One idea for verification of rule based or force based method is to apply the model to just one person and take all other trajectories from the experiment and compare the observed and the calculated trajectory. One problem with this is that the individual characteristics of the observed person are unknown, and thus those parameters of the model describing the person have to be determined by fitting the trajectory. That such a fit is possible does not prove the model, but it is certainly worthwhile to do this test and see if the parameters produced are possible for all persons and have a reasonable distribution. A second problem is that at high densities, the neighbors of a person form a 'cage' he cannot leave, and even very poor models can easily reproduce this.

It is therefore necessary to compare the simulation of larger groups or of all persons involved in the experiment. Time averages of densities, fluxes and local velocities can be compared for experiment and simulation. If these agree within the size of variations between different experiments producing the same state of movement (or alternatively the variations with time within an experiment), the model is confirmed. Unfortunately, the comparison can be a tricky problem. At high densities, the situation e.g. in a corridor may be in one of two phases: moving or standing [10]. The models should produce the same relative frequency of the phases, and within the phases similar densities and fluxes. The latter can be tested if both states have been observed experimentally. It is obvious that at the present state of knowledge, this comparison cannot be automated; it needs expert judgment as one component. Beside these verifications based on expensive experiments, there are a number of tests that can be done on simple experiments or common sense alone. For people following each other in a single file, there is much data available in literature [11, 12], and the modeling should reproduce the 1D fundamental diagram. Another simple test is the head on conflict in a narrow corridor. Both persons should stop in time and smoothly. Further tests are on qualitative features - if people cross each other's path, do they give way in time and sufficiently smooth? Does the model allow passing in a smooth maneuver? Do people cross walls or tunnel through each other - the crossing of walls certainly is a serious error, while the tunneling is sometimes used instead of a proper passing or crossing process.

3.3. *Verification process for the Hermes project*

For the Hermes project, about 170 experiments involving up to 360 persons each have been done. Within the arena, there have been multiple runs of leaving a grandstand through a port, walking up and down the stairs, and merging of traffic coming down the upper stairs with traffic from the gallery onto the lower part of the stairs. In specially built geometries there have been experiments of uni- and bidirectional traffic in corridors, in a T-merger ($^{\rightarrow}\Downarrow^{\leftarrow}$), round a corner and through a door, all with different widths and densities. All these experiments where documented by overhead video using mono- and stereo cameras. They have not all been analyzed yet, but they will together with older experiments [9] form the bases of software verification. A final test of the software will be a small number of egress simulations tested against the observations of normal leaving of the facility at the end of some

events to be performed in 2011, when all the instrumentation will be installed.

Acknowledgments

The ideas for verification presented here result from many discussions in the pedestrian dynamics group of the Jülich Supercomputing Centre, and all the members - staff and students - contributed to the results. All big experiments mentioned where conducted jointly by the pedestrian dynamics group of the Jülich Supercomputing Centre and the staff of the Institute for Building Materials and Fire Protection of the University of Wuppertal, some small ones were conducted by either group. The experiments done at the Esprit arena were funded by the the German Federal Ministry of Education and Research (BMBF) as part of the Hermes project, further experiments where funded by the German Research Foundation (DFG), grant No. KL 1873/1-1 and SE 1789/1-1.

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URBAN STRUCTURE ANALYSIS

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The built-up land represents an important type of overall landscape. We analyse the structure of built-up land in largest cities in the Czech Republic and selected cities in the USA using the framework of statistical physics. To do this, both the variance of the built-up area and the number variance of built-up landed plots in circles are calculated. In both cases the variance as a function of a circle radius follows a power law. The obtained value of the exponents are comparable to exponents typical for critical systems. The study is based on cadastral data in the Czech Republic and building footprints GIS data in the USA.

Keywords: Urban structure; critical systems; self-organized criticality.

1. Introduction

Urban land represents one of the most significant human touch on the Earth influenced by cultural, sociological, economic, political and other conditions. The vast amount of people lives in cities and the effort to understand the properties of those aggregates from various points of view always played a scientific attention. From physical point of view, it is interesting to study the spatial properties of urban pattern. Existing studies usually mention fractal self-similarity properties [1–4]. Recently the concept of self-organized criticality in connection to urban systems was introduced by Batty and Xie [5].

Our aim is to study the structure of built-up land pattern. We focus on the centres of cities, where the density of built-up land is roughly constant. That means similar probability for every location to be built-up. Together with the previously

mentioned self-similar properties the effort to study critical properties known from thermodynamics seems reasonable. The relation to critical systems and phase transitions can be also motivated by the fact, that from economic point of view, the change of land to built-up, represents the change of phase for type of land. The place is equipped with an additional property - a building. In the following we show the connection of built-up land to critical systems.

2. Critical phenomena

Let us now briefly recall some specific features of the so called critical systems [6–8]. Properties of different thermodynamic systems near the continuous (second-order) phase transition show specific universalities for which the term critical phenomena is used.

In order to describe explicitly these features one needs to define an order parameter $\langle M \rangle$ as a thermodynamic quantity that distinguishes between the two phases. Notation $\langle ... \rangle$ stands for ensemble average. It is also useful to define a local order parameter value $m(\boldsymbol{r})$ by the relation

$$M = \int_V m(\boldsymbol{r}) d\boldsymbol{r}, \qquad V \subset \mathbb{R}^2. \tag{1}$$

If the system is homogeneous and isotropic in the volume V then

$$\langle m(\boldsymbol{r}) \rangle = \langle m(0) \rangle = m = \frac{\langle M \rangle}{V}, \qquad \forall \boldsymbol{r} \in V. \tag{2}$$

The spatial properties of order parameter distribution can be described by the two-point correlation function defined as

$$G(\boldsymbol{r}_1, \boldsymbol{r}_2) = \langle (m(\boldsymbol{r}_1) - \langle m(\boldsymbol{r}_1) \rangle)(m(\boldsymbol{r}_2) - \langle m(\boldsymbol{r}_2) \rangle) \rangle \,. \tag{3}$$

This can be under homogeneity and isotropy assumptions simplified to

$$G(r) = \langle m(\boldsymbol{r}) m(0) \rangle - m^2, \tag{4}$$

where $r = |\boldsymbol{r}|$.

If one is interested in the static spacial structure of critical systems then certainly the most important property is the scaling invariance. For the correlation function it gives a restriction of its functional form to

$$G(r) = \frac{\Psi(r/\xi)}{r^\eta}, \tag{5}$$

where Ψ is some bounded function and ξ is the correlation length that diverges at the critical point. Index η appearing in the exponent of power law part of $G(r)$ is called the anomalous dimension.

2.1. *Parameter variance in spheres*

Useful tool to analyse experimental data is the variance of the parameter in spheres. For the parameter $m(\boldsymbol{r})$ with homogeneous and isotropic distribution $\langle m(\boldsymbol{r}) \rangle = m$ the cumulative value of the parameter in the sphere of radius R is given by

$$M(R) = \int_{S(R)} m(\boldsymbol{r}) d\boldsymbol{r}, \tag{6}$$

where the sphere is the set $S(R) \equiv \{\boldsymbol{r} \in \mathbb{R}^d | \, |\boldsymbol{r}| < R\}$ with a volume $|S(R)|$. The centre of the sphere is not important because of the homogeneity of the parameter distribution. The parameter variance is defined [9] as

$$\sigma^2(R) = \langle M(R)^2 \rangle - \langle M(R) \rangle^2. \tag{7}$$

It can be easily shown that in the thermodynamic limit $V \to +\infty$ outside of the critical point the following relation holds:

$$\sigma^2(R) \propto R^2 \sim \langle M(R) \rangle, \qquad R \gg 1. \tag{8}$$

A different situation arises when the system is approaching the critical point. Spatial correlations in this region are long-ranged and the correlation function is dominated by the power-law decay (5). In the region $R \gg 1$ and $R \ll \xi$ we obtain

$$\sigma^2(R) \propto R^{4-\eta} \sim \langle M(R) \rangle^{2-\frac{\eta}{2}}. \tag{9}$$

3. Data analysis

Our data contain all cadastral records from the Czech Republic and building footprints for few cities in the U.S.A. For Czech data every landed plot i is characterised by its definition point $\boldsymbol{r}_i$, size (acreage) λ_i, type of land and the ownership data. Since our interest is in the built-up structure we restrict our attention only to built-up landed plots. Building footprints are represented as polygons reflecting the true shape, and therefore size, of buildings. Since for our cadastral data the exact parcel shape is unknown, the most straightforward analysis is to represent them as points given by definition points $\boldsymbol{r}_i$ of the parcels. For this representation the order parameter is represented as the point density. In the case of building footprints, centroids of the parcels are used as definition points.

Another possibility is to define the order parameter as $m(\boldsymbol{r}) = 1$ if there is a building at $\boldsymbol{r}$ and $m(\boldsymbol{r}) = 0$ otherwise. The order parameter is here just the indicator of built-up subset. For the Czech cadastral data, the unknown shapes of parcels are approximated by circles with the same acreage.

All estimations are based on the assumption of self-averaging property [10]. It means that sufficiently large sample is a good representative of the whole ensemble. Mean values in formula (7) for fixed perimeter R are estimated in the following way. Inside the studied part of the city $A \subset \mathbb{R}^2$ centres $\boldsymbol{o}_j$ of N spheres are uniformly randomly chosen so that every sphere is inherited in A, $S(\boldsymbol{o}_j, R) \subset A$. For every sphere $S(\boldsymbol{o}_j, R)$ the cumulative parameter value (number of points and built-up area) $M_j(R)$ inside is calculated. The mean value and variance are estimated by usual unbiased estimators:

$$\langle M(R) \rangle = \frac{1}{N} \sum_j M_j(R), \quad \sigma^2(R) = \frac{1}{N-1} \sum_j \left(M_j(R) - \langle M(R) \rangle \right)^2. \tag{10}$$

3.1. *Results*

We analysed 6 largest cities in the Czech Republic and 6 cities form the U.S.A. For each city we calculate both number variance in spheres (point representation) and built-up area variance in spheres (set representation). The dependences of $\sigma^2(R)$

on $\langle M(R)\rangle$ for Czech cities in the case of set representation are plot in the log-log scale in figure 1.

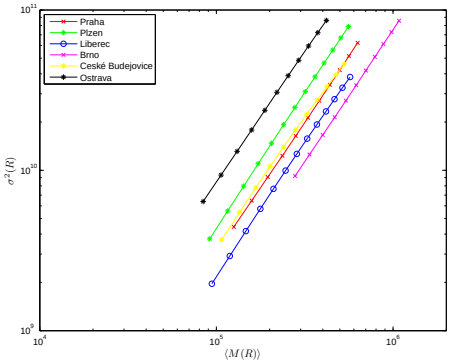

Fig. 1. Dependencies of $\sigma^2(R)$ on $\langle M(R)\rangle$ in log-log scale for different cities in the Czech republic.

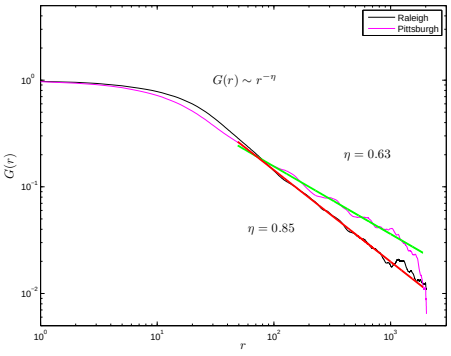

Fig. 2. Dependencies of $\sigma^2(R)$ on $\langle M(R)\rangle$ in log-log scale for different cities in the Czech republic.

It is clearly visible that the dependence for all cities follows a power law. It can be therefore fit by the straight line (in log-log scale). From this fit one can easily determine the exponent of power-law. The summary of resulting exponents α for studied cities according to the relation

$$\sigma^2(R) \propto \langle M(R)\rangle^{\alpha}, \quad \alpha = 2 - \frac{\eta}{2} \tag{11}$$

is given in the table 1. As it was expressed by (8), exponent $\alpha = 1$ express the system that is outside of the critical region, e.g. randomly positioned particles. One can see that this is not the case of built-up land pattern.

For polygon representation of building footprints from the U.S.A it is also possible to estimate the correlation function directly. Results for Raleigh and Pittsburgh are shown in the figure 2. Correlation function decay clearly follows the power law. Exponents obtained by fitting are consistent with the values of α from table 1 according to relation (11).

Table 1. Exponents α according to power law dependence (11) of $\sigma^2(R)$ on $\langle M(R)\rangle$.

City	Points	Area circle	City	Points	Area circle	Area polygon
Praha	1.47	1.64	Raleigh	1.73	1.58	1.58
Plzeň	1.61	1.69	Boston	1.62	1.62	1.62
Liberec	1.54	1.65	Pittsburgh	1.69	1.68	1.69
Brno	1.40	1.65	Spokane	1.69	1.57	1.59
České Budějovice	1.50	1.58	Tompkins	1.75	1.57	1.59
Ostrava	1.54	1.62	Springfield	1.52	1.3	1.3

4. Conclusion

The computations show, that for both representations the dependence of fluctuations on the mean value of the parameter follows a power law. Moreover the set representation, as can be expected, seems to be more universal. The values of exponent α in the relation $\sigma^2(R) \sim \langle M(R) \rangle^\alpha$, for different cities except of Springfield are very close to the value $\alpha = 1.62$. Different results for Springfield can be explained by strongly constrained lattice-like structure of that city.

We can conclude that the inner urban area structure is correlated with a long ranged power-law dependence. This shows the connection between critical systems and the urban system. The power-law exponent seems to be independent of the particular city, being therefore determined only by the fact that it represents an inner urban structure. Such an observation is very interesting and the connection between urban area and critical systems may be useful to development and verification of further urban models. The probable explanation is inherited in the connection of built-up land to various networks, e.g. transportation, water supply, sewerage, electricity.

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CONTRIBUTED TALKS

THE TOTALLY ASYMMETRIC EXCLUSION PROCESS IN TWO-DIMENSIONAL FINITE LATTICE, COMPARISON OF DENSITY PROFILES

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A two-dimensional model based on the totally asymmetric exclusion process is introduced. It's dynamics is inspired by pedestrian movement. We come out of the one-dimensional TASEP with open boundaries defined on a finite lattice of N sites. This model is solvable by means of the Matrix Product Ansatz method, which gives exact formulas for density profiles and phase diagram containing three phases, maximal current, low- and high-density phase; for both time continuous dynamics and discrete parallel updates. We define similar dynamics on a rectangle lattice of MxN sites with open boundaries. Several update procedures are discussed, and the permutation–parallel update is introduced. Via computer simulations the average density in steady state has been studied, and similar behavior to the one dimensional model has been observed. We have identified the same three phases and the same shape of the transition line between the low- and high-density phase. Finally, an idea of generalization for two particle species model is presented.

ELLIPTICAL VOLUME EXCLUSION OF PEDESTRIAN CROWD

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This paper introduces a spatially continuous force-based model for simulating pedestrian dynamics. By means of repulsive forces collision-avoidance is performed by moving pedestrians. A driving force models the intention of pedestrians to reach some destination. The main intention of the developed model is the quantitative description of

pedestrian movement in several geometries. Measurements of the fundamental diagram in narrow and wide corridors are performed. The results of the proposed model show a good agreement with empirical data. Having the ambition to describe with the same set of parameters the dynamics in one and two dimensional space we extend our model by introducing an elliptical volume exclusion. Given a pedestrian i we define an ellipse with velocity-dependent major semi-axis a and minor semi-axis b. The space requirement of pedestrian i is given by a, and b reflects the swaying of pedestrians while moving. To guarantee robust numerical integration of the equation of motion and to restrict the range of the repulsive force to those between adjacent pedestrians, a two-sided Hermite-interpolation of the repulsive force is implemented.

EMPLOYMENT, PRODUCTION AND CONSUMPTION MODEL: PATTERNS OF PHASE TRANSITION

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We have simulated the model of Employment, Production and Consumption (EPC) using Monte Carlo. The EPC model is an agent-based model that mimics very basic rules of industrial economy. From perspective of physics, the nature of the interactions in the EPC model represents multi-agent interactions where the relations among agents follow the key laws for circulation of capital and money. Monte Carlo simulations of the stochastic model reveal phase transition in the model economy. The two phases are the phase with full unemployment and the phase with nearly full employment. The economy switches between these two states suddenly as a reaction to a slight variation in the exogenous parameter, thus the system exhibits strong non-linear behavior as a response to the change of the exogenous parameters.

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Mathematical Results in QUANTUM PHYSICS

The volume collects papers from talks given at *QMath11 — Mathematical Results in Quantum Physics*, which was held in Hradec Králové, September 2010. These papers bring new and interesting results in quantum mechanics and information, quantum field theory, random systems, quantum chaos, as well as in the physics of social systems. Part of the contribution is dedicated to Ari Laptev on the occasion of his 60th birthday, in recognition of his mathematical results and his service to the community. The *QMath* conference series has played an important role in mathematical physics for more than two decades, typically attracting many of the best results achieved in the last three-year period, and the meeting in Hradec Králové was no exception.

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