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Chapter 1

Introduction

1.1 Préambule

En mécanique quantique relativiste, l'étude du comportement en temps long des solutions de l'équation de Schrödinger est déterminante. Un principe d'absorption limite (Limiting absorption principle en anglais, LAP dans le texte) est une estimation à poids de la résolvente d'un opérateur. Il permet d'apporter une information importante car il implique une estimation de propagation. Afin d'obtenir un LAP, il est naturel de s'appuyer sur la théorie de Mourre, voir Section 3.2. Dans celle-ci, on étudie les propriétés d'un opérateur auto-adjoint H avec l'aide d'un autre opérateur auto-adjoint A. Ce dernier s'appelle l'*opérateur conjugué.* C'est lui qui déterminera les poids dans le LAP. On s'appuie sur trois types d'hypothèses :

- $[H, \mathrm{i}A]$ est positif dans un certain sens.
- $[H, A]$ est borné par rapport à l'opérateur H.
- $[[H, A], A]$ est borné par rapport à l'opérateur H.

On appellera régularité de H par rapport à A les deux dernières hypothèses. Vérifier la positivité se résume souvent à construire un "bon" opérateur conjugué. La régularité est quant à elle parfois fausse. Il faut alors se tourner vers des versions alternatives de la théorie.

Dans le Chapitre 3, on expose les bases de la théorie en revenant à sa source, le théorème de C.R. Putnam. Puis on étudie des opérateurs de Schrödinger (magnétiques et de Hodge) sur les variétés. Les difficultés résident dans le calcul de l'asymptotique des valeurs propres dans le cas où le spectre est purement discret et dans le fait d'établir un LAP dans l'autre cas. Ici le choix de l'opérateur conjugué s'avère être déterminant afin de pouvoir contenir des perturbations très large de la métrique. Ensuite, dans le contexte d'un espace modulaire, on donne une justification de l'instabilité des valeurs propres plongées. La construction de l'opérateur conjugué est délicate et est intimement liée à la règle d'or de Fermi. Après cela, on présente une théorie de Mourre alternative que l'on a obtenue dans le contexte abstrait. Ceci nous permet de redémontrer un LAP par une autre méthode. Dans la section qui suit, on traite une extension du travail précédent : Une application dans le contexte des potentiels de Wigner-von Neumann. Pour ces derniers, les hypothèses de régularité ne permettent pas d'espérer un LAP avec l'approche classique. On s'appuie alors sur du calcul pseudo-différentiel. Enfin, nous passons en revue les difficultés liées à la première hypothèse de régularité et on donne un critère pratique que l'on a obtenu dans le cadre des variétés.

Dans le chapitre 4, on présente des résultats obtenus dans le cas où la positivité est vérifiée mais seulement dans un sens plus faible que dans la théorie classique. Ce sont des problèmes difficiles dit de *seuils.* On donne une première application pour un modèle de théorie quantique des champs. Le problème est lié à l'instabilité des valeurs propres plongées, sous une hypothèse de règle d'or de Fermi. Ici, une des difficultés supplémentaires vient du fait que le commutateur n'est pas H-borné. Puis, on travaille dans un contexte relativisite (particule très rapide), celui des équations de Dirac. Une difficulté vient du fait que l'opérateur est à valeurs matricielles. Notre analyse se réduit à l'étude d'une famille d'opérateurs elliptiques d'ordre 2, non-auto-adjoint et à paramètres. Enfin, on présente un résultat obtenu dans le cadre des opérateurs de Schrödinger non-auto-adjoints.

Dans ma thèse j'avais étudié les opérateurs de Schrödinger discrets agissant sur un arbre binaire. Depuis maintenant deux ans je m'intéresse plus particulièrement à des familles d'opérateurs discrets non-bornés agissant sur des graphes localement finis. Le fait d'être non-borné appelle naturellement des questions de domaine. On répond tout d'abord à la question de l'essentielle auto-adjonction (le fait d'avoir une unique extension auto-adjointe). Puis, on cherche à caractériser le fait d'avoir plusieurs extensions. Ensuite, on étudie le fait de pouvoir être non-borné mais tout de même borné inférieurementenent (ou supérieurement). Enfin, on donne des critères qui assurent le fait que l'opérateur est à spectre purement discret et on calcule l'asymptotique des valeurs propres.

Dans le Chapitre 6, on présente des résultats obtenus dans des domaines différents. Le travail exposé dans la Section 6.1 est l'aboutissement du stage de deux mois de Tristan Haugomat (L3 - magistère Rennes) que j'ai encadré. On y étudie l'opérateur de Dirac discret en dimension 1 et on prouve l'absolue continuité de la mesure spectrale associée (un résultat plus faible que le LAP) pour une classe de perturbations très large. Ce résultat ne peut être atteint par des techniques de commutateurs mais est basé sur une méthode de point fixe uni-dimensionnel. Enfin dans la Section 6.2, on s'intéresse à l'existence de cycles Hamiltoniens pour le cavalier sur des échiquiers de dimension supérieure.

1.2 Preamble

The study of the behavior the solutions of the Schrödinger equation for large time is essential part in relativistic quantum physics. A limiting absorption principle (LAP) is a weighted estimate of the resolvent of an operator. It brings an important information since it implies a propagation estimate. In order to obtain a LAP, it is natural to rely on Mourre's Theory, see Section 3.2. This theory is the study of the properties of a self-adjoint operator H with the help of another self-adjoint operator A. The latter is called the *conjugate operator*. It appears in the weights of the LAP. We rely on three types of hypothesis:

- $[H, \mathrm{i}A]$ is positive in a some sense.
- $[H, A]$ is relatively bounded with respect to the operator H.
- $[[H, A], A]$ is relatively bounded with respect to the operator H.

The two last hypotheses describe the regularity of H with respect to A. Checking the positivity follows usually from constructing a "good" conjugate operator. On the other hand, the regularity hypothesis is not always satisfied. We therefore rely on alternative versions of the theory.

In Chapter 3, we present the theory by going back to its roots, the Theorem of C.R. Putnam. Then we deal with (magnetic and Hodge) Schrödinger operators acting on manifolds. The difficulties come from the computation of the asymptotic of eigenvalues when the spectrum is purely discrete and from proving a LAP when it is not. Here, the choice of the conjugate is crucial in order to cover a very large class of perturbations of the metric. Next in the context of a modular space, we justify the instability of embedded eigenvalues. The construction of the conjugate operator is delicate and is intimately linked with the Fermi golden rule. Afterwards we present an alternative Mourre theory that we have obtained in the abstract context. We reprove a LAP with a different method. In the next section we give an extension of the previous work: an application in the context of Wigner-von Neumann potentials. For the latter, the regularity hypotheses are not satisfied and we cannot use the classical approach. We rely on pseudo-differential calculus. Finally we review the difficulties linked with the first hypothesis of regularity and we present a useful criteria which we have obtained in the context of manifolds.

In Chapter 4, we present some results obtained in the case when the positivity is obtained in a weaker context than in the classical theory. These are difficult problems called *threshold* problems. We give a first application in the quantum field theory setting. The problem is linked with the instability of embedded eigenvalue, under a hypothesis of the Fermi golden rule. Here, one supplementary difficulty lies in the fact that the commutator is not H-bounded. Next we work in the context of relativistic (i.e., very fast) particles, the one of Dirac equations. A difficulty comes from the fact that the operator is vector valued. Our analysis is reduced to the study of a family of non-self-adjoint elliptic operator of order 2, which depends on a parameter. Finally, we present a result obtained in the setting of non-self-adjoint Schrödinger operators.

In my Ph.D thesis I have studied discrete Schrödinger operators which acts on a binary tree. For the two last years I have been particularly interested in certain families of unbounded and discrete operators which act on locally finite graphs. The unboundedness is naturally associated with questions about domains. We first answer the question of essential self-adjointness (the fact that one has a unique self-adjoint extension). Then we characterize the fact that one could have many self-adjoint extensions. Afterwards we study the case when the operator is unbounded and yet bounded from below (or above). Finally, we give criteria that ensure the fact that the operator has purely discrete spectrum and we compute the asymptotic behavior of eigenvalues.

In Chapter 6, we present some results which were obtained in other domains. The work that we present in Section 6.1 is the outcome of the two-month training period of Tristan Haugomat (undergraduate - magistère Rennes) that I supervised. We study the discrete Dirac operator in dimension 1 and we prove that the spectrum is absolutely continuous (a result which is weaker than a LAP) for a large class of perturbations. This result cannot be reached by commutator techniques but is based on a one-dimensional fixed point method. Finally in Section 6.2, we are interested in the existence of Hamiltonian cycles for the knight acting on a higher dimensional chessboard.

1.3 Publications

The three first publications are part of my PhD thesis. The articles are sorted by date of creation.

1) S. Golénia: *C^*-algebras of anisotropic Schrödinger operators on trees*, Ann. H. Poincaré 5 (2004), no. 6, 1097–1115.

2) V. Georgescu and S. Golénia: *Isometries, Fock spaces, and spectral analysis of Schrödinger operators on trees*, J. Funct. Anal. 227 (2005), no. 2, 389–429.

3) V. Georgescu and S. Golénia: *Decay Preserving Operators and stability of the essential spectrum,*, J. Operator Theory 59 (2008), no. 1, 115–155.

4) S. Golénia and T. Jecko: *A new look at Mourre's commutator theory*, Complex Anal. Oper. Theory 1 (2007), no. 3, 399–422.

5) S. Golénia and S. Moroianu, *Spectral analysis of magnetic Laplacians on conformally cusp manifolds*, Ann. H. Poincaré 9 (2008), 131–179.

6) S. Golénia et S. Moroianu : *The spectrum of k-form Schrödinger Laplacians on conformally cusp manifolds*, Trans. Amer. Math. Soc. 364 (2012) 1–29.

7) S. Golénia : *Positive commutators, Fermi golden rule and the spectrum of the* 0 *temperature Pauli-Fierz Hamiltonians*, Journal of Functional Analysis, Volume 256, Issue 8, April 2009, Pages 2587–2620.

8) S. Golénia : *On the instability of eigenvalues*, Geometry-Exploratory Workshop on Differential Geometry and its Applications, 71–75, Cluj Univ. Press, Cluj-Napoca, 2011

9) N. Boussaid et S. Golénia : *Limiting absorption principle for some long range perturbations of Dirac systems at threshold energies.*, Communications in Mathematical Physics, Volume 299 (2010), Number 3, 677–708.

10) S. Golénia : *Unboundedness of adjacency matrices of locally finite graphs*, Letters in Mathematical Physics, Volume 93 (2010), Issue 2, 127–140.

11) S. Golénia et C. Schumacher : *The problem of deficiency indices for discrete Schrödinger operators on locally finite graphs*, Journal of Mathematical Physics 52, 063512 (2011).

12) S. Golénia and T. Jecko: *Rescaled Mourre's commutator theory, application to Schrödinger operators with oscillating potential*, To appear in J. Operator Theory.

13) S. Golénia : *Hardy inequality and asymptotic eigenvalue distribution for discrete Laplacians*, Preprint arXiv:1106.0658v2, 17 pages.

14) J. Erde, B. Golénia, and S. Golénia: *The closed knight tour problem in higher dimensions*, to appear in Electron. J. Combin., 17 pages.

15) S. Golénia, and T. Haugomat: *On the a.c. spectrum of 1D discrete Dirac operator*, preprint arXiv:1207.3516v1, 20 pages.

16) S. Golénia et C. Schumacher : *The problem of deficiency indices adjacency matrices on locally finite graphs*, preprint arXiv:1207.3518, 2 pages.

Chapter 2

On the continuous spectrum

2.1 Some notation

Given two Hilbert spaces $\mathscr{H}$ and $\mathscr{K}$, we denote by $\mathcal{B}(\mathscr{H}, \mathscr{K})$ and $\mathcal{K}(\mathscr{H}, \mathscr{K})$ the bounded and compact operators acting from $\mathscr{H}$ to $\mathscr{K}$, respectively. In $L^2(X)$, we denote by $f(Q)$ the operator of multiplication by a function $f : X \to \mathbb{C}$. We denote by $\mathbb{N}$ the set of non-negative integers and by $\mathbb{N}^*$ the set of positive ones.

2.2 The essential spectrum

Given a self-adjoint operator H acting on a complex and separable Hilbert space $\mathscr{H}$, we denote by $\sigma(H)$ its spectrum. It is included in $\mathbb{R}$. We refine this notion and set:

- $\sigma_{\mathrm{d}}(H) := \{\lambda \in \sigma(H),\ 0 < \dim\ker(H - \lambda) < \infty$ and λ is isolated in $\sigma(H)\}$,
- $\sigma_{\mathrm{ess}}(H) := \sigma(H) \setminus \sigma_{\mathrm{d}}(H)$,

the discrete spectrum and the essential spectrum, respectively.

Focus for a moment on the Schrödinger equation:

$$\mathrm{i}\partial_t f = Hf, \text{ where } f(0) := f_0 \in \mathscr{H}.$$

Since H is self-adjoint, there is a unique solution. It is given by the wave function $f(t) = e^{-\mathrm{i}tH} f_0$. If f_0 is an eigenfunction, we notice that f is periodic. We denote by $\mathscr{H}_{\mathrm{pp}}$ the closure of the span of the eigenfunctions of H. Being in the orthogonal of this subspace ensures some drastically different behavior:

Proposition 2.2.1 (RAGE)**.** *Suppose that f_0 is orthogonal to $\mathscr{H}_{\mathrm{pp}}$ and take K relatively compact to H, i.e., $K(H + \mathrm{i})^{-1}$ is a compact operator. Then one has:*

$$\frac{1}{T}\int_0^T \|Ke^{-\mathrm{i}tH} f_0\|^2 \to 0, \text{ as } T \to \pm\infty. \tag{2.2.1}$$

This result is originally due to Ruelle, see [Ru69] It was improved later by Amrein and Georgescu in [AmGe73] and by Enss in [En78]. A proof may be found in [ReSi79][Theorem XI.115].

Example 2.2.2. *Take $\mathscr{H} := L^2(\mathbb{R}^n)$ and $H_0 := -\Delta = -\sum_i \partial_i^2$. Here the domain of H_0 is the Sobolev Space $\mathscr{H}^2$ and by taking Fourier transformation one sees that its spectrum is given by $[0, \infty)$. Take now a bounded and real-valued function $V : \mathbb{R}^n \to \mathbb{R}$, which tends to 0 at infinity* *and consider the operator $H := H_0 + V(Q)$, where $V(Q)$ denotes the operator of multiplication by V. The domain of H is still $\mathscr{H}^2$. Moreover, we notice that*

$$(H + \mathrm{i})^{-1} - (-\Delta + \mathrm{i})^{-1} = -(H + \mathrm{i})^{-1} V (-\Delta + \mathrm{i})^{-1}. \tag{2.2.2}$$

is a compact operator. Indeed, by approximation, one can suppose that V has compact support and one extracts the compactness from the Rellich-Kondrakov Theorem. Then, by the Weyl Theorem, we infer that $\sigma_{\mathrm{ess}}(H) = [0, \infty)$. Finally, given a compact set $X \subset \mathbb{R}^n$, one can take $K := \mathbf{1}_X(Q)$, where $\mathbf{1}$ stands for the indicator function of X. Therefore, the RAGE Theorem tells that the particle will escape all compact set in a Cesàro sense.

2.3 Absolutely continuous spectrum

We aim to define the absolutely continuous spectrum and to improve (2.2.1).

Definition 2.3.1. *Let $f \in \mathscr{H}$ and H a self-adjoint operator. We define the measure μ_f on the Borel σ-algebra $\mathcal{B}(\mathbb{R})$ by*

$$\mu_f(.) = \langle f, E_H(.) f \rangle,$$

where $E_H(.)$ is the spectral projection associated to H.

By the Lebesgue Measure Decomposition Theorem we can decompose μ_f, with respect to the Lebesgue measure, into a pure point measure ($\mu_{f_{\mathrm{pp}}}$), an absolutely continuous measure ($\mu_{f_{\mathrm{ac}}}$) and a singularly continuous measure ($\mu_{f_{\mathrm{sc}}}$).

We now decompose the space into three parts. We set:

$$\begin{aligned} \mathscr{H}_{\mathrm{pp}} &= \overline{\{f \in \mathscr{H} : \mu_f = \mu_{f_{\mathrm{pp}}}\}}, \\ \mathscr{H}_{\mathrm{ac}} &:= \{f \in \mathscr{H} : \mu_f = \mu_{f_{\mathrm{ac}}}\}, \\ \mathscr{H}_{\mathrm{sc}} &:= \{f \in \mathscr{H} : \mu_f = \mu_{f_{\mathrm{sc}}}\}, \end{aligned}$$

the pure point subspace, the absolutely continuous subspace, and the singularly continuous subspace associated to H, respectively.

We infer the orthogonal decomposition:

$$\mathscr{H} = \mathscr{H}_{\mathrm{pp}} \oplus \mathscr{H}_{\mathrm{ac}} \oplus \mathscr{H}_{\mathrm{sc}}.$$

This induces the following definitions for the spectrum of the self-adjoint operator H:

- pure point spectrum: $\sigma_{\mathrm{pp}}(H) = \sigma(H_{|\mathscr{H}_{\mathrm{pp}}})$
- absolutely continuous spectrum: $\sigma_{\mathrm{ac}}(H) = \sigma(H_{|\mathscr{H}_{\mathrm{ac}}})$
- singularly continuous spectrum: $\sigma_{\mathrm{sc}}(H) = \sigma(H_{|\mathscr{H}_{\mathrm{sc}}})$

Adapting the Riemann-Lebesgue Theorem, we sharpen the RAGE Theorem:

Proposition 2.3.2. *Take K which is relatively compact to H and assume that $f \in \mathscr{H}_{\mathrm{ac}}$. Then one has:*

$$K e^{-\mathrm{i}tH} f \to 0, \text{ as } t \to \pm\infty. \tag{2.3.1}$$

Example 2.3.3. *In the setting of Example 2.2.2, if one take $V(x) = o(|x|^{-1-\varepsilon})$, as $|x| \to \infty$ and by taking $f \in \mathscr{H}_{\mathrm{pp}}^{\perp}$ then one has $f \in \mathscr{H}_{\mathrm{ac}}$. Finally, given a compact set $X \subset \mathbb{R}^n$, one can take $K := \mathbf{1}_X(Q)$ and (2.3.1) holds. The particle escapes all compact sets. One can also prove that $\sigma_{\mathrm{pp}}(H)$ is a compact set included in $(-\infty, 0]$ and that $\sigma_{\mathrm{ac}}(H) = [0, \infty)$. The fact that 0 is an eigenvalue or not is a much refined question.*

In our work we are especially interested in showing that

$$\sigma_{\mathrm{sc}}(S) = \emptyset.$$

Motivated by Example 2.3.3, one sees that this property is linked with the decay of potentials at infinity. We start with a down-to-earth and standard example:

Example 2.3.4. *Let $g \in \mathcal{C}^1(]a, b[)$ such that $\sharp\{x \mid g'(x) = 0\} < \infty$. Then the space $\mathscr{H}_{\mathrm{ac}}(g(Q)) = L^2(]a, b[)$.*

In actual cases, it can be very difficult to diagonalize explicitly a self-adjoint operator, i.e., to show that it is unitarily equivalent to an explicit $g(Q)$ acting in an explicit $L^2((a, b), \mu)$. The standard approach to prove purely a.c. spectrum, is the following one, e.g., [ReSi79][Theorem XIII.19]:

Proposition 2.3.5. *Let H be a self-adjoint operator of $\mathscr{H}$, let (x_1, x_2) be an interval and $f \in \mathscr{H}$. Suppose*

$$\sup_{\varepsilon>0} \sup_{\lambda \in (x_1, x_2)} \left| \left\langle f, \Im(H - \lambda - \mathrm{i}\varepsilon))^{-1} f \right\rangle \right| \leq c(f) < +\infty, \tag{2.3.2}$$

then the measure $\langle f, \mathbf{1}_{(\cdot)}(H) f\rangle$ is purely absolutely continuous w.r.t. the Lebesgue measure on (x_1, x_2).

Moreover, if (2.3.2) holds for a dense set of $f \in \mathscr{H}$, then the spectrum of H is purely absolutely continuous w.r.t. the Lebesgue measure on (x_1, x_2).

This proposition gives us an aim, i.e., to prove (2.3.2). However, one needs some techniques to achieve this. In this work, I will present two families of them. The first one is based on positive commutator techniques. It will be largely developed in the two next chapters. The second one is a 1-dimensional technique (transfer matrices) and will be discussed in Section 6.1.

Chapter 3

Positive commutator techniques

3.1 Basic ideas and General theory

The first stone was set by C.R. Putnam, see [Pu67].

Proposition 3.1.1. *Let H be a a bounded self-adjoint operator acting in a Hilbert space $\mathscr{H}$. Suppose that there is a bounded self-adjoint operator A, such that:*

$$[H, \mathrm{i}A] = C^*C,$$

where C is a bounded and injective operator. Then,

$$\sup_{\varepsilon>0} \sup_{\lambda\in(x_1,x_2)} \left|\left\langle f, \Im(H-\lambda-\mathrm{i}\varepsilon))^{-1} f\right\rangle\right| \leq 4\|A\| \cdot \|(C^*)^{-1}f\|^2, \tag{3.1.1}$$

for all $f \in \mathcal{D}((C^*)^{-1})$. In particular, the spectrum of H is purely absolutely continuous.

Proof. Set $R(z) := (H - z)^{-1}$. Then

$$\begin{aligned}
\|CR(\lambda \pm \mathrm{i}\varepsilon)\|^2 &= \|R(\lambda \mp \mathrm{i}\varepsilon)C^*CR(\lambda \pm \mathrm{i}\varepsilon)\| \\
&= \|R(\lambda \mp \mathrm{i}\varepsilon)[H, \mathrm{i}A]R(\lambda \pm \mathrm{i}\varepsilon)\| \\
&= \|R(\lambda \mp \mathrm{i}\varepsilon)[H - \lambda \mp \mathrm{i}\varepsilon, \mathrm{i}A]R(\lambda \pm \mathrm{i}\varepsilon)\| \\
&\leq \|AR(\lambda \pm \mathrm{i}\varepsilon)\| + \|R(\lambda \mp \mathrm{i}\varepsilon)A\| + 2\varepsilon\|R(\lambda \mp \mathrm{i}\varepsilon)AR(\lambda \pm \mathrm{i}\varepsilon)\| \leq 4\|A\|/\varepsilon.
\end{aligned}$$

Therefore, we obtain

$$2\|C\Im R(\lambda \pm \mathrm{i}\varepsilon)C^*\| = \|2\mathrm{i}\varepsilon CR(\lambda + \mathrm{i}\varepsilon)R(\lambda - \mathrm{i}\varepsilon)C^*\| \leq 8\|A\|.$$

Then, note that the domain of $(C^*)^{-1}$, which we denoted by $\mathcal{D}((C^*)^{-1})$, is dense in $\mathscr{H}$ since C is injective. Finally we conclude by Proposition 2.3.5. □

Here we have proved a stronger result than the absence of singularly continuous spectrum, (3.1.1) is in fact equivalent to the global propagation estimate:

$$\int_{\mathbb{R}} \|C^* e^{-\mathrm{i}tH} f\|^2 dt \leq c\|f\|^2,$$

for some $c > 0$. Kato provided a dynamical proof Putnam's Theorem in [Ka68]. The operator A was still bounded. Then Lavine in [La68] gave an interesting application, he extended the proof to some A which was H-bounded. But they all faced the same problem: the method excludes the presence of eigenvalue for H. Moreover, it is difficult to construct a bounded A and it would be much easier to take it unbounded (and not only H-bounded).

3.2 Mourre estimate - classical theory

In the beginning of the eighties, E. Mourre had the brilliant idea to localize (3.1.1) in energy. His theory was developed in [Mo81] to show the absolute continuity of the continuous spectrum of 3-body Schrödinger operators and to study their scattering theory. His work was immediately generalized to the N-body context in [PeSiSi81]. In particular, one wanted to show their asymptotic completeness and the Mourre estimate, c.f., (3.2.1), played a crucial role in the proof. Now, Mourre's commutator theory is fundamental tool to develop the stationary scattering theory of general self-adjoint operators. We refer to [AmBoGe96] for some historical developments.

To enter into the details of our approach, we need some notation and basic notions. We consider two self-adjoint (possibly unbounded) operators H and A acting in some complex separable Hilbert space $\mathscr{H}$. We shall study the spectral properties of H with the help of A. Since the commutator $[H, \mathrm{i}A]$ is going to play a central role in the theory, we need some regularity of H with respect to A to give an appropriate sense to this commutator. First there is a priori no reason that $[H, A]f$ can be taken directly, i.e., by setting $[H, A]f := HAf - AHf$. Indeed both A and H could be unbounded and the expression would have a meaning if $f \in \mathcal{D}(H) \cap \mathcal{D}(A)$, $Hf \in \mathcal{D}(A)$ and $Af \in \mathcal{D}(H)$. In application, it could happen that there is no dense subspace of f which satisfies those three conditions. We rely then on the form version:

$$\langle f, [H, A]g\rangle := \langle Hf, Ag\rangle - \langle Af, Hg\rangle.$$

Here we require that $f, g \in \mathcal{D}(A) \cap \mathcal{D}(H)$ which are much more chance to be a dense subspace. In most of the cases, the r.h.s. will have a closure. For instance using the Riesz lemma, we say that the closure of $[H, A]$ belongs to $\mathcal{B}(\mathcal{D}(H), \mathcal{D}(H)^*)$ if there is C

$$\langle f, [H, A]g\rangle \leq C\|(H + \mathrm{i})f\| \cdot \|(H + \mathrm{i})g\|,$$

for all $f, g \in \mathcal{D}(A) \cap \mathcal{D}(H)$ and if $\mathcal{D}(A) \cap \mathcal{D}(H)$ is dense in $\mathcal{D}(H)$. We shall denote it by $[H, A]_\circ$.

At the formal level, we expect two kinds of assumptions:

(a) the first commutator of H with A, $[H, A]_\circ$, is an element of $\mathcal{B}(\mathcal{D}(H), \mathcal{D}(H)^*)$

(b) the second commutator of H with A, $[H, [H, A]_\circ, A]_\circ$, is an element of $\mathcal{B}(\mathcal{D}(H), \mathcal{D}(H)^*)$.

The former would be the formal form of what we call $H \in \mathcal{C}^1(A)$ while the latter is expressed by $H \in \mathcal{C}^2(A)$. A rigorous version is that $H \in \mathcal{C}^k(A)$ if for a $z \in \mathbb{C} \setminus \sigma(H)$ [then for all]

$$\mathbb{R} \ni t \mapsto e^{\mathrm{i}tA}(H - z)^{-1}e^{-\mathrm{i}tA}f \in \mathscr{H}$$

has the usual $\mathcal{C}^k$ regularity for all $f \in \mathscr{H}$. We shall go into more detail about the $\mathcal{C}^1$ class in Section 3.8.

We say that the *Mourre estimate* holds true for H on a bounded interval $\mathcal{I}$ if there exist $c > 0$ and a compact operator K such that

$$E_{\mathcal{I}}(H)[H, \mathrm{i}A]_\circ E_{\mathcal{I}}(H) \geq cE_{\mathcal{I}}(H) + K, \tag{3.2.1}$$

in the form sense on $\mathscr{H} \times \mathscr{H}$. Here $E_{\mathcal{I}}(H)$ denotes the spectral measure of H above $\mathcal{I}$. Note that the $\mathcal{C}^1$ hypothesis ensures that the l.h.s. of (3.2.1) is a bounded operator.

Let $f \in \mathscr{H}$ and $\lambda \in \mathcal{I}$ with $Hf = \lambda f$. Then $E_{\mathcal{I}}(H)f = f$. Assume that $H \in \mathcal{C}^1(A)$. The Virial Theorem, e.g., [AmBoGe96, Proposition 7.2.10], implies that $\langle f, [H, \mathrm{i}A]_\circ f\rangle = 0$. If (3.2.1) holds true with $K = 0$ then f must be zero and there is no eigenvalue in $\mathcal{I}$. If (3.2.1) holds true then the total multiplicity of the eigenvalues in $\mathcal{I}$ is finite, e.g., [AmBoGe96, Corollary 7.2.11]. For a general discussion on the Virial Theorem see [GeGé99].

Moreover, choosing a sub-interval of $\mathcal{I}$ without any eigenvalue of H and by shrinking it, the spectral measure tends to 0 and then the compact part tends in norm to 0. Therefore, we always assume in the sequel the following *strict Mourre estimate*:

$$E_{\mathcal{I}}(H)[H, \mathrm{i}A]_\circ E_{\mathcal{I}}(H) \geq cE_{\mathcal{I}}(H), \text{ with } c > 0. \tag{3.2.2}$$

Before giving a result concerning the absence of absolutely continuous spectrum we give a heuristic explaination by means of the Heisenberg picture.

Given a state f and $f_t := e^{-\mathrm{i}tH}f$ its evolution at time $t \in \mathbb{R}$ under the dynamic generated by the Hamiltonian H, one looks at the Heisenberg picture:

$$\mathcal{H}_f(t) := \langle f_t, Af_t\rangle. \tag{3.2.3}$$

As A is an unbounded self-adjoint operator, we take $f := \varphi(H)g$, with $g \in \mathcal{D}(A)$ and $\varphi \in \mathcal{C}_c^\infty(\mathcal{I})$. Now $\mathcal{H}_f$ is well-defined as $e^{-\mathrm{i}tH}\varphi(H)$ stabilizes the domain of A by Lemma 3.8.5. This implies also that $\mathcal{H}_f \in \mathcal{C}^\infty(\mathbb{R})$.

Since $H \in \mathcal{C}^1(A)$, the commutator $[H, \mathrm{i}A]$ defined on $\mathcal{D}(H) \cap \mathcal{D}(A) \times \mathcal{D}(H) \cap \mathcal{D}(A)$ extends to a bounded operator from $\mathcal{D}(H)$ to $\mathcal{D}(H)^*$, see Section 3.8 for more details. We denote by C the norm $\|[H, \mathrm{i}A]_\circ\|_{\mathcal{B}(\mathcal{D}(H),\mathcal{D}(H)^*)}$. Moreover,

$$\mathcal{H}'_f(t) = \langle f_t, [H, \mathrm{i}A]_\circ f_t\rangle = \langle f_t, E_{\mathcal{I}}(H)[H, \mathrm{i}A]_\circ E_{\mathcal{I}}(H)f_t\rangle.$$

We now use the Mourre estimate above $\mathcal{I}$ and since $e^{\mathrm{i}tH}$ is unitary, one gets:

$$c\|f\|^2 \leq \mathcal{H}'_f(t) \leq C\|f\|^2. \tag{3.2.4}$$

Now integrate (3.2.4) and obtain

$$ct\|f\|^2 \leq \mathcal{H}_f(t) - \mathcal{H}_f(0) \leq Ct\|f\|^2, \qquad \text{for } t \geq 0 \tag{3.2.5}$$

The transport of the particle is therefore ballistic with respect to A. Purely absolutely continuous spectrum is therefore expected. This is a hard and open question. The question already appeared in [Si90]. Some links between a.c. spectrum and ballistic transport have been recently pointed out in [AiWa12].

The positive lower bound on $\mathcal{H}_f(t)$ is usually the heuristic justification of why $Ke^{-\mathrm{i}tH}f$ should tend to 0 as $t \mapsto \infty$ where K is relatively compact with respect to H and the hope that the spectral measure of H is purely absolutely continuous with respect to the Lebesgue measure. This is however formal as it is unclear whether a part of f_t remains localized in energy, with respect to A. In spite of that, this lower bound implies that A is neither bounded from below nor from above:

Proposition 3.2.1. *Assume that the Mourre estimate* (3.2.2) *holds true, that* $H \in \mathcal{C}^1(A)$ *and also that* $E_{\mathcal{I}}(H)$ *is not zero. Then* A *is not semi-bounded and* A *is not* H*-bounded.*

Proof. If A is bounded from above, for instance. Then, there is c_0 such that $\langle\phi, A\phi\rangle \leq c_0\|\phi\|$ for all $\phi \in \mathcal{D}(A)$. Now, since $E_{\mathcal{I}}(H) \neq 0$ and that $\mathcal{D}(A)$ is dense in $\mathscr{H}$, there are $\varphi \in \mathcal{C}_c^\infty(\mathcal{I})$, $g \in \mathcal{D}(A)$ and a *non-zero* element of $\mathcal{D}(A)$ given by $f := \varphi(H)g$ such that $f_t \in \mathcal{D}(A)$ for all $t \in \mathbb{R}$, c.f., Lemma 3.8.5. By letting t tend to infinity in (3.2.5), one obtains a contradiction. The proof for A being not H-bounded goes along the same line. □

In the Putnam theory, one has that $\mathcal{H}_f(\cdot)$ is also strictly increasing. The difference is that there is no lower bound for $\mathcal{H}'_f$. This is why the boundedness of A is allowed. In this setting, note also that $\mathcal{H}_f(t)$ as a limit has t tends to $\pm\infty$.

In [Mo81], using a method of differential inequalities and assuming a second-commutator hypothesis, $H \in \mathcal{C}^2(A)$ in the setting of [AmBoGe96], one gets a limiting absorption principle (LAP) on any compact sub-interval $\mathcal{J}$ of $\mathcal{I}$:

$$\sup_{\lambda\in\mathcal{J},\varepsilon>0} |\langle f, (H-\lambda-\mathrm{i}\varepsilon)^{-1} f|\rangle \leq C\|\langle A\rangle^s f\|^2, \tag{3.2.6}$$

for $s > 1/2$ and where $\langle x\rangle := \sqrt{1+x^2}$. This immediately gives the absence of singularly continuous spectrum and propagation estimate:

$$\int_{\mathbb{R}} \|\langle A\rangle^s e^{\mathrm{i}tH} E_I(H) f\|^2 dt \leq c\|f\|^2,$$

for some $c > 0$.

Taking two commutators is however very restrictive in the applications. Therefore, it was crucial to weaken this hypothesis. For the question of the LAP, a lot of energy has been devoted to reach the optimal class, $H \in \mathcal{C}^{1,1}(A)$, i.e.,

$$\int_0^1 \left\|[[(H-z)^{-1}, e^{\mathrm{i}tA}], e^{\mathrm{i}tA}]\right\| \frac{dt}{t^2} \ < \ \infty,$$

for some $z \notin \sigma(H)$. We refer to [AmBoGe96][Section 7] for proofs and references therein. This condition is rather subtle. For instance, when H is the multiplication by a real-valued function and $A = -\mathrm{i}\partial_x$ in $L^2(\mathbb{R})$, $H \in \mathcal{C}^{1,1}(A)$ if and only if its resolvent belongs to the Besov space $\mathcal{B}_2^{1,1}(\mathbb{R})$. The optimality of the condition $\mathcal{C}^{1,1}$ is pointed out in [AmBoGe96][section 7.B].

We present a classical example of construction of the Mourre estimate. Set $d \geq 1$. For the sake of simplicity, we shall present an intermediate situation. In the sequel we denote by $V(Q)$ the operator of multiplication by the function V.

Theorem 3.2.2. *Set H_0 to be the self-adjoint realization of the Laplace operator $-\Delta$ in $L^2(\mathbb{R}^d)$. Set*

$$H := H_0 + V(Q),$$

where $V := V_{\mathrm{sr}} + V_{\mathrm{lr}}$ is the sum of real-valued functions, $V_{\mathrm{sr}} \in L^\infty(\mathbb{R}^d)$ is the short-range component and $V_{\mathrm{lr}} \in L^\infty(\mathbb{R}^d)$ the long-range one. Suppose that the distribution $x \mapsto x\cdot\nabla V_{\mathrm{lr}}(x)$ is a function and that

$$\lim_{\|x\|\to\infty} V_{\mathrm{sr}}(x) = \lim_{\|x\|\to\infty} V_{\mathrm{lr}}(x) = 0. \tag{3.2.7}$$

Then, $\sigma_{\mathrm{ess}}(H) = [0,\infty)$. Take $A := (P\cdot Q + Q\cdot P)/2$, where $P := -\mathrm{i}\nabla$.

a) Assume that

$$x \mapsto \langle x\rangle V_{\mathrm{sr}}(x) \text{ and } x \mapsto x\cdot\nabla V_{\mathrm{lr}}(x) \in L^\infty. \tag{3.2.8}$$

Then, $H \in \mathcal{C}^1(A)$ and there is $\kappa > 0$ such that (3.2.1) holds true for all interval $\mathcal{I}$ such that $\inf \mathcal{I} \geq \kappa$.

b) Assume that

$$\lim_{\|x\|\to\infty} \langle x\rangle V_{\mathrm{sr}}(x) = \lim_{\|x\|\to\infty} x\cdot\nabla V_{\mathrm{lr}}(x) = 0. \tag{3.2.9}$$

Then, $H \in \mathcal{C}^1(A)$ and (3.2.1) holds true for all interval $\mathcal{I}$ such that $\inf \mathcal{I} > 0$.

c) Assume there is $\varepsilon > 0$ such that

$$\lim_{\|x\|\to\infty} \langle x\rangle^{1+\varepsilon} V_{\rm sr}(x) = \lim_{\|x\|\to\infty} \langle x\rangle^{\varepsilon} x\cdot \nabla V_{\rm lr}(x) = 0. \tag{3.2.10}$$

Then, $H \in \mathcal{C}^{1,1}(A)$, (3.2.1) for for all interval $\mathcal{I}$ such that $\inf \mathcal{I} > 0$, (3.2.6) hold true. In particular H has no singularly continuous spectrum.

We mention that it is well-known that there is no positive eigenvalue, see [FrHe82].

Remark 3.2.3. *Assume that*

$$\lim_{\|x\|\to\infty} \langle x\rangle^{2} V_{\rm sr}(x) = \lim_{\|x\|\to\infty} \langle x\rangle^{2} x\cdot \nabla V_{\rm lr}(x) = 0. \tag{3.2.11}$$

Then, $H \in \mathcal{C}^2(A)$.

Partial proof. We present the proof of the point b) and refer to [AmBoGe96, Theorem 7.6.8] for a full proof. The domain of H is the Sobolev space $\mathscr{H}^2$. Consider the strongly continuous one-parameter unitary group $\{\mathcal{W}_t\}_{t\in\mathbb{R}}$ acting by:

$$(\mathcal{W}_t f)(x) = e^{dt/2} f(e^t x), \text{ for all } f \in L^2.$$

This is the C_0-group of dilation. A direct computation shows that

$$\mathcal{W}_t\, \mathscr{H}^2 \subset \mathscr{H}^2, \text{ for all } t\in\mathbb{R}. \tag{3.2.12}$$

We denote by A its generator. It is self-adjoint and given by the closure of $(P\cdot Q + Q\cdot P)/2$ on $\mathcal{C}_c^\infty$ in L^2, where $P := -\mathrm{i}\nabla$. Since

$$[H_0, \mathrm{i}A]_\circ = 2H_0 \tag{3.2.13}$$

and (3.2.12) holds, Theorem 3.8.3 ensures that $H_0 \in \mathcal{C}^1(A)$. We now compute the commutators with the potentials on $\mathscr{H}^2 \cap \mathcal{D}(A) \times \mathscr{H}^2 \cap \mathcal{D}(A)$. The easy one is: $[V_{\rm lr}(Q), \mathrm{i}A]_\circ = Q\cdot \nabla V_{\rm lr}(Q)$. Note that it is a compact operator from $\mathscr{H}^1$ to L^2, by Rellich-Kondrakov. We turn to

$$\begin{aligned}\langle f, [V_{\rm sr}(Q), \mathrm{i}A] g\rangle &= \langle V_{\rm sr}(Q) f, \mathrm{i}Ag\rangle - \langle Af, \mathrm{i}V_{\rm sr}(Q) g\rangle\\ &= \langle \langle Q\rangle V_{\rm sr}(Q) f, \langle Q\rangle^{-1}(Q\cdot P + d/2) g\rangle\\ &\quad + \langle \langle Q\rangle^{-1}(Q\cdot P + d/2) f, \langle Q\rangle V_{\rm sr}(Q) g\rangle\end{aligned}$$

Note that we did not commute $V_{\rm sr}$ with a derivative. Its closure is a compact operator from $\mathscr{H}^1$ into $\mathscr{H}^{-1}$. Indeed, we consider for instance the first term. We have $\langle Q\rangle^{-1}(Q\cdot P + d/2)$ bounded from $\mathscr{H}^1$ into L^2 and $\langle Q\rangle V_{\rm sr}(Q)$ compact from L^2 into $\mathscr{H}^{-1}$ by Rellich-Kondrakov. We summarize:

$$[V_{\rm sr}(Q), \mathrm{i}A]_\circ + [V_{\rm lr}(Q), \mathrm{i}A]_\circ \in \mathcal{K}(\mathscr{H}^1, \mathscr{H}^{-1}). \tag{3.2.14}$$

Recalling Theorem 3.8.1, we infer that $H \in \mathcal{C}^1(A)$.

We focus now on the Mourre estimate. Take $\lambda \in (0,\infty)$ and $\varphi \in \mathcal{C}_c^\infty(\mathbb{R}; [0,1])$ being 1 in a neighborhood of λ and with support in $(0,\infty)$. By (3.2.13), there is $c > 0$ such that

$$\varphi(H_0)[H_0, \mathrm{i}A]_\circ \varphi(H_0) \geq c\,\varphi^2(H_0)$$

holds. Now recalling (3.2.14) and that $\varphi(H) - \varphi(H_0)$ is compact from $\mathscr{H}^2$ to L^2, this follows from the Helffer-Sjøstrand Formula and (3.2.14), we derive that there is a compact K such that:

$$\varphi(H)[H, \mathrm{i}A]_\circ \varphi(H) \geq c\,\varphi^2(H) + K$$

Finally, by taking an interval $\mathcal{I}$ which contains λ and where $\varphi|_{\mathcal{I}} = 1$, we obtain (3.2.1). □

When $d = 1$, we point out that if $V = \mathcal{O}(1/\|x\|)$, A. Kiselev proved in [Ki05] that there is no singularly continuous spectrum for H. The case $o(1/\|x\|)$ was previously obtained by C. Remling in [Re98]. The decay assumption is in fact optimal. Indeed, for any positive function h which grows at infinity, there is a potential V such that $V = \mathcal{O}(h(|x|)/|x|)$ and $-\Delta + V(Q)$ has some singularly continuous spectrum, see [Ki05], or has dense point spectrum, see [Na86, Si97].

3.3 Application to magnetic Laplacians on manifolds

In this section we explain a first application of the Mourre theory in the context of differential operators acting on manifolds with finite volume.

Let X be a smooth manifold of dimension n, diffeomorphic outside a compact set to a cylinder $(1,\infty)\times M$, where M is a possibly disconnected closed (= compact without boundary) manifold. On X we consider asymptotically conformally cylindrical metrics, i.e., perturbations of the metric given near the border $\{\infty\}\times M$ by:

$$g_p = y^{-2p}(dy^2 + h), \qquad y \to \infty \tag{3.3.1}$$

where h is a metric on M and $p > 0$. If $p = 1$ and h is flat, the ends are *cusps*, i.e., complete hyperbolic of finite volume. For $p > 1$ one gets the (incomplete) metric horns. For our presentation, we focus on the complete case, i.e., $p \leq 1$ and refer to [GoMo08] for further discussions about the incomplete case.

The refined properties of the essential spectrum of the Laplace-Beltrami operator $\Delta_p := d^*d$ have been studied by Froese and Hislop [FrHi89] in the complete case. For the unperturbed metric (3.3.1), they get

$$\sigma_{\rm ess}(\Delta_p) = [\kappa(p), \infty), \text{ where } \begin{cases} \kappa(p) := 0, & \text{for } p < 1 \\ \kappa(1) := \left(\frac{n-1}{2}\right)^2. \end{cases} \tag{3.3.2}$$

The singular continuous part of the spectrum is empty and the eigenvalues distinct from $\kappa(p)$ are of finite multiplicity and may accumulate only at $\kappa(p)$. Froese and Hislop actually show a limiting absorption principle, a stronger result, see also [DeHiSi92, FrHiPe91, FrHiPe91b, Hi94] for the continuation of their ideas. Their approach relies on a Mourre estimate. See for instance [Gu98, Ku06] for different methods.

As seen in Section 2.3, a dynamical consequence of the absence of singular continuous spectrum and of the local finiteness of the point spectrum is that for an interval $\mathcal{J}$ that contains no eigenvalue of the Laplacian, for all $\chi \in \mathcal{C}_c^\infty(X)$ and $\phi \in L^2(X)$, the norm $\|\chi e^{it\Delta_p}E_{\mathcal{J}}(\Delta_p)\phi\|$ tends to 0 as t tends to $\pm\infty$. In other words, if you let evolve long enough a particle which is located at scattering energy, it eventually becomes located very far on the exits of the manifold. Add now a magnetic field B with compact support and look how strongly it can interact with the particle. Classically there is no interaction as B and the particle are located far from each other. One looks for a quantum effect.

The Euclidean intuition tells that there is no essential difference between the free Laplacian and the magnetic Laplacian Δ_A, when A is a magnetic potential arising from a magnetic field B with compact support. They still share the spectral properties of absence of singular continuous spectrum and local finiteness of the point spectrum, although a long-range effect does occur and destroys the asymptotic completeness of the couple (Δ, Δ_A); one needs to modify the wave operators to compare the two operators, see [LoTh87]. However, we point out that the situation is dramatically different in our setting and therefore on hyperbolic manifolds of finite volume, even if the magnetic field is very small in size and with compact support. We now go into definitions and describe our results.

A magnetic field B is a smooth real exact 2-form on X. There exists a real 1-form A, called vector potential, satisfying $dA = B$. Set $d_A := d + \mathrm{i}A\wedge : \mathcal{C}_c^\infty(X) \to \mathcal{C}_c^\infty(X, T^*X)$. The magnetic Laplacian on $\mathcal{C}_c^\infty(X)$ is given by $\Delta_A := d_A^* d_A$. When the manifold is complete, Δ_A is known to be essentially self-adjoint, see [Sc01]. Given two vector potentials A and A' such that $A - A'$ is exact, the two magnetic Laplacians Δ_A and $\Delta_{A'}$ are unitarily equivalent, by gauge invariance. Hence when the first cohomogical group is trivial, i.e., $H^1_{\mathrm{dR}}(X) = 0$, the spectral properties of the magnetic Laplacian do not depend on the choice of the vector potential, so we may write Δ_B instead of Δ_A. To simplify our presentation we shall focus on $H^1_{\mathrm{dR}}(X) = 0$ and assume that the boundary is connected.

Definition 3.3.1. *Let X be the interior of a compact manifold with boundary $\partial\overline{X}$. Suppose that $H^1_{\mathrm{dR}}(X) = 0$ and that $M = \partial\overline{X}$ is connected. Let B be a magnetic field on X which is compactly supported. We say that B is* trapping *if*

1) *either B does not vanish identically on M, or*

2) *B vanishes on M but defines a non-integral cohomology class $[2\pi B]$ inside the relative cohomology group $H^2_{\mathrm{dR}}(X, M)$.*

Otherwise, we say that B is *non-trapping*. This terminology is motivated by the spectral consequences a) and c) of Theorem 3.3.2. The definition can be generalized to the case where M is disconnected. The condition of B being trapping can be expressed in terms of any vector potential A. We mention that when $H^1_{\mathrm{dR}}(X) \neq 0$, the trapping condition makes sense only for vector potentials, see Theorem 3.3.3.

Let us fix some notation. To measure the size of the perturbation, we compare it to the lengths of geodesics. Let $L \in \mathcal{C}^\infty(X)$ be defined by

$$L \geq 1, \quad L(y) = \begin{cases} \frac{y^{1-p}}{1-p} & \text{for } p < 1 \\ \ln(y) & \text{for } p = 1 \end{cases}, \text{ for } y \text{ big enough.} \tag{3.3.3}$$

Given $s \geq 0$, let $\mathscr{L}_s$ be the domain of L^s equipped with the graph norm. We set $\mathscr{L}_{-s} := \mathscr{L}_s^*$ where the adjoint space is defined so that $\mathscr{L}_s \subset L^2(X, g_p) \subset \mathscr{L}_s^*$, using the Riesz lemma. Given a subset I of $\mathbb{R}$, let $I_\pm$ be the set of complex numbers $x \pm \mathrm{i}y$, where $x \in I$ and $y > 0$. For simplicity, we state our result only for the unperturbed metric (3.3.1).

Theorem 3.3.2. *Let $1 \geq p > 0$, g_p the metric given by* (3.3.1)*. Suppose that $H_1(X, \mathbb{Z}) = 0$ and that M is connected. Let B be a magnetic field with compact support. If B is trapping then:*

a) *The spectrum of Δ_B is purely discrete.*

b) *The asymptotic of its eigenvalues is given by*

$$N_{B,p}(\lambda) \approx \begin{cases} C_1 \lambda^{n/2} & \text{for } 1/n < p, \\ C_2 \lambda^{n/2} \log \lambda & \text{for } p = 1/n, \\ C_3 \lambda^{1/2p} & \text{for } 0 < p < 1/n \end{cases} \tag{3.3.4}$$

in the limit $\lambda \to \infty$, where C_3 is given [GoMo08], and

$$C_1 := \frac{\mathrm{Vol}(X, g_p)\,\mathrm{Vol}(S^{n-1})}{n(2\pi)^n}, \quad C_2 := \frac{\mathrm{Vol}(M, h)\,\mathrm{Vol}(S^{n-1})}{2(2\pi)^n}. \tag{3.3.5}$$

If B is non-trapping with compact support in X then

c) The essential spectrum of Δ_B is $[\kappa(p), \infty)$.

d) The singular continuous spectrum of Δ_B is empty.

e) The eigenvalues of Δ_B are of finite multiplicity and can accumulate only in $\{\kappa(p)\}$.

f) Let $\mathcal{J}$ a compact interval such that $\mathcal{J} \cap \big(\{\kappa(p)\} \cup \sigma_{\rm pp}(H)\big) = \emptyset$. Then, for all $s \in]1/2, 3/2[$ and all A such that $dA = B$, there is c such that

$$\|(\Delta_A - z_1)^{-1} - (\Delta_A - z_2)^{-1}\|_{\mathcal{B}(\mathscr{L}_s, \mathscr{L}_{-s})} \leq c\|z_1 - z_2\|^{s-1/2},$$

for all $z_1, z_2 \in \mathcal{J}_\pm$.

Note that the condition of being trapping (resp. non-trapping) is equivalent to having empty (resp. non-empty) essential spectrum in the complete case. The terminology arises from the dynamical consequences of this theorem and should not be confused with the classical terminology. Indeed, when B is trapping, the spectrum of Δ_B is purely discrete and for all non-zero ϕ in $L^2(X)$, there is $\chi \in \mathcal{C}_c^\infty(X)$ such that $1/T \int_0^T \|\chi e^{it\Delta_B}\phi\|^2 dt$ tends to a non-zero constant as T tends to $\pm\infty$. On the other hand, taking $\mathcal{J}$ as in f), for all $\chi \in \mathcal{C}_c^\infty(X)$ one obtains that $\chi e^{it\Delta_B} E_{\mathcal{J}}(\Delta_A)\phi$ tends to zero, when B is non-trapping and with compact support.

The statements a) and b) follow from general results from [Mo08]. This part relies on the Melrose calculus of cusp pseudodifferential operators (see e.g., [MeNi96]). The result still hold for some quasi-isometric perturbation of (3.3.1). The statement *c*) follows directly by the diagonalisation of Δ_A. As announced c), d), e), and f) are consequences of our use of the Mourre Theory. Moreover, short-range and long-range perturbation of a potential and of a magnetic field are also allowed. Let us discuss the perturbation of the metric and consider more generally a conformal perturbation of the metric (3.3.1). Let $\rho \in \mathcal{C}^\infty(X, \mathbb{R})$ be such that $\inf_{y \in X}(\rho(y)) > -1$. Consider the same problem as above for the metric

$$\tilde{g}_p = (1 + \rho)g_p, \text{ for large } y. \tag{3.3.6}$$

In [FrHi89], one essentially assumes that

$$L^2\rho, L^2 d\rho \text{ and } L^2\Delta_g\rho \text{ are in } L^\infty(X),$$

in order to obtain the absence of singular continuous spectrum and local finiteness of the point spectrum. On one hand, one knows from the perturbation of a Laplacian by a short-range potential V that only the speed of the decay of V is important to conserve these properties. On the other hand, in [GeGo08] and in a general setting, one shows that only the fact that ρ tends to 0 is enough to ensure the stability of the essential spectrum. Therefore, it is natural to ask whether the decay of the metric (without decay conditions on the derivatives) is enough to ensure the conservation of these properties. Here, we consider that $\rho = \rho_{\rm sr} + \rho_{\rm lr}$ decomposes in short-range and long-range components. We ask the long-range component to be radial, i.e., that it depends only on the parameter y. We also assume that there exists $\varepsilon > 0$ such that

$$\begin{gathered} L^{1+\varepsilon}\rho_{\rm sr} \text{ and } d\rho_{\rm sr}, \Delta_g\rho_{\rm sr} \in L^\infty(X), \\ L^\varepsilon\rho_{\rm lr},\ L^{1+\varepsilon}d\rho_{\rm lr} \text{ and } \Delta_g\rho_{\rm sr} \in L^\infty(X). \end{gathered} \tag{3.3.7}$$

Going from 2 to $1 + \varepsilon$ is not a significant improvement as it relies on the use of an optimal version of the Mourre theory instead of the original theory, see [AmBoGe96] and references therein. Nevertheless, the fact that the derivatives are asked only to be bounded and no longer to decay is a real improvement due to our method. The conjugate operator introduced in [FrHi89] is too rough to handle very singular perturbations. Here, we introduce a conjugate operator, which is local in energy, in order to avoid the problem. We believe that our approach could be implemented easily in the manifold settings from [Bo06, DeHiSi92, FrHi89, FrHiPe91, FrHiPe91b, Hi94, KrTi04] to improve results on perturbations of the metric.

Partial proof of Theorem 3.3.2. After some transformations and some choice of the vector potential A, we are pursuing the analysis on the manifold $X_0 = X$ endowed with the Riemannian metric

$$dr^2 + h, \qquad\qquad r \to \infty, \tag{3.3.8}$$

on the end $X_0' = [1/2, \infty) \times M$. The magnetic Laplacian is unitarily sent into an elliptic operator of order 2 denoted by Δ_0. On $\mathcal{C}_c^\infty(X_0')$, it acts by

$$\Delta_0 := Q_p \otimes d_{\tilde\theta}^{\,*} d_{\tilde\theta} + (-\partial_r^2 + V_p(Q)) \otimes 1,$$

on the tensor product $L^2([1/2, \infty), dr) \otimes L^2(M, h)$, where

$$V_p(r) = \begin{cases} ((n-1)/2)^2 \\ c_0 r^{-2} \end{cases} \quad \text{and} \quad Q_p(r) = \begin{cases} e^{2r} \\ ((1-p)r)^{2p/(1-p)} \end{cases} \quad \text{for} \quad \begin{cases} p = 1 \\ p < 1. \end{cases}$$

for some c_0 and where $d_{\tilde\theta} = d_M + i\theta_0 \wedge$ for some θ_0. Intuitively, eigenvalues come from $\ker(d_{\tilde\theta}^{\,*} d_{\tilde\theta})^\perp$ and the continuous spectrum from $\ker(d_{\tilde\theta}^{\,*} d_{\tilde\theta})$. One proves that the trapping condition is equivalent to the fact that $P_0 := \ker d_{\tilde\theta}^{\,*} d_{\tilde\theta} = \{0\}$.

We focus on the non-trapping case and explain how to establish the Mourre estimate. By mimicking the case of the Laplacian, see [FrHi89], one may use the following localization of the generator of dilation. Let $\xi \in \mathcal{C}^\infty([1/2, \infty))$ such that the support of ξ is contained in $[2, \infty)$ and that $\xi(r) = r$ for $r \geq 3$ and let $\tilde\chi \in \mathcal{C}^\infty([1/2, \infty))$ with support in $[1, \infty)$, which equals 1 on $[2, \infty)$. By abuse of notation, we denote $\tilde\chi \otimes 1 \in \mathcal{C}^\infty(X_0)$ with the same symbol. Let $\chi := 1 - \tilde\chi$. On $\mathcal{C}_c^\infty(X_0)$ we set:

$$S_\infty := (-\mathrm{i}(\xi\partial_r + \partial_r\xi) \otimes P_0)\, \tilde\chi, \tag{3.3.9}$$

However this operator is *not* suitable for very singular perturbations like that of the metric we consider. To solve this problem, one should consider a conjugate operator more "local in energy". Concerning the Mourre estimate, as it is local in energy for the Laplacian, one needs only a conjugate operator which fits well on this level of energy. Considering singular perturbation theory, the presence of differentials in (3.3.9) is a serious obstruction to deal with (3.3.7); the idea is to replace the conjugate operator with a multiplication operator in the analysis of perturbations, therefore reducing the role of derivatives within it. The approach has been used for Dirac operators for instance in [GeMă01] to treat very singular perturbations. We set:

$$S_R := \tilde\chi \left(\left(\Phi_R(-\mathrm{i}\partial_r)\xi + \xi\Phi_R(-\mathrm{i}\partial_r) \right) \otimes P_0 \right) \tilde\chi,$$

where $\Phi_R(x) := \Phi(x/R)$ for some $\Phi \in \mathcal{C}_c^\infty(\mathbb{R})$ satisfying $\Phi(x) = x$ for all $x \in [-1, 1]$. The operator $\Phi_R(-i\partial_r)$ is defined on $\mathbb{R}$ by $\mathscr{F}^{-1}\Phi_R\mathscr{F}$, where $\mathscr{F}$ is the unitary Fourier transform. Let us also denote by S_R the closure of this operator. Then, we are able to prove that $\Delta_0 \in \mathcal{C}^2(S_R)$. Moreover, given an interval $\mathcal{J}$ inside $\sigma_{\mathrm{ess}}(\Delta_0)$, there exist $\varepsilon_R > 0$ and a compact operator K_R such that

$$E_{\mathcal{J}}(\Delta_0)[\Delta_0, \mathrm{i}S_R]_\circ E_{\mathcal{J}}(\Delta_0) \geq (4\inf(\mathcal{J}) - \varepsilon_R)E_{\mathcal{J}}(\Delta_0) + K_R$$

holds in the sense of forms, and such that ε_R tends to 0 as R goes to infinity. To handle the perturbations (3.3.7), we prove that, after some transformations, the associated Laplacian is a perturbation Δ_0 which is in $\mathcal{C}^{1,1}(S_R)$. □

If $H^1_{\rm dR}(M) \neq 0$ (take $M = S^1$ for instance), there exist some trapping magnetic fields with *compact support*. We construct an explicit example in [GoMo08]. We are able to construct some examples in dimension 2 and higher than 4 but there are topological obstructions in dimension 3. As pointed out previously regarding the Euclidean case, the fact that a magnetic field with compact support can turn off the essential spectrum and even a situation of limiting absorption principle is somehow unexpected and should be understood as a strong long-range effect.

We discuss other interesting phenomena. Consider $M = S^1$ and take a trapping magnetic field B with compact support and a coupling constant $g \in \mathbb{R}$. Now remark that Δ_{gB} is non-trapping if and only if g belongs to the discrete group $c_B\mathbb{Z}$, for a certain $c_B \neq 0$. When $g \notin c_B\mathbb{Z}$ and $p \geq 1/n$, the spectrum of Δ_{gB} is discrete and the eigenvalue asymptotics do not depend either on B or on g. It would be very interesting to know whether the asymptotics of embedded eigenvalues, or more likely of resonances, remain the same when $g \in c_B\mathbb{Z}$, (see [Ch01] for the case $g = 0$). It would be also interesting to study the inverse spectral problem and ask if the magnetic field could be recovered from the knowledge of the whole spectrum, since the first term in the asymptotics of eigenvalues does not feel it.

Assume now that gauge invariance does not hold, i.e., $H^1_{\rm dR}(X) \neq 0$. In quantum mechanics, it is known that the choice of a vector potential has a physical meaning. This is known as the Aharonov-Bohm effect [AhBo59]. Two choices of magnetic potential may lead to in-equivalent magnetic Laplacians. In $\mathbb{R}^2$ with a bounded obstacle, this phenomenon can be seen through a difference of wave phase arising from two non-homotopic paths that circumvent the obstacle. Some long-range effect appears, for instance in the scattering matrix like in [Ro03, RoYa02, RoYa03], in an inverse-scattering problem [Ni00, We02] or in the semi-classical regime [BiRo01]. See also [He88] for the influence of the obstacle on the bottom of the spectrum. In all of these cases, the essential spectrum remains the same.

We discuss briefly the Aharonov-Bohm effect in our setting. In light of Theorem 3.3.2, one expects a drastic effect. We show that the choice of a vector potential can indeed have a significant spectral consequence. For one choice of vector potential, the essential spectrum could be empty and for another choice it could be a half-line. This phenomenon is generic for hyperbolic surfaces of finite volume, and also appears for hyperbolic 3-manifolds. We focus the presentation on magnetic fields B with compact support. We say that a smooth vector potential A (i.e., a smooth 1-form on $\overline{X}$) is trapping if Δ_A has compact resolvent, and non-trapping otherwise. It also follows that when the metric is of type (3.3.1), A is trapping if and only if a)–b) of Theorem 3.3.2 hold for Δ_A, while A is non-trapping if and only if Δ_A satisfies c)–f) of Theorem 3.3.2.

Theorem 3.3.3. *Let X be a complete oriented hyperbolic surface of finite volume and B a smooth magnetic field on the compactification $\overline{X}$.*

- *If X has at least 2 cusps, then for all B there exists both trapping and non-trapping vector potentials A such that $B = dA$.*
- *If X has precisely 1 cusp, choose $B = dA = dA'$ where A, A' are smooth vector potentials for B on $\overline{X}$. Then*

$$A \textit{ is trapping} \iff A' \textit{ is trapping} \iff \int_X B \in 2\pi\mathbb{Z}.$$

This implies on one hand that for a choice of A, as one has the points c), d), and e), a particle located at a scattering energy escapes from any compact set; on the other hand taking a trapping choice, the particle will behave like an eigenfunction and will remain bounded.

3.4 Application to the Hodge Laplacian on manifolds

There exist complete, noncompact manifolds on which the scalar Laplacian has purely discrete spectrum, see e.g. [Do79]. The goal of this note is to understand such phenomena for the Laplacian on differential forms in a more geometric setting. We aim to provide eigenvalue asymptotics whenever the spectrum is purely discrete, and to clarify the nature of the essential spectrum when it arises.

As in the previous section, we study n-dimensional Riemannian manifolds X with ends diffeomorphic to a cylinder $[0,\infty)\times M$, where M is a closed (= compact without boundary), possibly disconnected Riemannian manifold. The metric on X near the boundary is assumed to be quasi-isometric to the unperturbed model metric

$$g_p = y^{-2p}(dy^2 + h), \qquad y\to\infty \tag{3.4.1}$$

where h is a metric on M and $p>0$.

We denote by $\Delta = d^*d + \delta^*\delta$ the Hodge Laplacian defined on smooth forms with compact support in X. It is a symmetric non-negative operator in $L^2(X,\Lambda^*X,g_p)$ and we also denote by Δ its self-adjoint Friedrichs extension. If $p\leq 1$, i.e. if (X,g_p) is complete, then Δ is essentially self-adjoint, see [Ga55]. Since Δ preserves the space of k-forms, we can define Δ_k as its restriction to $\Lambda^k X$, which is also self-adjoint.

The essential spectrum of the Laplacian acting on forms on non-compact manifolds and has been extensively studied, as it provides informations on the Hodge decomposition of the space of L^2 forms. Without attempting to give an exhaustive bibliography, we mention here the papers [Bu99, Ca02, GoWa04, Lo01, Ma88, MaPh90]. We are interested in some refined (and less studied) properties of the essential spectrum, namely the absence of singularly continuous spectrum and estimate of the resolvent. For the metric (3.4.1), in the complete case, a refined analysis was started in [An04] and [An06]. For technical reasons, Antoci is unable to decide whether 0 is isolated in the essential spectrum of Δ_k except in the case where $M=S^{n-1}$ with the standard metric, assuming that the metric on X is globally rotationally-symmetric. For the metric (3.4.1) and for a general M, by Theorems 3.4.1 and 3.4.2, we deduce that 0 is never isolated in the essential spectrum of Δ_k for any k.

We investigate first the absence of the essential spectrum and improve along the way the results of [An06, An04]. We replace the condition $M=S^{n-1}$ with a weaker topological condition on the boundary at infinity M. Related results were obtained in [Bä00, GoMo08, Mo08]. The following theorem holds for some conformally cusp metrics and is an application of [Mo08].

Theorem 3.4.1. *Set $p>0$ and fix an integer k between 0 and n. If the Betti numbers $b_k(M)$ and $b_{k-1}(M)$ of the boundary at infinity M both vanish, then:*

- *the Laplacian Δ_k acting on k-forms on X is essentially self-adjoint in L^2 for the metric g_p;*
- *the spectrum of Δ_k is purely discrete;*
- *the asymptotic of its eigenvalues, in the limit $\lambda\to\infty$, is given by*

$$N_p(\lambda) \approx \begin{cases} C_1\lambda^{n/2} & \text{for } 1/n < p,\\ C_2\lambda^{n/2}\log\lambda & \text{for } p = 1/n,\\ C_3\lambda^{1/2p} & \text{for } 0<p<1/n, \end{cases} \tag{3.4.2}$$

where C_3 is given [GoMo08] and where

$$C_1 := \binom{n}{k} \frac{\operatorname{Vol}(X, g_p)\operatorname{Vol}(S^{n-1})}{n(2\pi)^n}, \quad C_2 := \binom{n}{k} \frac{\operatorname{Vol}(M, h)\operatorname{Vol}(S^{n-1})}{2(2\pi)^n}.$$

Note that the hypothesis $b_k(M) = b_{k-1}(M) = 0$ does not hold for $k = 0, 1$; it also does not hold for $k = n, n-1$ if M has at least one orientable connected component. In particular, Theorem 3.4.1 does not apply to the Laplacian acting on functions.

We stress that Δ_k is essentially self-adjoint and has purely discrete spectrum solely based on the hypothesis $b_k(M) = b_{k-1}(M) = 0$ *without* any condition like completeness of the metric or finiteness of the volume. Intuitively, the continuous spectrum of Δ_k is governed by zero-modes of the form Laplacian on M in dimensions k and $k-1$ (both dimensions are involved because of algebraic relations in the exterior algebra). By Hodge theory, the kernel of the k-form Laplacian on the compact manifold M is isomorphic to $H^k(M)$, hence these zero-modes (harmonic forms) exist precisely when the Betti numbers do not vanish. We mention that, in the study of the scalar magnetic Laplacian [GoMo08] the role of the Betti numbers was played by an integrability condition on the magnetic field.

We next attack the more demanding question of determining the nature of the essential spectrum by positive commutator techniques. The case of the Laplacian on functions has been treated originally by this method in [FrHi89], and by many other methods in the literature, see for instance [Gu98, Ku06] for different techniques. In [GoMo08] we introduced a conjugate operator which was "local in energy", in order to deal with a bigger class of perturbations of the metric. We use the same idea here, however the analysis of the Laplacian on k-forms turns out to be more involved than that of the scalar magnetic Laplacian. Indeed, one could have two thresholds and the positivity is harder to extract between them. The difficulty arises from the compact part of the manifold, since we can diagonalize the operator only on the cusp ends. The resolvent of the operator does *not* stabilize this decomposition. To deal with this, we introduce a perturbation of the Laplacian which uncouples the compact part from the cusps in a gentle way.

Let L be the operator on $\mathcal{C}_c^\infty(X, \Lambda^* X)$ of multiplication by the function $L \geq 1$ such that for y large enough,

$$L(y) = \begin{cases} \ln(y) & \text{for } p = 1, \\ \frac{y^{1-p}}{1-p} & \text{for } p < 1. \end{cases} \tag{3.4.3}$$

Given $s \geq 0$, let $\mathscr{L}_s$ be the domain of L^s equipped with the graph norm. We set $\mathscr{L}_{-s} := \mathscr{L}_s^*$ where the adjoint space is defined so that $\mathscr{L}_s \subset L^2(X, \Lambda^* X, g_p) \subset \mathscr{L}_s^*$, using the Riesz lemma. Given a subset I of $\mathbb{R}$, let $I_\pm$ be the set of complex numbers $a \pm \mathrm{i}b$, where $a \in I$ and $b > 0$.

Perturbations of *short-range* (resp. *long-range*) type are denoted with the subscript sr (resp. lr); they are supported in $(2, \infty) \times M$. We ask long-range perturbations to be *radial*. In other words, a perturbation $W_{\rm lr}$ satisfies $W_{\rm lr}(y, m) = W_{\rm lr}(y, m')$ for all $m, m' \in M$.

Theorem 3.4.2. *Let $\varepsilon > 0$. We consider the metric $\tilde g = (1 + \rho_{\rm sr} + \rho_{\rm lr}) g_p$, with $0 < p \leq 1$ and where the short-range and long-range components satisfy*

$$\begin{gathered} L^{1+\varepsilon}\rho_{\rm sr}, d\rho_{\rm sr} \text{ and } \Delta_g \rho_{\rm sr} \in L^\infty(X), \\ L^\varepsilon \rho_{\rm lr},\ L^{1+\varepsilon} d\rho_{\rm lr} \text{ and } \Delta_g \rho_{\rm sr} \in L^\infty(X). \end{gathered} \tag{3.4.4}$$

Suppose that at least one of the two Betti numbers $b_k(M)$ and $b_{k-1}(M)$ is non zero . Let $V = V_{\rm loc} + V_{\rm sr}$ and $V_{\rm lr}$ be some potentials, where $V_{\rm loc}$ is measurable with compact support and Δ_k-compact, and $V_{\rm sr}$ and $V_{\rm lr}$ are in $L^\infty(X)$ such that:

$$\|L^{1+\varepsilon} V_{\rm sr}\|_\infty < \infty, V_{\rm lr} \to 0, \text{ as } y \to +\infty \text{ and } \|L^{1+\varepsilon} dV_{\rm lr}\|_\infty < \infty.$$

Consider the Schrödinger operators $H_0 = \Delta_{k,p} + V_{\rm lr}(Q)$ *and* $H = H_0 + V(Q)$. *Then*

(a) *The essential spectrum of* H *is* $[\inf\{\kappa(p)\}, \infty)$, *where the set of* thresholds $\kappa(p) \subset \mathbb{R}$ *is defined as follows:*

$$\text{for } p < 1,\ \kappa(p) = \begin{cases} \emptyset, & \text{if } b_k(M) = b_{k-1}(M) = 0, \\ \{0\}, & \text{otherwise.} \end{cases}$$
$$\text{for } p = 1,\ \kappa(p) = \left\{c_i^2 \in \{c_0^2, c_1^2\}; b_{k-i}(M) \neq 0\right\}.$$
$$\text{for } p > 1,\ \kappa(p) = \emptyset.$$

(b) H *has no singular continuous spectrum.*

(c) *The eigenvalues of* H *have finite multiplicity and no accumulation points outside* $\kappa(p)$.

(d) *Let* $\mathcal{J}$ *a compact interval such that* $\mathcal{J} \cap \big(\kappa(p) \cup \sigma_{\rm pp}(H)\big) = \emptyset$. *Then, for all* $s \in (1/2, 3/2)$, *there exists c such that*

$$\|(H - z_1)^{-1} - (H - z_2)^{-1}\|_{\mathcal{B}(\mathscr{L}_s, \mathscr{L}_{-s})} \leq c|z_1 - z_2|^{s-1/2},$$

for all $z_1, z_2 \in \mathcal{J}_\pm$.

(e) *Let* $\mathcal{J} = \mathbb{R} \setminus \kappa(p)$ *and let* E_0 *and* E *be the continuous spectral component of* H_0 *and* H, *respectively. Then, the wave operators defined as the strong limit*

$$\Omega_\pm = \text{s}-\lim_{t \to \pm\infty} e^{\text{i}tH} e^{-\text{i}tH_0} E_0(\mathcal{J})$$

exist and are complete, i.e., $\Omega_\pm \mathscr{H} = E(\mathcal{J})\mathscr{H}$, *where* $\mathscr{H} = L^2(X, \Lambda^k, g_p)$.

Here we have used the convention that $\inf \emptyset = +\infty$ and we point out that in (e), the long-range part of the potential is included in H_0.

The point (a) remains true for a wide family of metrics asymptotic to (3.4.1). The fact that every eigenspace is finite-dimensional (in particular, for the eigenvalue $\kappa(p)$, the bottom of the continuous spectrum) is due to [GoMo08, Lemma B.1] and holds for an arbitrary conformally cusp metric. The proof of the rest, (b)–(e) where in (3) we consider eigenvalues with energy different from $\kappa(p)$, relies on the Mourre theory. These wide classes of perturbation of the metric have been introduced in [GoMo08]. We point out that the treatment of long-range perturbations is different from the one in [GoMo08].

We now turn to question of the perturbation of the Laplacian Δ_k by some non relatively compact potential. In the Euclidean $\mathbb{R}^n$, using Persson's formula, one sees that $\sigma_{\rm ess}(H)$ is empty for $H = \Delta + V(Q)$ if $V \in L^\infty_{\rm loc}$ tends to ∞ at infinity. However, the converse is wrong as noted in [Si83] by taking $V(x_1, x_2) = x_1^2 x_2^2$ which gives rise to a compact resolvent. Intuitively, a particle can not escape in the direction of finite energy at infinity which is too narrow compared to the very attracting part of V which tends to infinity. In our setting, the space being smaller at infinity, it is easier to create this type of situation even if most of the potential tends to $-\infty$. To our knowledge, the phenomenon is new.

Proposition 3.4.3. *Let* $p > 0$ *and* (X, g_p) *be a conformally cusp manifold. Let* $V \in y^{2p}\mathcal{C}^\infty(\overline{X})$ *be a smooth potential with Taylor expansion* $y^{-2p}V = V_0 + y^{-1}V_1 + O(y^{-2})$ *at infinity. Assume that* V_0 *is non-negative and not identically zero on any connected component of* M. *Then the Schrödinger operator* $\Delta_k + V(Q)$ *is essentially self-adjoint and has purely discrete spectrum. The eigenvalues obey the generalized Weyl law* (3.4.2) *and the constants* C_1, C_2 *do not depend on* V.

As in Theorem 3.4.1, the completeness of the manifold is not required to obtain the essential self-adjointness of the operator. Note that by assuming $p > 1/2$ (in particular, on finite-volume hyperbolic manifolds, for which $p = 1$) and $V_1 < 0$, we get $V \sim y^{2p-1}V_1 \to -\infty$ as we approach $M \setminus \mathrm{supp}(V_0)$. The support of the non-negative leading term V_0 must be nonempty, but otherwise it can be chosen arbitrarily small.

3.5 Instability of eigenvalues

Let $\mathbb{H} := \{(x, y) \in \mathbb{R}^2, y > 0\}$ be the Poincaré half-plane and we endow it with the metric $g := y^{-2}(dx^2+dy^2)$. Consider the group $\Gamma := PSL_2(\mathbb{Z})$. It acts faithfully on $\mathbb{H}$ by homographies, from the left. The interior of a fundamental domain of the quotient $\mathbb{H}\backslash\Gamma$ is given by $X := \{(x, y) \in \mathbb{H}, |x| < 1, x^2 + y^2 > 1\}$. Let $\mathscr{H} := L^2(X, g)$ be the set of L^2 integrable function acting on X, with respect to the volume element $dx\, dy/y^2$. Let $\mathcal{C}_b^\infty(X)$ be the restriction to X of the smooth bounded functions acting on $\mathbb{H}$ which are $\mathbb{C}$-valued and invariant under Γ. The (non-negative) Laplace operator is defined as the closure of

$$\Delta := -y^2(\partial_x^2 + \partial_y^2), \text{ on } \mathcal{C}_b^\infty(X).$$

It is a (unbounded) self-adjoint operator on $L^2(X)$. Using Eisenstein series, for instance, one sees that its essential spectrum is given by $[1/4, \infty)$ and that it has no singularly continuous spectrum, with respect to the Lebesgue measure. It is well-known that Δ has infinitely many eigenvalues accumulating at $+\infty$ and that every eigenspace is of finite dimension. We refer to [Fi87] for an introduction to the subject.

We consider the Schrödinger operator $H_\lambda := \Delta + \lambda V(Q)$, where V is the multiplication by a bounded, real-valued function and $k \in \mathbb{R}$. We focus on an eigenvalue $k > 1/4$ of Δ and assume that the following hypothesis of *Fermi golden rule* holds true. Namely, there is $c_0 > 0$ so that:

$$\lim_{\varepsilon \to 0^+} PV(Q)\overline{P}\,\Im(H_0 - k + \mathrm{i}\varepsilon)^{-1}\overline{P}V(Q)P \geq c_0 P, \tag{3.5.1}$$

in the form sense and where $P := P_k$, the projection on the eigenspace associated to k, and $\overline{P} := 1 - P$. As P is of finite dimension, the limit can be taken in the weak or in the strong sense. At least formally, $\overline{P}\,\Im(H_0 - k + \mathrm{i}\varepsilon)^{-1}\overline{P}$ tends to the Dirac mass $\pi\delta_k(\overline{P}H_0)$. Therefore, the potential V couples the eigenspace of H_0 associated to the energy k and $\overline{P}H_0$ over k in a non-trivial way. This is a key assumption in the second-order perturbation theory of embedded eigenvalues, e.g., [ReSi79], and all the art is to prove that it implies there is $\lambda_0 > 0$ that H_λ has no eigenvalue in a neighborhood of k for $\lambda \in (0, |\lambda_0|)$.

In [Co83], one shows that generically the eigenvalues disappear under the perturbation of a potential (or of the metric) on a compact set. Here, we are interested about the optimal decay at infinity of the perturbation given by a potential, namely $VL = o(1)$, as $y \to +\infty$. Using the general result obtained in [CaGrHu06] and under a hypothesis of Fermi golden rule, one is only able to cover the assumption $VL^3 = o(1)$, as $y \to +\infty$, where L denotes the operator of multiplication by $L := (x, y) \mapsto 1 + \ln(y)$. We give the main result:

Theorem 3.5.1. *Let $k > 1/4$ be an L^2-eigenvalue of Δ. Suppose that $VL = o(1)$, as $y \to +\infty$ and that the Fermi golden rule* (3.5.1) *holds true, then there is $\lambda_0 > 0$, so that H_λ has no eigenvalue in a neighborhood of k, for all $\lambda \in (0, |\lambda_0|)$. Moreover, if $VL^{1+\varepsilon} = o(1)$, as $y \to +\infty$ for some $\varepsilon > 0$, then H_λ has no singularly continuous spectrum.*

Partial proof. Standardly, for y large enough and up to some isometry $\mathcal{U}$, the Laplace operator can be written as

$$\tilde{\Delta} = (-\partial_r^2 + 1/4) \otimes P_0 + \tilde{\Delta}(1 \otimes P_0^\perp)$$

on $\mathcal{C}_c^\infty\big((c,\infty), dr\big)\otimes\mathcal{C}^\infty(S^1)$, for some $c>0$ and where P_0 is the projection on constant functions and $P_0^\perp := 1-P_0$. The Friedrichs extension of the operator $\tilde\Delta(1\otimes P_0^\perp)$ has compact resolvent.

Then, as in [GoMo08, GoMo12], we construct a conjugate operator. One chooses $\Phi\in\mathcal{C}_c^\infty(\mathbb{R})$ with $\Phi(x)=x$ on $[-1,1]$, and sets $\Phi_\Upsilon(x):=\Upsilon\Phi(x/\Upsilon)$, for $\Upsilon\geq 1$. Let $\tilde\chi$ be a smooth cut-off function being 1 for r big enough and 0 for r being close to c. We define on $\mathcal{C}_c^\infty\big((c,\infty)\times S^1\big)$ a micro-localized version of the generator of dilation:

$$S_{\Upsilon,0} := \tilde\chi(Q)\,\Big(\big(\Phi_\Upsilon(-\mathrm{i}\partial_r)Q + Q\Phi_\Upsilon(-\mathrm{i}\partial_r)\big)\otimes P_0\,\Big)\,\tilde\chi(Q).$$

The operator $\Phi_\Upsilon(-\mathrm{i}\partial_r)$ is defined on the real line by $\mathscr{F}^{-1}\Phi_\Upsilon(\cdot)\mathscr{F}$, where $\mathscr{F}$ is the unitary Fourier transform. We also denote its closure by $S_{\Upsilon,0}$ and it is self-adjoint. In [FrHi89] for instance, one does not use a micro-localization and one is not able to deal with really singular perturbation of the metric as in [GoMo08, GoMo12].

Now, one obtains

$$[\partial_r^2, \tilde\chi(Q)(\Phi_\Upsilon(-\mathrm{i}\partial_r)Q + Q\Phi_\Upsilon(-\mathrm{i}\partial_r))\tilde\chi(Q)]_\circ = 4\tilde\chi(Q)\partial_r\Phi_\Upsilon(-\mathrm{i}\partial_r)\tilde\chi(Q) + \text{remainder}.$$

Using a cut-off function $\tilde\mu$ being 1 on the cusp and 0 for $y\leq 2$, we set

$$S_\Upsilon := \widetilde{\mu}(Q)\,\mathcal{U}^{-1}S_{\Upsilon,0}\,\mathcal{U}\,\widetilde{\mu}(Q) \tag{3.5.2}$$

This is self-adjoint in $L^2(X)$. Now by taking Υ big enough, one can show, as in [GoMo08, GoMo12] that given an interval $\mathcal{J}$ around k, there exist $\varepsilon_\Upsilon>0$ and a compact operator K_Υ such that the inequality

$$E_{\mathcal{J}}(\Delta)[\Delta, \mathrm{i}S_\Upsilon]_\circ E_{\mathcal{J}}(\Delta) \geq (4\inf(\mathcal{J})-\varepsilon_\Upsilon)E_{\mathcal{J}}(\Delta) + E_{\mathcal{J}}(\Delta)K_\Upsilon E_{\mathcal{J}}(\Delta) \tag{3.5.3}$$

holds in the sense of forms, and such that ε_Υ tends to 0 as Υ goes to infinity.

Now, we apply $\overline{P}$ to the left and right of (3.5.3). Easily one has $\overline{P}E_{\mathcal{J}}(\Delta) = \overline{P}E_{\mathcal{J}}\big(\Delta\overline{P}\big)$. We get:

$$\begin{aligned}\overline{P}E_{\mathcal{J}}(\overline{P}\Delta)\big[\,\overline{P}\Delta, \mathrm{i}\overline{P}S_\Upsilon\overline{P}\,\big]_\circ E_{\mathcal{J}}(\overline{P}\Delta)\overline{P} \geq{}& (4\inf(\mathcal{J})-\varepsilon_\Upsilon)\overline{P}E_{\mathcal{J}}(\Delta\overline{P})\overline{P}\\ &+\overline{P}E_{\mathcal{J}}(\overline{P}\Delta)K_\Upsilon E_{\mathcal{J}}(\overline{P}\Delta)\overline{P}\end{aligned}$$

One can show that $\overline{P}S_\Upsilon\overline{P}$ is self-adjoint in $\overline{P}L^2(X)$ and that $\big[\,P\overline{\Delta}, \overline{P}S_\Upsilon\overline{P}\,\big]_\circ$ extends to a bounded operator.

We now shrink the size of the interval $\mathcal{J}$. As $\overline{P}\Delta$ has no eigenvalue in $\mathcal{J}$, then the operator $\overline{P}E_{\mathcal{J}}(\overline{P}\Delta)K_\Upsilon E_{\mathcal{J}}(\overline{P}\Delta)\overline{P}$ tends to 0 in norm. Therefore, by shrinking enough, one obtains a smaller interval $\mathcal{J}$ containing k and a constant $c>0$ so that

$$\overline{P}E_{\mathcal{J}}(\overline{P}\Delta)\big[\,\overline{P}\Delta, \mathrm{i}\overline{P}S_\Upsilon\overline{P}\,\big]_\circ E_{\mathcal{J}}(\overline{P}\Delta)\overline{P} \geq c\overline{P}E_{\mathcal{J}}(\Delta\overline{P})\overline{P} \tag{3.5.4}$$

holds true in the form sense on $\overline{P}L^2(X)$. At least formally, the positivity on $\overline{P}L^2(X)$ of the commutator $\big[\,H_\lambda, \mathrm{i}\overline{P}S_\Upsilon\overline{P}\,\big]_\circ$, up to some spectral measure and to some small λ, should be a general fact and should not rely on the Fermi golden rule hypothesis.

We now try to extract some positivity on $PL^2(X)$. First, we set

$$R_\varepsilon := \big((H_0-k)^2+\varepsilon^2\big)^{-1/2},\ \overline{R_\varepsilon} := \overline{P}R_\varepsilon \text{ and } F_\varepsilon := \overline{R_\varepsilon}^{\,2}. \tag{3.5.5}$$

Note that $\varepsilon R_\varepsilon^2 = \Im(H_0-k+\mathrm{i}\varepsilon)^{-1}$ and that R_ε commutes with P. Using (3.5.1), we get:

$$(c_1/\varepsilon)P \geq PV(Q)\overline{P}\,F_\varepsilon\,\overline{P}V(Q)P \geq (c_2/\varepsilon)P, \tag{3.5.6}$$

for $\varepsilon_0 > \varepsilon > 0$.

We follow an idea of [BaFrSiSo99], which was successfully used in [Go09, Me01] and set

$$B_\varepsilon := \Im(\overline{R_\varepsilon}^2 V(Q)P).$$

It is a finite rank operator. Observe now that we gain some positivity as soon as $\lambda \neq 0$:

$$P[H_\lambda, \mathrm{i}\lambda B_\varepsilon]_\circ P = \lambda^2 PV(Q)F_\varepsilon V(Q)P \geq (c_2\lambda^2/\varepsilon)P. \tag{3.5.7}$$

It is therefore natural to modify the conjugate operator S_Υ to obtain some positivity on $PL^2(X)$. We set

$$\hat{S}_\Upsilon := \overline{P}S_\Upsilon\overline{P} + \lambda\theta B_\varepsilon. \tag{3.5.8}$$

It is self-adjoint on $\mathcal{D}(S_\Upsilon)$ and is diagonal with respect to the decomposition $\overline{P}L^2(X) \oplus PL^2(X)$.

Here $\theta > 0$ is a technical parameter. We choose ε and θ, depending on λ, so that $\lambda = o(\varepsilon)$, $\varepsilon = o(\theta)$ and $\theta = o(1)$ as λ tends to 0. We summarize this into:

$$|\lambda| \ll \varepsilon \ll \theta \ll 1, \text{ as } \lambda \text{ tends to } 0. \tag{3.5.9}$$

With respect to the decomposition $\overline{P}E_\mathcal{J}(\Delta) \oplus PE_\mathcal{J}(\Delta)$, as λ goes to 0, we have:

$$E_\mathcal{J}(\Delta)\left[\lambda V(Q), \mathrm{i}\overline{P}S_\Upsilon\overline{P}\right]_\circ E_\mathcal{J}(\Delta) = \begin{pmatrix} O(\lambda) & O(\lambda) \\ O(\lambda) & 0 \end{pmatrix},$$
$$E_\mathcal{J}(\Delta)[\Delta, \mathrm{i}\lambda\theta B_\varepsilon]_\circ E_\mathcal{J}(\Delta) = \begin{pmatrix} 0 & O(\lambda\theta\varepsilon^{-1/2}) \\ O(\lambda\theta\varepsilon^{-1/2}) & 0 \end{pmatrix},$$
$$\text{and } E_\mathcal{J}(\Delta)[\lambda V(Q), \mathrm{i}\lambda\theta B_\varepsilon]_\circ E_\mathcal{J}(\Delta) = \begin{pmatrix} O(\lambda^2\theta\varepsilon^{-3/2}) & O(\lambda^2\theta\varepsilon^{-3/2}) \\ O(\lambda^2\theta\varepsilon^{-3/2}) & \lambda^2\theta F_\varepsilon \end{pmatrix}.$$

Now comes the delicate point. Under the condition (3.5.9) and by choosing $\mathcal{I}$, slightly smaller than $\mathcal{J}$, we use the previous estimates and a Schur Lemma to deduce:

$$E_\mathcal{I}(H_\lambda)[H_\lambda, \mathrm{i}\hat{S}_\Upsilon]_\circ E_\mathcal{I}(H_\lambda) \geq \frac{c\lambda^2\theta}{\varepsilon}E_\mathcal{I}(H_\lambda), \tag{3.5.10}$$

for some positive c and as λ tends to 0. Now it is a standard use of the Mourre theory. We mention that only the decay of VL is used to establish the last estimate. In fact, one uses that $[V(Q), \mathrm{i}\hat{S}_\Upsilon]_\circ(\Delta + 1)^{-1}$ is a compact operator. □

3.6 An alternative approach in the Mourre theory

In the setting of the Mourre estimate and in order to obtain a LAP, there was one way: to go through a differential inequality. In [GoJe07], which is strongly inspired by results in semi-classical analysis (cf., [Bu02, CaJe06, Je04, Je05]), we provided the first alternative proof of Mourre Theory. We did not use differential inequalities. Our proof was implicit as we had an argument by contradiction. In [Gé08], C. Gérard showed that the method can be followed using traditional "energy estimates". His proof is no more by contradiction. The result is:

Theorem 3.6.1. *Let $H \in \mathcal{C}^2(A)$ and assume* (3.2.2)*, then* (3.2.6) *holds true.*

We present briefly the ideas. To simplify, we set H bounded.

Partial proof. Step 1: This is the most technical part, we follow the presentation of [Gé08]. Take $s > 1/2$ and set $\psi : \mathbb{R} \longrightarrow \mathbb{R}$ by

$$\psi(t) := \int_{-\infty}^{t} \langle u\rangle^{-2s}\, du. \tag{3.6.1}$$

We start form (3.2.2). We assume $H \in \mathcal{C}^2(A)$ in order to justify of the following commutator expansions. Take $\mathcal{I}'$ an open interval such that its closure is included in $\mathcal{I}$. Take $\theta \in \mathcal{C}_c^\infty(\mathcal{I}; [0,1])$ being 1 above $\mathcal{I}'$. We use the Helffer-Sjøstrand Formula and denote by $\psi^{\mathbb{C}}$ an almost analytic extension of ψ. We have:

$$\begin{aligned}\theta(H)[H, \mathrm{i}\psi(A/R)]_\circ\theta(H) &= \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \partial_{\bar z}\psi^{\mathbb{C}}(z)\theta(H)(z - A/R)^{-1}[H, \mathrm{i}A/R]_\circ \\ &\qquad\qquad (z - A/R)^{-1}\theta(H)dz\wedge d\bar z \\ &= \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \partial_{\bar z}\psi^{\mathbb{C}}(z)(z - A/R)^{-1}\theta(H)[H, \mathrm{i}A/R]_\circ\theta(H) \\ &\qquad\qquad (z - A/R)^{-1}dz\wedge d\bar z + \text{small terms} \\ &\geq c\frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \partial_{\bar z}\psi^{\mathbb{C}}(z)(z - A/R)^{-1}\theta(H)\theta(H) \\ &\qquad\qquad (z - A/R)^{-1}dz\wedge d\bar z + \text{small terms} \\ &= c\,\theta(H)\langle A/R\rangle^{-2s}\theta(H) + \text{small terms}\end{aligned}$$

By taking R large enough, we obtain:

$$E_{\mathcal{I}'}(H)[H, \mathrm{i}\psi(A/R)]_\circ E_{\mathcal{I}'}(H) \geq c_1 E_{\mathcal{I}'}(H)\langle A/R\rangle^{-2s}E_{\mathcal{I}'}(H), \tag{3.6.2}$$

We mention that, as in the Putnam Theory, all the operators which are appearing on the l.h.s. are bounded.

Step 2: Using solely $H \in \mathcal{C}^1(A)$, one derives from (3.6.2) the LAP (3.2.6). We follow the presentation of [GoJe07].

Definition 3.6.2. *A* special sequence $(f_n, z_n)_n$ *for* H *associated to* $(\mathcal{J}, s, A)$*, i.e., to the LAP* (3.2.6)*, is a sequence* $(f_n, z_n)_n \in (\mathscr{H} \times \mathbb{C})^{\mathbb{N}}$ *such that, for certain* $\lambda \in \mathcal{J}$ *and* $\eta \geq 0$*,* $\mathcal{J} \ni \Re(z_n) \to \lambda$*,* $0 \neq \Im(z_n) \to 0$*,* $\|\langle A\rangle^{-s}f_n\| \to \eta$*,* $(H - z_n)f_n \in \mathcal{D}(\langle A\rangle^s)$*, and* $\|\langle A\rangle^s(H - z_n)f_n\| \to 0$*. The limit* η *is called the* mass *of the special sequence.*

This terminology has first appeared in [Je04] in a semi-classical context. We give the link between this notion and the LAP.

Proposition 3.6.3. *Given* $s \geq 0$ *and a compact interval* $\mathcal{I}$*, the LAP for* H *respectively to* $(\mathcal{I}, s, A)$ *is false if and only if there exists a special sequence* $(f_n, z_n)_n$ *for* H *associated to* $(\mathcal{I}, s, A)$ *with a positive mass.*

Proof. Suppose the LAP to be false. There exist a sequence $(k_n)_n$ of nonnegative numbers, going to infinity, a sequence $(g_n)_n$ of non-zero elements of $\mathscr{H}$, and a sequence $(z_n)_n$ of complex numbers such that $\Re(z_n) \in \mathcal{I}$, $0 \neq \Im(z_n) \to 0$, and

$$\left\|\langle A\rangle^{-s}(H - z_n)^{-1}\langle A\rangle^{-s}g_n\right\| \;=\; k_n\,\|g_n\| \;= 1. \tag{3.6.3}$$

Setting $f_n = (H - z_n)^{-1}\langle A\rangle^{-s}g_n$, $f_n \in \mathscr{H}$, $(H - z_n)f_n \in \mathcal{D}(\langle A\rangle^s)$, and, by (3.6.3),

$$\left\|\langle A\rangle^{-s}f_n\right\| \;=\; 1 \text{ and } \|\langle A\rangle^s(H - z_n)f_n\| \;= 1/k_n \to 0.$$

Up to a subsequence, we can assume that $\Re(z_n) \to \lambda \in \mathcal{I}$. Now, we assume the LAP true and consider $(f_n, z_n)_n$, a special sequence for H associated to $(\mathcal{I}, s, A)$. By (3.2.6), there exists $c > 0$ such that

$$\left\|\langle A\rangle^{-s} f_n\right\| \ \leq \ c\|\langle A\rangle^{s}(H - z_n) f_n\|.$$

This implies $\eta = 0$. □

Finally, our approach is based on the following Virial-like result.

Proposition 3.6.4. *Let $(f_n, z_n)_n$ be a special sequence for a* bounded*, self-adjoint operator H respectively to $(\mathcal{I}, s, A)$, as in* (3.2.6) *with $s \geq 0$. For any* bounded *borelian function ϕ,*

$$\lim_{n\to\infty} \langle f_n, [H, \phi(A)]_\circ f_n\rangle = 0.$$

Proof. Since $[H, \phi(A)]_\circ = [H - z_n, \phi(A)]_\circ$,

$$\begin{aligned}\langle f_n, [H, \phi(A)]_\circ f_n\rangle &= 2\mathrm{i}\Im(z_n)\langle f_n, \phi(A) f_n\rangle \\ &\quad + \langle (H - z_n) f_n, \phi(A) f_n\rangle + \langle \phi(A)^* f_n, (H - z_n) f_n\rangle.\end{aligned}$$

By Definition 3.6.2, there exists $C > 0$ such that

$$\begin{aligned}|\langle (H - z_n) f_n, \phi(A) f_n\rangle| &\leq |\langle \langle A\rangle^{s}(H - z_n) f_n, \langle A\rangle^{-s}\phi(A) f_n\rangle| \\ &\leq C\|\phi(A)\| \cdot \|\langle A\rangle^{s}(H - z_n) f_n\| \underset{n\to\infty}{\to} 0.\end{aligned}$$

Similarly, $\lim\langle \phi(A)^* f_n, (H - z_n) f_n\rangle = 0$. By Definition 3.6.2,

$$\begin{aligned}\Im(z_n) \cdot \|f_n\|^2 &= \Im\langle f_n, (H - z_n) f_n\rangle \\ &= \Im\langle \langle A\rangle^{-s} f_n, \langle A\rangle^{s}(H - z_n) f_n\rangle \underset{n\to\infty}{\to} 0.\end{aligned}$$

Since

$$|\Im(z_n)\langle f_n, \phi(A) f_n\rangle| \leq |\Im(z_n)| \cdot \|f_n\|^2 \cdot \|\phi(A)\|,$$

we obtain the desired result. □

To conclude, take $\theta \in \mathcal{C}_c^\infty(\mathcal{I}'; [0, 1])$ such that $\theta|_{\mathcal{J}} = 1$. Then take a special sequence f_n for $(\mathcal{J}, s, A)$, apply it to (3.6.2) and notice that $(1 - \theta)(f_n)$ tends to 0. □

3.7 Application to Wigner-von Neumann potentials

Neither [GoJe07] nor [Gé08] brought an example that was unreachable from the classical Mourre theory. It was finally done in [GoJe10]. Keeping in mind Theorem 3.2.2, the point is to consider a potential which is in $\mathcal{C}^1(A)$ and not in $\mathcal{C}^{1,1}(A)$. In order to obtain the LAP, we establish directly the rescalled Mourre estimate (3.6.2) and conclude by using $H \in \mathcal{C}^1(A)$. The difficulty dwells therefore in proving this estimate. We cannot use straightforwadly the commutator expansion of the previous section as it relies on the $\mathcal{C}^2(A)$ hypothesis. Our result is:

Theorem 3.7.1. *Set $\rho_0 \in]0, 1]$. Assume that the functions $\langle x\rangle^{\rho_0} V_{\mathrm{lr}}$, $\langle x\rangle^{1+\rho_0} V_{\mathrm{sr}}$, and the distribution $\langle x\rangle^{\rho_0} x \cdot \nabla V_{\mathrm{lr}}(x)$ belong to $\mathrm{L}^\infty(\mathbb{R}^d)$. Suppose also that $V_{\mathrm{lr}} + V_{\mathrm{sr}} \in \mathcal{C}^m(\mathbb{R}^d)$, with $m > d/2$. Take $q, k > 0$ and set $H_1 := H + W(Q)$, where $H := -\Delta + V_{\mathrm{lr}}(Q) + V_{\mathrm{sr}}(Q)$ and where $W : \mathbb{R}^d \longrightarrow \mathbb{R}$ is defined by*

$$W(x) := q(\sin k|x|)/|x|.$$

Take a closed interval $\mathcal{I}$ such that $\inf \mathcal{I} > 0$ *and such that*

- $k^2/4 \cap \mathcal{I} = \emptyset$, *if* $d = 1$,
- $\sup \mathcal{I} < k^2/4$, *if* $d > 1$.

Then the LAP (3.2.6) *holds true.*

As in Theorem 3.2.2, the positivity in (3.6.2) comes from the Laplacian. We deal with the short and long range parts of the potential with the help of some compactness of the commutator. Note that they are not in $\mathcal{C}^2(A)$ and that the strategy of the previous section does not apply. Finally the hard part is the one coming from the Wigner-von Neumann potential, which is $\mathcal{C}^1(A)$ and not better. Here we cannot use any compactness for it. We rely on the use of some pseudo-differential calculus in (3.7.3), see [GoJe10] for the details. The cost is that we have to avoid the energy $k^2/4$, it acts like a threshold (a point where one cannot prove a Mourre estimate). We mention also that when $V_{\rm lr} = 0$ and for some $V_{\rm sr}$, then H_1 has an embedded eigenvalue in $\{k^2/4\}$, see [ReSi79][Section XIII.13].

We stress that even for $q = 0$ and still in the setting of c) from Theorem 3.2.2, our approach is interesting. Indeed it gives an alternative approach (which is based on some compactness and some commutator expansion) to the use of the class $\mathcal{C}^{1,1}(A)$ can be difficult to check in some situations.

From the point of view of the Mourre theory, this result is new. Furthermore we can allow a long-range perturbation which is not covered by previous results in [Ki05, DeMoRe91, ReTa97, ReTa97]. A similar situation is considered in [MoUc78] but at different energies. We did not optimize our study of Schrödinger operators with oscillating potential. We believe that we can handle more general perturbations. For instance, we did not consider intervals $\mathcal{I}$ above $k^2/4$ for $d > 1$ so far. However we believe that a variant of the present theory is applicable in this case. We think that a general study of long range perturbations of the Schrödinger operator with Wigner-Von Neumann potential is interesting in itself and hope to develop it in a forthcoming paper.

Partial proof. We focus on the energies contained in an open interval $\mathcal{I} \subset]0; k^2/4[$. We denote by A the generator of dilations and by P_1 the orthogonal projection onto the eigenspaces of H_1. Let $\theta, \chi, \tau \in \mathcal{C}_c^\infty(]0; k^2/4[)$ such that $\tau\chi = \chi$, $\chi\theta = \theta$, and $\theta = 1$ near $\mathcal{I}$. Later we shall adjust the size of the support of χ. First $\chi(H_1) \in \mathcal{C}^1(A)$ by Lemma 3.8.5. Then, elliptic regularity ensures that $E_{\mathcal{I}}(H_1)P_1 L^2(\mathbb{R}^d) \subset \mathcal{C}^2(\mathbb{R}^2)$. Using a Lithner-Agmon type estimate, see [GoJe10][Lemma 4.10], we infer that $E_{\mathcal{I}}(H_1)P_1 L^2(\mathbb{R}^d) \subset \mathcal{D}(A)$. From here, recalling that $\dim E_{\mathcal{I}}(H_1)P_1 L^2(\mathbb{R}^d)$ is finite and that $|f\rangle\langle g| \in \mathcal{C}^1(A)$ if $f, g \in \mathcal{D}(a)$, we derive that $E_{\mathcal{I}}(H_1)P_1$ and $\chi(H_1)P_1^\perp = \chi(H_1) - \chi(H_1)E_{\mathcal{I}}(H_1)P_1$ are also in $\mathcal{C}^1(A)$.

Let $s \in]1/2; 1[$. As in [Gé08], we define $\psi : \mathbb{R} \longrightarrow \mathbb{R}$ by (3.6.1). Note that $\psi \in \mathcal{S}^0$ and is in particular bounded. Let $R \geq 1$. Using the fact that $H_1\tau(H_1)$ is a bounded operator which belongs to $\mathcal{C}^1(A)$ and some commutator expansion, we get:

$$\begin{aligned} F &:= P_1^\perp \theta(H_1)[H_1, \mathrm{i}\psi(A/R)]_\circ \theta(H_1)P_1^\perp = P_1^\perp \theta(H_1)[H_1\tau(H_1), \mathrm{i}\psi(A/R)]_\circ \theta(H_1)P_1^\perp \\ &= \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \partial_{\overline{z}}\psi^{\mathbb{C}}(z) P_1^\perp \theta(H_1)(z - A/R)^{-1}[H_1\tau(H_1), \mathrm{i}A/R]_\circ \\ &\qquad\qquad (z - A/R)^{-1}\theta(H_1)P_1^\perp dz \wedge d\overline{z}\,. \end{aligned}$$

Next to $P_1^\perp \theta(H_1)$ we let appear $\chi(H_1)P_1^\perp$ and commute it with $(z - A/R)^{-1}$. Since we have $\chi(H_1)P_1^\perp \in \mathcal{C}^1(A)$, using some properties of $\psi^{\mathbb{C}}$, we obtain some uniformly bounded operator

B_1 w.r.t. $R \geq 1$,

$$\begin{aligned} F =& \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \partial_{\overline{z}}\psi^{\mathbb{C}}(z) P_1^{\perp}\theta(H_1)(z - A/R)^{-1}P_1^{\perp}\chi(H_1)[H_1\tau(H_1), \mathrm{i}A/R]_\circ \\ & \qquad \chi(H_1)P_1^{\perp}(z - A/R)^{-1}\theta(H_1)P_1^{\perp} dz \wedge d\overline{z} \\ &+ \ P_1^{\perp}\theta(H_1)\langle A/R\rangle^{-s}R^{-2}B_1\langle A/R\rangle^{-s}\theta(H_1)P_1^{\perp} . \end{aligned} \tag{3.7.1}$$

Let $\varepsilon := \rho_0/2$. Using $(\varphi(H_1) - \varphi(H_0))\langle A\rangle^{\varepsilon} \in \mathcal{K}(L^2, \mathscr{H}^2)$, notice that

$$\begin{aligned} G &:= P_1^{\perp}\chi(H_1)[H_1\tau(H_1), \mathrm{i}A/R]_\circ\chi(H_1)P_1^{\perp} = P_1^{\perp}\chi(H_1)[H_1, \mathrm{i}A/R]_\circ\chi(H_1)P_1^{\perp} \\ &= P_1^{\perp}\chi(H_1)[H_1, \mathrm{i}A/R]_\circ\chi(H_0)P_1^{\perp} + P_1^{\perp}\chi(H_1)K_1R^{-1}B_2\langle A/R\rangle^{-\varepsilon}P_1^{\perp}, \end{aligned}$$

where the operator $K_1 := \tau(H_1)[H_1, \mathrm{i}A]_\circ(\chi(H_1)-\chi(H_0))\langle A\rangle^{\varepsilon}$ is compact and $B_2 := \langle A/R\rangle^{\varepsilon}\langle A\rangle^{-\varepsilon}$ is uniformly bounded. Similarly, there is K_2 compact so that

$$\begin{aligned} G =& P_1^{\perp}\chi(H_0)[H_1, \mathrm{i}A/R]_\circ\chi(H_0)P_1^{\perp} + P_1^{\perp}\chi(H_1)K_1R^{-1}B_2\langle A/R\rangle^{-\varepsilon}P_1^{\perp} \\ &+ \ P_1^{\perp}\langle A/R\rangle^{-\varepsilon}B_2K_2R^{-1}\chi(H_0)P_1^{\perp}. \end{aligned} \tag{3.7.2}$$

We focus on the potential contribution in G. Choosing τ appropriately and by using the decay of V and some pseudo-differential calculus for W, see [GoJe10][Proof of Lemma 5.5], we obtain that there exist a compact operator K_3 and an uniformly bounded operator B_3 such that

$$\chi(H_0)[(W + V)(Q), \mathrm{i}A/R]_\circ\chi(H_0) = R^{-1}\chi(H_0)K_3B_3\langle A/R\rangle^{-\varepsilon}\chi(H_0). \tag{3.7.3}$$

Taking advantage of $[H_0, \mathrm{i}A]_\circ = 2H_0$, of (3.7.3), and of (3.7.2), we rewrite (3.7.1):

$$\begin{aligned} F =& \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \partial_{\overline{z}}\psi^{\mathbb{C}}(z) P_1^{\perp}\theta(H_1)(z - A/R)^{-1}P_1^{\perp}2R^{-1}H_0\chi^2(H_0) \\ & \qquad P_1^{\perp}(z - A/R)^{-1}\theta(H_1)P_1^{\perp} dz \wedge d\overline{z} \\ &+ \ P_1^{\perp}\theta(H_1)\langle A/R\rangle^{-s}(R^{-2}B_1 + R^{-1}K_4)\langle A/R\rangle^{-s}\theta(H_1)P_1^{\perp} , \end{aligned} \tag{3.7.4}$$

with compact K_4 such that, for some $c_1 > 0$,

$$\|K_4\| \ \leq \ c_1(\|P_1^{\perp}\chi(H_1)K_1\| + \|K_2\chi(H_0)\| + \|\chi(H_0)K_3\|) . \tag{3.7.5}$$

Next we commute $(z-A/R)^{-1}$ with $P_1^{\perp}2R^{-1}H_0\chi^2(H_0)P_1^{\perp}$. Next, there are B_4 and B_5, uniformly bounded, such that

$$\begin{aligned} F &= P_1^{\perp}\theta(H_1)\psi'(A/R)P_1^{\perp}2R^{-1}H_0\chi^2(H_0)P_1^{\perp}\theta(H_1)P_1^{\perp} \\ &\qquad + \ P_1^{\perp}\theta(H_1)\langle A/R\rangle^{-s}(R^{-2}B_4 + R^{-1}K_4)\langle A/R\rangle^{-s}\theta(H_1)P_1^{\perp} , \\ &= P_1^{\perp}\theta(H_1)\langle A/R\rangle^{-s}2R^{-1}H_0\chi^2(H_0)\langle A/R\rangle^{-s}\theta(H_1)P_1^{\perp} \\ &\qquad + \ P_1^{\perp}\theta(H_1)\langle A/R\rangle^{-s}(R^{-2}B_5 + R^{-1}K_4)\langle A/R\rangle^{-s}\theta(H_1)P_1^{\perp} , \\ &\geq 2R^{-1}c_2P_1^{\perp}\theta(H_1)\langle A/R\rangle^{-s}\chi^2(H_0)\langle A/R\rangle^{-s}\theta(H_1)P_1^{\perp} \\ &\qquad + \ P_1^{\perp}\theta(H_1)\langle A/R\rangle^{-s}(R^{-2}B_5 + R^{-1}K_4)\langle A/R\rangle^{-s}\theta(H_1)P_1^{\perp} , \end{aligned}$$

where $c_2 > 0$ is the infimum of $\mathcal{I}$. Finally, since $K_5 := \chi^2(H_0) - \chi^2(H_1)$ is compact, we find an uniformly bounded B_6, such that

$$\begin{aligned} F &\geq 2R^{-1}c_2P_1^{\perp}\theta(H_1)\langle A/R\rangle^{-s}\chi^2(H_1)\langle A/R\rangle^{-s}\theta(H_1)P_1^{\perp} \\ &\qquad + \ P_1^{\perp}\theta(H_1)\langle A/R\rangle^{-s}(R^{-2}B_5 + R^{-1}K_4 + R^{-1}K_5)\langle A/R\rangle^{-s}\theta(H_1)P_1^{\perp} \\ &\geq 2R^{-1}c_2P_1^{\perp}\theta(H_1)\langle A/R\rangle^{-2s}\theta(H_1)P_1^{\perp} + \ P_1^{\perp}\theta(H_1)\langle A/R\rangle^{-s} \cdot \\ &\qquad (R^{-2}B_6 + R^{-1}K_4 + R^{-1}K_5\chi(H_1)P_1^{\perp})\langle A/R\rangle^{-s}\theta(H_1)P_1^{\perp} . \end{aligned}$$

To conclude, using (3.7.5), we decrease the support of χ to ensure that

$$\|K_4\| + \|K_5\chi(H_1)P_1^\perp\| < c_2.$$

Subsequently, we choose $R > 1$ large enough to guarantee

$$F \geq R^{-1}c_2 P_1^\perp \theta(H_1)\langle A/R\rangle^{-2s}\theta(H_1)P_1^\perp.$$

Letting act the projector $E_\mathcal{I}(H_1)$ on both sides of this inequality and recalling the definition of F, we get

$$P_1^\perp E_\mathcal{I}(H_1)[H_1, \mathrm{i}\psi(A/R)]_\circ E_\mathcal{I}(H_1)P_1^\perp \;\geq \frac{c_1}{R}\, P_1^\perp E_\mathcal{I}(H_1)\langle A/R\rangle^{-2s}E_\mathcal{I}(H_1)P_1^\perp$$

By an adapted Virial-like Theorem, we obtain the result. □

3.8 The C^1 hypothesis

In this section, we gather some well-known properties about the so-called C^1 class. In the following A is a fixed self-adjoint operator. Given a bounded operator H acting in a complex Hilbert space $\mathscr{H}$ and $k \in \mathbb{N}$, one says that $H \in \mathcal{C}^k(A)$ if $t \mapsto e^{-\mathrm{i}tA}He^{\mathrm{i}tA}f$ is $\mathcal{C}^k$ for all $f \in \mathscr{H}$. Let now H be a (possibly unbounded) self-adjoint operator. We denote by $R(z)$ its resolvent $(H-z)^{-1}$ in $z \notin \sigma(H)$. We say that $H \in \mathcal{C}^k(A)$ if for one $z \notin \sigma(H)$ (then for all $z \notin \sigma(H)$), $(H-z)^{-1} \in \mathcal{C}^k(A)$. When H is bounded the two definitions are equivalent. More generally, we recall a result following from Lemma 6.2.9 and Theorem 6.2.10 of [AmBoGe96].

Theorem 3.8.1. *Let A and H be two self-adjoint operators in the Hilbert space $\mathscr{H}$. The following points are equivalent:*

(a) $H \in \mathcal{C}^1(A)$.

(b) for one (then for all) $z \notin \sigma(H)$, there is a finite c such that

$$|\langle Af, R(z)f\rangle - \langle R(\overline{z})f, Af\rangle| \leq c\|f\|^2, \quad \forall f \in \mathcal{D}(A).$$

(c) a. *There is a finite c such that for all $f \in \mathcal{D}(A)\cap\mathcal{D}(H)$:*

$$|\langle Af, Hf\rangle - \langle Hf, Af\rangle| \leq c(\|Hf\|^2 + \|f\|^2), \tag{3.8.1}$$

b. *for some (then for all) $z \notin \sigma(H)$, the set $\{f \in \mathcal{D}(A) \mid R(z)f \in \mathcal{D}(A)$ and $R(\overline{z})f \in \mathcal{D}(A)\}$ is a core for A.*

From here one obtains that the commutator from H with A extends to the bounded operator $[H,A]_\circ \in \mathcal{B}(\mathcal{D}(H), \mathcal{D}(H)^*)$, where $\mathcal{D}(H) \subset \mathscr{H} \simeq \mathscr{H}^* \subset \mathcal{D}(H)^*$ by the Riesz theorem. This allows one to give a meaning to the Mourre estimate (3.2.1). Moreover, if $H \in \mathcal{C}^1(A)$ and $z \notin \sigma(H)$,

$$\left[A, (H-z)^{-1}\right]_\circ = \underbrace{(H-z)^{-1}}_{\mathscr{H}\leftarrow\mathcal{D}(H)^*} \quad \underbrace{[H,A]_\circ}_{\mathcal{D}(H)^*\leftarrow\mathcal{D}(H)} \quad \underbrace{(H-z)^{-1}}_{\mathcal{D}(H)\leftarrow\mathscr{H}}. \tag{3.8.2}$$

Note that, in practice, the condition (3.a) is usually easy and follows with the construction of the conjugate operator. The condition (3.b) could be delicate to check. This is addressed in the next lemma. It was proved in [GoMo08][Lemma A.2] and inspired by [Bo06]. We refer to [GéŁa90][Lemma 3.2.2] for an other approach.

Lemma 3.8.2. *Let $\mathscr{D}$ be a subspace of $\mathscr{H}$ such that $\mathscr{D} \subset \mathcal{D}(H) \cap \mathcal{D}(A)$, $\mathscr{D}$ is a core for A and $H\mathscr{D} \subset \mathscr{D}$. Let $(\chi_n)_{n\in\mathbb{N}}$ be a family of bounded operators such that*

(a) $\chi_n\mathscr{D} \subset \mathscr{D}$, χ_n tends strongly to 1 as $n \to \infty$, and $\sup_n \|\chi_n\|_{\mathcal{B}(\mathcal{D}(H))} < \infty$.

(b) $A\chi_n f \to Af$, for all $f \in \mathscr{D}$, as $n \to \infty$,

(c) There is $z \notin \sigma(H)$, such that $\chi_n R(z)\mathscr{D} \subset \mathscr{D}$ and $\chi_n R(\overline{z})\mathscr{D} \subset \mathscr{D}$.

Suppose also that for all $f \in \mathscr{D}$

$$\lim_{n\to\infty} A[H, \chi_n]R(z)f = 0 \text{ and } \lim_{n\to\infty} A[H, \chi_n]R(\overline{z})f = 0. \tag{3.8.3}$$

Finally, suppose that there is a finite c such that

$$|\langle Af, Hf\rangle - \langle Hf, Af\rangle| \le c(\|Hf\|^2 + \|f\|^2), \quad \forall f \in \mathscr{D}. \tag{3.8.4}$$

Then one has $H \in \mathcal{C}^1(A)$.

Note that (3.8.3) is well defined by expanding the commutator $[H, \chi_n]$ and by using (3) and $H\mathscr{D} \subset \mathscr{D}$. We refer to [GoMo08, GoMo12] for a use of this Lemma.

It turns out that an easier characterization is available if the domain of H is conserved under the action of the unitary group generated by A.

Theorem 3.8.3. *([AmBoGe96, p. 258]) Let A and H be two self-adjoint operators in the Hilbert space $\mathscr{H}$ such that $e^{itA}\mathcal{D}(H) \subset \mathcal{D}(H)$, for all $t \in \mathbb{R}$. Then $H \in \mathcal{C}^1(A)$ if and only if* (3.8.1) *holds true.*

The invariance of the domain can be proved by the following result of [GeGé99].

Lemma 3.8.4. *If $H \in \mathcal{C}^1(A)$ and $[H, iA]_\circ : \mathcal{D}(H) \to \mathscr{H}$ then $e^{itA}\mathcal{D}(H) \subset \mathcal{D}(H)$, for all $t \in \mathbb{R}$.*

Finally, it is also important to have in mind the following application of the Helffer-Sjøstrand Formula, e.g., [GoJe07][Appendix B]:

Lemma 3.8.5. *Let $H \in \mathcal{C}^1(A)$. Then for all $z \notin \sigma(H)$ and $\varphi \in \mathcal{C}_c^\infty(\mathbb{R})$, $(H - z)^{-1}$ and $\varphi(H)$ are in $\mathcal{C}^1(A)$ and stabilize the domain of A.*

Even though the hypothesis $[H, A]_\circ \in \mathcal{B}(\mathcal{D}(H), \mathcal{D}(H)^*)$ is enough to state a Mourre estimate like (3.2.1), there is an example where the Virial Theorem does not hold, see [GeGé99].

Chapter 4

Non-classical positive commutator theories

4.1 The spectrum of the zero temperature Pauli-Fierz Hamiltonians

Pauli-Fierz operators are often used in quantum physics as generator of approximate dynamics of a (small) quantum system interacting with a free Bose gas. They describe typically a non-relativistic atom interacting with a field of massless scalar bosons. Pauli-Fierz operators appear also in solid state physics. They are used to describe the interaction of phonons with a quantum system with finitely many degrees of freedom. Our result is devoted to the justification of the second-order perturbation theory for a large class of perturbation. For positive temperature system, this property is related to the return to equilibrium, see for instance [DeJa03] and reference therein.

This question has been studied in many places, see for instance the references [BaFrSi98, BaFrSi99, BaFrSiSo99, DeJa01, FaMøSk11, FrPi09, HaHeHu] for zero temperature systems and [DeJa01, JaPi95, Me01] for positive temperature. We mention also [FrGrSi08, GeGéMø04, HüSp95, Sk98] who studied certain spectral properties using positive commutator techniques. Here, we focus on the zero temperature setting. In [BaFrSi98], one initiates the analysis using analytic deformation techniques. In [BaFrSiSo99] and in [DeJa01], one introduces some kind of Mourre estimate approach. In the former, one enlarges the class of perturbation studied in [BaFrSi98] and in the latter, one introduces another class. These two classes do not fully overlap. This is due to the choice of the conjugate operator. Here, we enlarge the class of perturbations used in [DeJa01] for the question of the Virial theorem (one-commutator theory) and also for the limiting absorption principal (two-commutator theory).

Now, we present the model. For the sake of simplicity and as in [DeJa01], we start with a n-level atom. It is described by a self-adjoint matrix K acting on a finite dimensional Hilbert space $\mathscr{K}$. Let $(k_i)_{i=0,\dots,n}$ be its eigenvalues, with $k_i < k_{i+1}$. On the other hand, we have the Bosonic field $\Gamma_s(\mathbf{h})$ with the 1-particle Hilbert space $\mathbf{h} := L^2(\mathbb{R}^d, dk)$. We recall its construction. Set

$$\mathbf{h}^{0\otimes} = \mathbb{C} \text{ and } \mathbf{h}^{n\otimes} = \mathbf{h} \otimes \cdots \otimes \mathbf{h}.$$

Given a closed operator A, we define the closed operator $A^{n\otimes}$ defined on $\mathbf{h}^{n\otimes}$ by $A^{0\otimes} = 1$ if $n = 0$ and by $A \otimes \ldots \otimes A$ otherwise. Let S_n be the group of permutation of n elements. For each $\sigma \in S_n$, one defines the action on $\mathbf{h}^{n\otimes}$ by

$$\sigma(f_{i_1} \otimes \ldots \otimes f_{i_n}) = f_{\sigma^{-1}(i_1)} \otimes \ldots \otimes f_{\sigma^{-1}(i_n)},$$

where (f_i) is a basis of $\mathbf{h}$. The action extends to $\mathbf{h}^{n\otimes}$ by linearity to a unitary operator. The definition is independent of the choice of the basis. On $\mathbf{h}^{n\otimes}$, we set

$$\Pi_n := \frac{1}{n!}\sum_{\sigma\in S_n}\sigma \text{ and } \Gamma_n(\mathbf{h}) := \Pi_n(\mathbf{h}^{n\otimes}). \tag{4.1.1}$$

Note that Π_n is an orthogonal projection. We call $\Gamma_n(\mathbf{h})$ the n-particle bosonic space. The bosonic space is defined by

$$\Gamma(\mathbf{h}) := \bigoplus_{n=0}^{\infty}\Gamma_n(\mathbf{h}).$$

We denote by Ω the *vacuum*, the element $(1,0,0,\ldots)$ and by $P_\Omega := \Gamma(\mathbf{h}) \to \Gamma_0(\mathbf{h})$ the projection associated to it. We define $\Gamma_{\text{fin}}(\mathbf{h})$ the set of finite particle vectors, i.e. $\Psi = (\Psi_1, \Psi_2, \ldots)$ such that $\Psi_n = 0$ for n big enough.

We now define the second quantized operators. We recall that a densely defined operator A is closable if and only if its adjoint A^* is densely defined. Given a closable operator q in $\mathbf{h}$. We define $\Gamma_{\text{fin}}(q)$ acting from $\Gamma_{\text{fin}}(\mathcal{D}(q))$ into $\Gamma_{\text{fin}}(\mathbf{h})$ by

$$\Gamma_{\text{fin}}(q)|_{\Pi_n(\mathcal{D}(q)^{n\otimes})} := q\otimes\ldots\otimes q.$$

Since q is closable, q^* is densely defined. Using that $\Gamma_{\text{fin}}(q^*) \subset \Gamma_{\text{fin}}(q)^*$, we see that $\Gamma_{\text{fin}}(q)$ is closable and we denote by $\Gamma(q)$ its closure. Note that $\Gamma(q)$ is bounded if and only if $\|q\| \leq 1$.

Let b be a closable operator on $\mathbf{h}$. We define $d\Gamma_{\text{fin}}(b) : \Gamma_{\text{fin}}\big(\mathcal{D}(b)\big) \longrightarrow \Gamma_{\text{fin}}(\mathbf{h})$ by

$$d\Gamma_{\text{fin}}(b)|_{\Pi_n(\mathcal{D}(b)^{n\otimes})} := \sum_{j=1}^{n} 1\otimes\ldots\otimes 1\otimes \underbrace{b}_{j^{\text{th}}} \otimes 1\otimes\ldots\otimes 1.$$

As above, $d\Gamma_{\text{fin}}(b)$ is closable and $d\Gamma(b)$ denotes also its closure.

The Hamiltonian is given by the second quantization $d\Gamma(\omega)$ of ω, where $\omega(k) = |k|$. This is a massless and zero temperature system. The free operator is given by

$$H_0 = K\otimes 1_{\Gamma(\omega)} + 1_{\mathscr{K}}\otimes d\Gamma(\omega)$$

on $\mathscr{K}\otimes\Gamma(\mathbf{h})$. Its spectrum is $[k_0, \infty)$. It has no singularly continuous spectrum. Its point spectrum is the same as K, with the same multiplicity. We recall also the definition of the *number operator*

$$N := 1_{\mathscr{K}}\otimes d_G(\text{Id}).$$

We now define the interaction. Let $\alpha \in \mathcal{B}(\mathscr{K}, \mathscr{K}\otimes\mathbf{h})$. This is a *form-factor*. We set $b(\alpha)$ on $\mathscr{H}$ by $b(\alpha) := \mathscr{K}\otimes h^{n\otimes} \to \mathscr{K}\otimes h^{(n-1)\otimes}$, where

$$b(\alpha)(\Psi\otimes\phi_1\otimes\ldots\phi_n) := \alpha^*(\Psi\otimes\phi_1)\otimes\phi_2\otimes\ldots\phi_n,$$

for $n \geq 1$ and by 0 otherwise. This operator is bounded and its norm is given by $\|\alpha\|_{\mathcal{B}(\mathscr{K},\mathscr{K}\otimes\mathbf{h})}$. We define the *annihilation operator* on $\mathscr{K}\otimes\Gamma(\mathbf{h})$ with domain $\mathscr{K}\otimes\Gamma_{\text{fin}}(\mathbf{h})$ by

$$a(\alpha) := (N+1)^{1/2} b(\alpha)\big(1\otimes\Pi\big),$$

where $\Pi := \sum_n \Pi_n$, see (4.1.1). As above, it is closable and its closure is denoted by $a(\alpha)$. Its adjoint is the *creation operator*. It acts as $a^*(\alpha) = b^*(\alpha)(N+1)^{1/2}$ on $\mathscr{H}$. Note that

$$b^*(\alpha)(\psi\otimes\phi_1\otimes\ldots\otimes\phi_n) = (\alpha\phi)\otimes\phi_1\otimes\ldots\otimes\phi_n.$$

The *(Segal) Field operator* is defined by

$$\phi(\alpha) := \frac{1}{\sqrt{2}}\big(a(\alpha) + a^*(\alpha)\big).$$

We consider its closure on $\mathscr{K} \otimes \mathcal{D}(N^{1/2})$. Under the condition

(I0) $(1 \otimes \omega^{-1/2})\alpha \in \mathcal{B}(\mathscr{K}, \mathscr{K} \otimes \mathbf{h})$,

we define the interacting Hamiltonian on $\mathscr{K} \otimes \Gamma(\mathbf{h})$ by

$$H_\lambda := K \otimes 1_{\Gamma(\mathbf{h})} + 1_{\mathscr{K}} \otimes d\Gamma(\omega) + \lambda\phi(\alpha), \text{ where } \lambda \in \mathbb{R}. \tag{4.1.2}$$

The operator is self-adjoint with domain $\mathscr{K} \otimes \mathcal{D}\big(d\Gamma(\omega)\big)$.

We now focus on a selected eigenvalue k_{i_0}, with $i_0 > 0$. Our aim is to give hypotheses on the form-factor α to ensure that H_λ has no eigenvalue in a neighborhood of k_{i_0} for λ small enough (and non-zero). First, we have to ensure that the perturbation given by the field operator will really couple the system at energy k_{i_0}; we have to avoid form-factors like $\alpha(x) = 1 \otimes b$ for all $x \in \mathscr{K}$ and some $b \in \mathbf{h}$. Here comes the second-order perturbation theory, namely the hypothesis of *Fermi golden rule* for the couple (H_0, α) at energy k_{i_0}:

$$\text{w-}\lim_{\varepsilon \to 0^+} P\phi(\alpha)\overline{P}\,\Im(H_0 - k + \mathrm{i}\varepsilon)^{-1}\overline{P}\phi(\alpha)P > 0, \text{ on } P\mathscr{H}, \tag{4.1.3}$$

where $P := P_{k_{i_0}} \otimes P_\Omega$ and $\overline{P} := 1 - P$. At first sight, this is pretty implicit. This condition involves the form-factor, the eigenvalues of H_0 lower than k_{i_0} and its eigenfunctions. We make it explicit:

Let e_i be an orthonormal basis of eigenvectors of K relative to the eigenvalue k_i. To simplify the computation, say that k_{i_0} is simple. Since k_{i_0} is simple and since $\phi(\alpha)(e_{i_0} \otimes \Omega) = \alpha(e_{i_0}) \in \mathscr{K} \otimes \mathbf{h}$, (4.1.3) is equivalent to:

$$c_1 \geq \big\langle \alpha(e_{i_0}), \Im(H_0 - k_{i_0} + \mathrm{i}\varepsilon)^{-1}\alpha(e_{i_0})\big\rangle \geq c_2 > 0, \text{ for } 0 < \varepsilon \leq \varepsilon_0.$$

We have $\alpha(e_{i_0}) = \sum_{i=1,\dots,n} e_i \otimes f_{i,i_0} \in \mathscr{K} \otimes \mathbf{h}$, where $f_{i,i_0} = \big\langle e_i \otimes 1_{\mathbf{h}}, \alpha(e_{i_0})\big\rangle$. As $\mathbf{h} = L^2(\mathbb{R}^d, dk)$, we write f_{i,i_0} as a function of k. We go into *polar coordinates* and of the unitary map:

$$T := \begin{cases} L^2(\mathbb{R}^d, dk) & \longrightarrow \quad L^2(\mathbb{R}^+, dr) \otimes L^2(S^{d-1}, d\theta) := \tilde{\mathbf{h}} \\ \quad u & \longmapsto \quad Tu := (r, \theta) \mapsto r^{(d-1)/2}u(r\theta). \end{cases} \tag{4.1.4}$$

We infer

$$c_1 \geq \sum_{i=1,\dots,n} \int_0^\infty \int_{S^{d-1}} \varepsilon \frac{|f_{i,i_0}|^2(r\theta)r^{d-1}}{(r + \lambda_i - \lambda_{i_0})^2 + \varepsilon^2}\, d\sigma\, dr \geq c_2 > 0$$

Suppose now that $(r, \theta) \mapsto |f_{i,i_0}|^2(r\theta)r^{d-1}$ is continuous and in L^1. Then by dominated convergence, we let ε go to zero and get:

$$c_1 \geq \sum_{i=1,\dots,i_0} c_i(\lambda_{i_0} - \lambda_i)^{d-1} \int_{S^{d-1}} \varepsilon|f_{i,i_0}|^2\big(\theta(\lambda_{i_0} - \lambda_i)\big)\, d\sigma \geq c_2 > 0 \tag{4.1.5}$$

Here note that, up to the constant c_i, $r \mapsto \varepsilon/\big((r + \lambda_i - \lambda_{i_0})^2 + \varepsilon^2\big)$ is an approximate delta function if and only if $\lambda_i \leq \lambda_{i_0}$.

To satisfy the Fermi golden rule, it is enough to have a non-zero term in (4.1.5). When $d \geq 2$, we stress that the sum is taken till $i_0 - 1$ and therefore is empty at ground state energy. When the 1-particle space is over $\mathbb{R}$, it cannot be satisfied at this level of energy as well. Indeed, one would obtain a contradiction with the hypothesis **(I0)** and the continuity of $(r, \theta) \mapsto |f_{i,i_0}|^2(r\theta)$.

Here, we are establishing an extended Mourre estimate, in the spirit of [GeGéMø04b, Sk98]; this is an extended version of the positive commutator technique initiated by E. Mourre. Due to the method, we make further hypotheses on the form-factor. To formulate them, we shall take advantage of the polar coordinates. We identify $\mathbf{h}$ and $\tilde{\mathbf{h}}$ through this transformation. We write ∂_r for $\partial_r \otimes 1$. We first give a meaning to the commutator via:

(I1a) $\alpha \in \mathcal{B}\big(\mathscr{K}, \mathscr{K} \otimes \mathscr{H}_0^1(\mathbb{R}^+) \otimes L^2(S^{d-1})\big)$, $1 \otimes \omega^{-1/2}\partial_r \alpha \in \mathcal{B}(\mathscr{K}, \mathscr{K} \otimes \mathbf{h})$.

Here, $\mathscr{H}_0^1$ denotes the completion of $\mathcal{C}_c^\infty(\mathbb{R}^+)$ under the norm given by the space $\mathscr{H}^1$. We denote by $\|\cdot\|_2$ the L^2 norm. Recall the norm of $\mathscr{H}^1$ is given by $\|\cdot\|_2 + \|\partial_r \cdot\|_2$.

We explain the method on a formal level. We start by choosing a conjugate operator so as to obtain some positivity of the commutator. We choose $A := 1_{\mathscr{K}} \otimes d\Gamma(\mathrm{i}\partial_{|r|})$. Note this operator is not self-adjoint and only maximal symmetric. Thanks to **(I1a)**, one obtains

$$[H_\lambda, \mathrm{i}A]_\circ = \underbrace{N + 1_{\mathscr{K}} \otimes P_\Omega}_{\geq 1} + \underbrace{\lambda\phi(\partial_r \alpha) - 1_{\mathscr{K}} \otimes P_\Omega}_{H_\lambda\text{-bounded}} =: M + S.$$

Consider a compact interval $\mathcal{J}$. Since $d\Gamma(\omega)$ is non-negative, we have:

$$E_{\mathcal{J}}(H_0) = \sum_{0 \leq i \leq \sup(\mathcal{J})} P_{k_i} \otimes E_{\mathcal{J}-k_i}\big(d\Gamma(\omega)\big). \tag{4.1.6}$$

We infer $(1_{\mathscr{K}} \otimes P_\Omega)E_{\mathcal{J}}(H_0) = 0$ if and only if $\mathcal{J}$ contains no eigenvalues of K. We evaluate the commutator at an energy $\mathcal{J}$ which contains k_{i_0} and no other k_i. Thus,

$$M + E_{\mathcal{J}}(H_0) S E_{\mathcal{J}}(H_0) \geq 1 + \big(-1 + O(\lambda)\big)E_{\mathcal{J}}(H_0) \geq O(\lambda)E_{\mathcal{J}}(H_0), \tag{4.1.7}$$

since $\phi(\mathrm{i}\partial_r\alpha)$ is H_0-bounded. We keep M outside the spectral measure as it is not H_λ-bounded. Note we have no control on the sign of $O(\lambda)$ so far. We have not yet used the Fermi golden rule assumption. We follow an idea of [BaFrSiSo99] and set

$$B_\varepsilon := \Im\big((H_0 - k_{i_0})^2 + \varepsilon^2\big)^{-1}\overline{P}\phi(\alpha)P\big)$$

Observe that (4.1.3) implies there exists $c > 0$ such that

$$P[H_\lambda, \mathrm{i}\lambda B_\varepsilon]_\circ P = \frac{\lambda^2}{\varepsilon} P\phi(\alpha)\overline{P}\,\Im(H_0 - k_{i_0} + \mathrm{i}\varepsilon)^{-1}\,\overline{P}\phi(\alpha)P \geq \frac{c\lambda^2}{\varepsilon}P,$$

holds true for ε small enough. Let $\hat{A} := A + \lambda B_\varepsilon$ and $\hat{S} := S + \lambda[H_\lambda, iB_\varepsilon]_\circ$. We have $[H_\lambda, \mathrm{i}\hat{A}]_\circ = M + \hat{S}$. We go back to (4.1.7) and infer:

$$M + E_{\mathcal{J}}(H_0)\hat{S}E_{\mathcal{J}}(H_0) \geq \big(c\lambda^2/\varepsilon + O(\lambda)\big)E_{\mathcal{J}}(H_0) + \text{ error terms}. \tag{4.1.8}$$

By taking $\varepsilon := \varepsilon(\lambda)$, one hopes to obtain the positivity of the constant in front of $E_{\mathcal{J}}(H_0)$, to control the errors terms and to replace the spectral measure by the one of H_λ. Using the Feshbach method and with a more involved choice of conjugate operator, we show that there are $\lambda_0, c', \eta > 0$ so that

$$M + E_{\mathcal{J}}(H_\lambda)\hat{S}E_{\mathcal{J}}(H_\lambda) \geq c'|\lambda|^{1+\eta}E_{\mathcal{J}}(H_\lambda), \text{ for all } |\lambda| \leq \lambda_0, \tag{4.1.9}$$

on the sense of forms on $\mathcal{D}(N^{1/2})$.

One would like to deduce there is no eigenvalue in $\mathcal{J}$ from (4.1.9). To apply a Virial theorem, one has at least to check that the eigenvalues of H_λ are in the domain of $N^{1/2}$. One may proceed like in [Me01]. Here, we follow [GeGéMø04, Sk98] and construct a sequence of approximated conjugate operators $\hat{A}_n$ such that $[H_\lambda, \mathrm{i}\hat{A}_n]_\circ$ is H_λ-bounded, converges to $[H_\lambda, \mathrm{i}\hat{A}]_\circ$ and such that one may apply the Virial theorem with A_n. To justify these steps, we make a new assumption:

(I1b) $1_{\mathscr{K}} \otimes \omega^{-a}\alpha \in \mathcal{B}(\mathscr{K}, \mathscr{K} \otimes \mathbf{h})$, for some $a > 1$.

We now give our first result, based on the Virial theorem.

Theorem 4.1.1. *Let $\mathcal{I}$ be an open interval containing k_{i_0} and no other k_i. Assume the Fermi golden rule hypothesis* (4.1.3) *at energy k_{i_0}. Suppose that* **(I0)**, **(I1a)** *and* **(I1b)** *are satisfied. Then, there is $\lambda_0 > 0$ such that H_λ has no eigenvalue in $\mathcal{I}$, for all $|\lambda| \in (0, \lambda_0)$.*

We now give more information on the resolvent $R_\lambda(z) := (H_\lambda - z)^{-1}$ as the imaginary part of z tends to 0. We show it extends to an operator in some weighted spaces around the real axis. This is a standard result in the Mourre theory, when one supposes some 2-commutators-like hypothesis, see [AmBoGe96]. Here, as the commutator is not H_λ-bounded, one relies on an adapted theory. We use [GeGéMø04] which is a refined version of [Sk98]. Using again (4.1.4), we state our class of form-factors:

(I2) $\alpha \in \mathcal{B}\big(\mathscr{K}, \mathscr{K} \otimes \dot{\mathscr{B}}_2^{1,1}(\mathbb{R}^+) \otimes L^2(S^{d-1})\big)$.

Here the dot denotes the completion of $\mathcal{C}_c^\infty$. One choice of norm for $\mathscr{B}_2^{1,1}$ is:

$$\|f\|_{\mathscr{B}_2^{1,1}(\mathbb{R}^+)} = \|f\|_2 + \int_0^1 \big\|f(2t+\cdot) - 2f(t+\cdot) + f(\cdot)\big\|_2 \frac{dt}{t^2}.$$

We refer to [AmBoGe96, Tr78] for Besov spaces and real interpolation. To express the weights, consider $\tilde{b}$ the square root of the Dirichlet Laplacian on $L^2(\mathbb{R}^+, dr)$. Using (4.1.4), we define $b := 1_{\mathscr{K}} \otimes T^{-1}\tilde{b}T$ in $\mathscr{H}$. Set $\mathscr{P}_s := 1_{\mathscr{K}} \otimes (d\Gamma(b) + 1)^{-s}(N+1)^{1/2}$.

Theorem 4.1.2. *Let $\mathcal{I}$ be an open interval containing k_{i_0} and no other k_i. Assume the Fermi golden rule hypothesis* (4.1.3) *at energy k_{i_0}. Suppose that* **(I0)**, **(I1a)** *and* **(I2)** *(and not necessarily* **(I1b)***), there is $\lambda_0 > 0$ such that H_λ has no eigenvalue in $\mathcal{I}$, for all $|\lambda| \in (0, \lambda_0)$. Moreover, H_λ has no singularly continuous spectrum in $\mathcal{I}$. For each compact interval $\mathcal{J}$ included in $\mathcal{I}$, and for all $s \in (1/2, 1]$, the limits*

$$\mathscr{P}_s^* R_\lambda(x \pm \mathrm{i}0)\, \mathscr{P}_s := \lim_{y \to 0^+} \mathscr{P}_s^* R_\lambda(x \pm \mathrm{i}y) \mathscr{P}_s$$

exist in norm uniformly in $x \in \mathcal{J}$. Moreover the maps:

$$\mathcal{J} \ni x \mapsto \mathscr{P}_s^* R_\lambda(x \pm \mathrm{i}0)\mathscr{P}_s$$

are Hölder continuous of order $s - 1/2$ for the norm topology of $\mathcal{B}(\mathscr{H})$

To our knowledge, the condition **(I2)** is new, even for the question far from the thresholds. We believe it to be optimal in the Besov scale associated to L^2 for limiting absorption principle.

We now compare our result with the literature. In [DeJa01][Theorem 6.3], one shows the absence of embedded eigenvalues by proving a limiting absorption principal with the weights $1_{\mathscr{K}} \otimes (d\Gamma(b) + 1)^{-s}$, for $s > 1/2$, without any contribution in N. They suppose essentially **(I0)** and that $\alpha \in \mathcal{B}\big(\mathscr{K}, \mathscr{K} \otimes \dot{\mathscr{H}}^s(\mathbb{R}^+) \otimes L^2(S^{d-1})\big)$, for $s > 1$. The class of perturbations is chosen in relation with the weights. Their strategy is to take advantage the Fermi golden rule at the level of the limiting absorption principle, with the help of the Feshbach method. The drawback is that they are limited by the relation weight/class of form-factors and they cannot give a Virial-type theorem. On the other hand, their method allows to cover some positive temperature systems and we do not deal with this question. Their method leads to fewer problems with domains questions. We mention that they do not suppose the second condition of **(I1a)**.

Therefore, concerning merely the disappearance of the eigenvalues, the conditions **(I1a)** and **(I1b)** do not imply α to be better than $\dot{\mathscr{H}}^1(\mathbb{R}^+)$, in the Sobolev scale. Hence, Theorem

4.1.1 is a new result. We point out that the condition **(I2)** is weaker than the one used in [DeJa01]. The weights obtained in the limiting absorption principle are also better than the ones given in [DeJa01]. We mention that one could improve them by using some Besov spaces, see [GeGéMø04]. To simplify the presentation, we do not present them here. We believe they could hardly be reached by the method exposed in [DeJa01] due to the interplay between weights and form-factors.

In [GeGéMø04b] and in [Sk98], one cares about showing that the point spectrum is locally finite, i.e. without clusters and of finite multiplicity. Here, they use a Virial theorem. Between the eigenvalues, one shows a limiting absorption principle, and uses a hypothesis on the second commutator, something stronger than **(I2)**. In our approach, we use the Virial theorem and the limiting absorption principle in an independent way. In particular, if one is interested only in the limiting absorption principle, one does not need to suppose the more restrictive condition **(I1b)** but only **(I0)**, **(I1a)** and **(I2)**. This is due to the fact that we are showing a strict Mourre estimate, i.e. without compact contribution.

In [BaFrSiSo99], one proves some version of Theorems 4.1.1 and 4.1.2 for a different class of perturbation. They use the second quantization of the generator of dilation:

$$A_{\text{dil}} := \mathrm{i}1_{\mathscr{K}} \otimes d\Gamma(k \cdot \nabla_k + \nabla_k \cdot k),$$

which is a self-adjoint operator. One motivation being that:

$$[H_\lambda, \mathrm{i}A_{\text{dil}}]_\circ = 1_{\mathscr{K}} \otimes d\Gamma(\omega) + \mathcal{O}(\lambda).$$

Then, one modifies the conjugate operator in the same way as we do but the choice of parameters is more involved. Note that the commutator is H_λ-bounded if and only if the dimension of $\mathscr{K}$ is finite. When the dimension is not finite, like in QED models, $\theta(H_\lambda)[H_\lambda, \mathrm{i}A_{\text{dil}}]_\circ\theta(H_\lambda)$ is bounded when the support of θ contains only a finite number of eigenvalues of K. This approach leads to less questions of domains but one relies on another alternate Mourre theory, see [Sa97].

We point out this choice of conjugate operator has proved to be better to treat the infrared singularities present in QED. By choosing a function G_x acting in $\mathbf{h}$ and depending on $x \in X$, where $\mathscr{K} = L^2(X)$, one may consider

$$\phi(\alpha) = \int G_x(k) \otimes a^*(k) + \overline{G_x(k)} \otimes a(k)dk,$$

where a and a^* are the standard photon creation and annihilation operators. They are operator-valued distribution in $\mathbf{h}$. In QED, the behavior of $\omega^{-1}G_x$ near $k = 0$ determines the infrared problem. One has $G_x(k) \approx |k|^{-1/2}$ in the vicinity of $k = 0$, in this case. Since applying A_{dil} recreates this singularity, this somehow explains why the generator of dilatation is efficient with infrared problems. The choice of conjugate operator A is inferior in this regard. The first condition **(I1a)** requires α to be bounded; This can be fulfilled if the atomic part has a particular shape by using some gauge transformations, see for instance [GeGéMø04b][Section 2.4] and [DeJa01][Section 1.6]. After this, one considers $G_x(k) \approx |k|^{1/2}$. The problem dwells in the second condition of **(I1a)** which cannot be checked. Albeit one is not able to recover the physical case, this choice of conjugate operator remains popular in the literature. From mathematical standpoint, note the classes of pertubation induced by the two operators do not cover one another.

4.2 Dirac systems at threshold energies

We study properties of relativistic massive charged particles with spin-1/2 (e.g., electron, positron, (anti-)muon, (anti-)tauon,...). We follow the Dirac formalism, see [Di82]. Because of the spin, the configuration space of the particle is vector valued. To simplify, we consider finite dimensional and trivial fiber. Let $\nu \geq 2$ be an integer. The movement of the free particle is given by the Dirac equation,

$$\mathrm{i}\hbar\frac{\partial\varphi}{\partial t} = D_m\varphi, \text{ in } L^2(\mathbb{R}^3;\mathbb{C}^{2\nu}),$$

where $m > 0$ is the mass, c the speed of light, $\hbar$ the reduced Planck constant, and

$$D_m := c\hbar\,\alpha\cdot P + mc^2\beta = -\mathrm{i}c\hbar\sum_{k=1}^{3}\alpha_k\partial_k + mc^2\beta. \tag{4.2.1}$$

Here we set $\alpha := (\alpha_1, \alpha_2, \alpha_3)$ and $\beta := \alpha_4$. The α_i, for $i \in \{1, 2, 3, 4\}$, are linearly independent self-adjoint linear maps, acting in $\mathbb{C}^{2\nu}$, satisfying the anti-commutation relations:

$$\alpha_i\alpha_j + \alpha_j\alpha_i = 2\delta_{i,j}\mathbf{1}_{\mathbb{C}^{2\nu}}, \text{ where } i, j \in \{1, 2, 3, 4\}. \tag{4.2.2}$$

For instance, when $\nu = 2$, one may choose the Pauli-Dirac representation:

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} \mathrm{Id}_{\mathbb{C}^\nu} & 0 \\ 0 & -\mathrm{Id}_{\mathbb{C}^\nu} \end{pmatrix} \tag{4.2.3}$$

$$\text{where } \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

for $i = 1, 2, 3$. We refer to [Th92][Appendix 1.A] for various equivalent representations. Here, we do not choose any specific basis and work intrinsically with (4.2.2). We refer to [LaMi89] for a discussion of the representations of the Clifford algebra generated by (4.2.2). We also renormalize and consider $\hbar = c = 1$. The operator D_m is essentially self-adjoint on $\mathcal{C}_c^\infty(\mathbb{R}^3;\mathbb{C}^{2\nu})$ and the domain of its closure is $\mathscr{H}^1(\mathbb{R}^3;\mathbb{C}^{2\nu})$, the Sobolev space of order 1 with values in $\mathbb{C}^{2\nu}$. We denote the closure with the same symbol. Easily, using Fourier transformation and some symmetries, one deduces the spectrum of D_m is purely absolutely continuous and given by $(-\infty, -m] \cup [m, \infty)$.

In this introduction, we focus on the dynamical and spectral properties of the Hamiltonian describing the movement of the particle interacting with n fixed, charged particles. We model them by fixed points $\{a_i\}_{i=1,\dots,n} \in \mathbb{R}^{3n}$ with respective charges $\{z_i\}_{i=1,\dots,n} \in \mathbb{R}^n$. Doing so, we tacitly suppose that the particles $\{a_i\}$ are far enough from one another, so as to neglect their interactions. Note we make no hypothesis on the sign of the charges. The new Hamiltonian is given by

$$H_\gamma := D_m + \gamma V_c(Q), \text{ where } V_c := v_c \otimes \mathrm{Id}_{\mathbb{C}^{2\nu}} \text{ and } v_c(x) := \sum_{k=1,\dots,n}\frac{z_i}{|x - a_i|}, \tag{4.2.4}$$

acting on $\mathcal{C}_c^\infty(\mathbb{R}^3 \setminus \{a_i\}_{i=1,\dots,n};\mathbb{C}^{2\nu})$, with $a_i \neq a_j$ for $i \neq j$. The $\gamma \in \mathbb{R}$ is the coupling constant. The index c stands for *coulombic multi-center*. The notation $V(Q)$ indicates the operator of multiplication by V. Here, we identify $L^2(\mathbb{R}^3;\mathbb{C}^{2\nu}) \simeq L^2(\mathbb{R}^3) \otimes \mathbb{C}^{2\nu}$, canonically. Remark the perturbation V_c is not relatively compact with respect to D_m, then one needs to be careful to define a self-adjoint extension for D_m. Assuming

$$Z := |\gamma| \max_{i=1,\dots,n}(|z_i|) < \sqrt{3}/2, \tag{4.2.5}$$

the theorem of Levitan-Otelbaev ensures that H_γ is essentially self-adjoint and its domain is the Sobolev space $\mathscr{H}^1(\mathbb{R}^3;\mathbb{C}^{2\nu})$, see [ArYa82, Ka98, Kl80, LaRe79, LaReKl80, LeOt77] for various generalizations. This condition corresponds to the nuclear charge $\alpha_{\mathrm{at}}^{-1}Z \leq 118$, where

$\alpha_{\rm at}^{-1} = 137.035999710(96)$. Note that using the Hardy-inequality, the Kato-Rellich theorem will apply till $Z < 1/2$ and is optimal in the matrix-valued case, see [Th92][Section 4.3] for instance. For $Z < 1$, one shows there exists only one self-adjoint extension so that its domain is included in $\mathscr{H}^{1/2}(\mathbb{R}^3;\mathbb{C}^{2\nu})$, see [Ne75]. When $n = 1$ and $Z = 1$, this property still holds true, see [EsLo07]. Surprisingly enough, when $n = 1$ and $Z > 1$, there is no self-adjoint extension with domain included in $\mathscr{H}^{1/2}(\mathbb{R}^3;\mathbb{C}^{2\nu})$, see [Xi99][Theorem 6.3]. We mention also the work of [VoGiTy07] for $Z > 1$.

In [Ne75], one shows for $Z < 1$ that the essential spectrum is given by $(-\infty, -m] \cap [m, \infty)$ for all self-adjoint extension. For all Z, one refers to [GeMă01][Proposition 4.8.], which relies on [Xi99]. In [GeGo08] one gives some criteria of stability of the essential spectrum for some very singular cases. In [BeGe87], one proves there is no embedded eigenvalues for a more general model and till the coupling constant $Z < 1$. For all energies being in a compact set included in $(-\infty, -m) \cap (m, \infty)$, [GeMă01] obtains some estimates of the resolvent. This implies some propagation estimates and that the spectrum of H_γ is purely absolutely continuous. Similar results have been obtained for magnetic potential of constant direction, see [Yo01] and more recently [RiTi07].

Here, we are interested in uniform estimates of the resolvent at threshold energies. The energy m is called the *electronic threshold* and $-m$ the *positronic threshold*. In Theorem (4.2.2), we obtain a uniform estimate of the resolvent over $[-m - \delta, -m] \cup [m, m + \delta]$, see (4.2.6) and deduce some propagation properties, see (4.2.7). One difficulty is that in the case $n = 1$ and $z_i < 0$, it is well known there are infinitely many eigenvalues in the gap $(-m, m)$ converging to the m as soon as $\gamma \neq 0$ (see for instance [Th92][Section 7.4] and references therein). This is a difficult problem and, to our knowledge, this result is new for the multi-center case. There is a larger literature for non-relativist models, e.g., $-\Delta + V(Q)$ in $L^2(\mathbb{R}^n;\mathbb{C})$. The question is intimately linked with the presence of resonances at threshold energy, [JeNe01, FoSk04, Na94, Ri06, Ya82]. We mention also [BuPlStTaZa04] for applications to Strichartz estimates and [DeSk09, DeSk09b] for applications to scattering theory. We refer to [BoHa10, Bo11] for perturbations in divergence form and to [GuHa08, GuHa08b, VaWu10] for some more geometrical setting.

As we are concern about thresholds, Mourre's method does not seem enough, as the estimate of the resolvent is given on an interval which is strictly smaller than the one used in the commutator estimate. In [BoMă97] one generalizes the result of Putnam's approach. Under some conditions, one allows A to be unbounded. They obtain a global estimate of the resolvent. Note this implies the absence of eigenvalue. In [FoSk04], in the non-relativistic context, by asking some positivity on the Virial of the potential, see below, one is able to conciliate the estimate of the resolvent above the threshold energy and the accumulation of eigenvalues under it. In [Ri06], one presents an abstract version of the method of [FoSk04]. To give an idea, we shall compare the theories on a non-optimal example. Take $H := -\Delta + V(Q)$ in $L^2(\mathbb{R}^3)$, with V being in the Schwartz space. Consider the generator of dilation $A := (P \cdot Q + Q \cdot P)/2$, where $P := -\mathrm{i}\nabla$. One looks at the quantity

$$[H, \mathrm{i}A]_\circ - cH = -(2-c)\Delta - W_V(Q), \text{ where } W_V(Q) := Q \cdot \nabla V(Q) + cV(Q),$$

with $c \in (0, 2)$ and seeks some positivity. The expression W_V is called the *Virial* of V. In [FoSk04], one uses extensively that $W_V(x) \leq -c\langle x\rangle^{-\alpha}$ for some $\alpha, c > 0$ and $|x|$ big enough. In [Ri06], one notices that it suffices to suppose that $W_V(x) \leq 0$ and to take advantage of the positivity of the Laplacian. We take the opportunity to mention that it is enough to suppose that $W_V(x) \leq c'|x|^{-2}$, for some small positive constant c'. Observe also that these methods give different weights. For instance, [FoSk04] obtains better weights in the scale of $\langle Q\rangle^\alpha$ and [Ri06] can obtain singular weights like $|Q|$. Finally, [FoSk04] deals only with low energy estimates and [Ri06] works globally on $[0, \infty)$. We also point out [He91] which relies on commutator techniques and deals with smooth homogeneous potentials.

We revisit the approach of [Ri06] and make several improvements. Our aim is twofold: to treat dispersive non self-adjoint operator, see also Section 4.3, and to obtain estimates of the resolvent uniformly in a parameter. At first sight, these improvements are pointless from the standpoint of the Coulomb-Dirac problem we treat. In reality, they are the key-stone of our approach.

As the Dirac operator is vector-valued, coulombic interactions are singular and as we are interested in both thresholds, we were not able to use directly the ideas of [FoSk04, Ri06]. Indeed, it is unclear for us if one can actually deal with thresholds energy and keep the "positivity" of something close to the quantity $[H_\gamma, \mathrm{i}A] - cH_\gamma$, for some self-adjoint operator A. We avoid this fundamental problem. First of all we cut-off the singularities of the potential V_c and consider the operator $H_\gamma^{\mathrm{bd}} = D_m + \gamma V(Q)$. We recover at the end the singularities of the operator by perturbation of the LAP. Then, similarly to [DoEs00], we specify the resolvent of $H_\gamma^{\mathrm{bd}} - z$ relatively to a spin-down/up decomposition.

Lemma 4.2.1. . *Take $z \in \mathbb{C} \setminus \mathbb{R}$ such that $\Re(z) \geq 0$. We have* $(H_1^{\mathrm{bd}} - z)^{-1} =$

$$\begin{pmatrix} (\Delta_{m,v,z} + m - z)^{-1} & (\Delta_{m,v,z} + m - z)^{-1} \alpha\cdot P \dfrac{1}{m - v(Q) + z} \\ \dfrac{1}{m - v(Q) + z} \alpha\cdot P (\Delta_{m,v,z} + m - z)^{-1} & \dfrac{1}{m - v(Q) + z} \alpha\cdot P (\Delta_{m,v,z} + m - z)^{-1} \alpha\cdot P \dfrac{1}{m - v(Q) + z} - \dfrac{1}{m - v(Q) + z} \end{pmatrix},$$

where

$$\Delta_{m,v,z} := \alpha\cdot P \frac{1}{m - v(Q) + z} \alpha\cdot P + v(Q).$$

This transfers the analysis to the one of the elliptic operator of second order $\Delta_{m,v,z}$. The drawback is that this operator is dispersive and also depends on the spectral parameter z. We bypass the latter difficulty by studying the family $\{\Delta_{m,v,\xi}\}_{\xi \in \mathcal{E}}$ uniformly in $\mathcal{E}$. The main result is the following one.

Theorem 4.2.2. *There are $\kappa, \delta, C > 0$ such that*

$$\sup_{|\lambda| \in [m, m+\delta],\, \varepsilon > 0, |\gamma| \leq \kappa} \| \langle Q \rangle^{-1} (H_\gamma - \lambda - \mathrm{i}\varepsilon)^{-1} \langle Q \rangle^{-1} \| \leq C. \tag{4.2.6}$$

In particular, H_γ has no eigenvalue in $\pm m$. Moreover, there is C' so that

$$\sup_{|\gamma| \leq \kappa} \int_{\mathbb{R}} \| \langle Q \rangle^{-1} e^{-\mathrm{i}tH_\gamma} E_{\mathcal{I}}(H_\gamma) f \|^2 dt \leq C' \|f\|^2, \tag{4.2.7}$$

where $\mathcal{I} = [-m - \delta, -m] \cup [m, m + \delta]$ and where $E_{\mathcal{I}}(H_\gamma)$ denotes the spectral measure of H_γ.

We mention that using some kernel estimates, one can obtain (4.2.6) directly for the free Dirac operator, i.e., $\gamma = 0$, see for instance [Th92][Section 1.E] and [KaYa89]. One may find an alternative proof of this fact in [IfMă99] which relies on some positive commutator techniques.

In this study, we are mainly interested by long range perturbations of Dirac operators. Concerning limiting absorption principle for short range perturbations of Dirac operators there are some interesting works such as [D'AFa07] for small perturbations without discrete spectrum or [Bo06] for potentials producing discrete spectrum. These authors were mainly interested by time decay estimates similar to (4.2.7). In the short range case, the limiting absorption principle is a key ingredient to establish Strichartz estimates for perturbed Dirac type equations see [Bo08, D'AFa08]. For free Dirac equations there are some direct proofs, see [EsVe97, MaNaOz04, MaNaNaOz05]. Related time decay estimates are crucial tools to establish well posedness results [EsVe97, MaNaOz04, MaNaNaOz05] and stability results [Bo06, Bo08] for nonlinear Dirac equations.

4.3 Application to non-relativistic dispersive Hamiltonians

In this section, we expose a by-product result obtained in [BoGo10]. We discuss shortly the Helmholtz equation, see [BeCaKaPe02, BeLaSeSo03, Wa87, WaZh06]. In [Ro10], one studies the size of the resolvent of

$$H_h := -h^2\Delta + V_1(Q) - \mathrm{i}hV_2(Q), \text{ as } h \to 0.$$

The term V_2 corresponds to the absorption coefficient of the laser energy by material medium absorption term in the Helmholtz model, see [Ja99] for instance. The important improvement between [Ro10] and the previous ones, is that he allows V_2 to be a smooth function tending to 0 without any assumption on the size of $\|V_2\|_\infty$. Note he supposes the coefficients are smooth as some pseudo-differential calculus is used to apply the non self-adjoint Mourre theory which he develops. Then, he discusses trapping conditions in the spirit of [Wa87]. Here, we will stick to the quantum case and choose $h = -1$. To simplify the presentation, we focus on $L^2(\mathbb{R}^n;\mathbb{C})$, with $n \geq 3$.

Theorem 4.3.1. *Suppose that $V_1, V_2 \in L^1_{\mathrm{loc}}(\mathbb{R}^n;\mathbb{R})$ satisfy:*

(H0) $V_i(Q)$ are Δ-operator bounded with a relative bound $a < 1$, for $i \in \{1, 2\}$.

(H1) ∇V_i, $Q\cdot\nabla V_i(Q)$ are in $\mathcal{B}(\mathscr{H}^2(\mathbb{R}^n); L^2(\mathbb{R}^n))$ and $\langle Q\rangle(Q\cdot\nabla V_i)^2(Q)$ is bounded, for $i \in \{1, 2\}$.

(H2) There are $c_1 \in [0, 2)$ and $c_1' \in \big[0, 4(2 - c_1)/(n - 2)^2\big)$ such that

$$W_{V_1}(x) := x \cdot (\nabla V_1)(x) + c_1 V_1(x) \leq \frac{c_1'}{|x|^2}, \text{ for all } x \in \mathbb{R}^n.$$

and

$$V_2(x) \geq 0 \text{ and } -c_1 x \cdot (\nabla V_2)(x) \geq 0, \text{ for all } x \in \mathbb{R}^n.$$

On $\mathcal{C}_c^\infty(\mathbb{R}^n)$, we define $H := -\Delta + V(Q)$, where $V := V_1 + \mathrm{i}V_2$. The closure of H defines a dispersive closed operator with domain $\mathscr{H}^2(\mathbb{R}^n)$. We keep denoting it with H. Its spectrum included in the upper half-plane. Moreover, H has no eigenvalue in $[0, \infty)$ and

$$\sup_{\lambda\in[0,\infty),\, \mu>0} \big\| \, |Q|^{-1}(H - \lambda + \mathrm{i}\mu)^{-1}|Q|^{-1} \big\| < \infty. \tag{4.3.1}$$

If $c_1 = 0$, H has no eigenvalue in $\mathbb{R}$ and (4.3.1) holds true for $\lambda \in \mathbb{R}$.

The quantity W_{V_1} is called the *virial* of V_1. For h fixed and for a compact $\mathcal{I}$ included in $(0, \infty)$, [Ro10] shows some estimates of the resolvent above $\mathcal{I}$. Here we deal with the threshold 0 and with high energy estimates. On the other hand, as he avoids the threshold, he reaches some very sharp weights. As mentioned previously, one can improve the weights $|Q|$ to some extend by the use of Besov spaces, see [Ri06]. In [Ro10] one makes an hypothesis on the sign of V_2 but not on the one of $x \cdot (\nabla V_2)(x)$. Supposing $c_1 = 0$, we are also in this situation. We take the opportunity to point out [Wa11], where one discusses the presence of possible eigenvalues in 0 for non self-adjoint problems.

Remark 4.3.2. *Taking $V_2 = 0$, we can compare the results with [FoSk04, Ri06]. In [FoSk04], one uses in a crucial way that $W_{V_1}(x) \leq -c\langle x\rangle^{\alpha}$ in a neighborhood of infinity, for some $\alpha, c > 0$. In [Ri06], one remarks that the condition $W_{V_1}(x) \leq 0$ is enough to obtain the estimate. Here we mention that the condition (H2) is sufficient. Note this example is not explicitly discussed in [Ri06] but is covered by his abstract approach. In [BoKaMă96], for the special case $c_1 = 0$, one uses extensively the condition (H2). This implies* (4.3.1) *for $\lambda \in \mathbb{R}$.*

Remark 4.3.3. *Unlike in [Ro10], we stress that V is* not *supposed to be a relatively compact perturbation of H and that the essential spectrum of H can be different from $[0, \infty)$. In [He91], see also [BoKaMă96], one studies $V_2 = 0$ and $V_1(x) := v(x/|x|)$, with $v \in \mathcal{C}^{\infty}(S^{n-1})$. We improve the weights of [He91][Theorem 3.2] from $\langle Q\rangle$ to $|Q|$. We can also give a non-self-adjoint version. Consider V_1 satisfying (H1) and being relatively compact with respect to Δ and $V_2(x) := v(x/|x|)$, where $v \in \mathcal{C}^0(S^{n-1})$, non-negative. If $v^{-1}(0)$ is non-empty, one shows $[0, \infty)$ is included in the essential spectrum of H by using some Weyl sequences.*

Chapter 5

Spectral analysis on graphs

5.1 Notation

The spectral theory of discrete Laplace operators and adjacency matrices acting on graphs in useful for the study, among others, of some electrical networks, some gelling polymers and number theory, e.g. [CcDoSa82, DoSn84, DaSaVa03].

We start with some definitions and fix our notation for graphs. Let $\mathscr{V}$ be a countable set. Let $\mathscr{E} := \mathscr{V} \times \mathscr{V} \to [0, \infty)$ and assume that

$$\mathscr{E}(x, y) = \mathscr{E}(y, x), \quad \text{for all } x, y \in \mathscr{V}.$$

We say that $G := (\mathscr{V}, \mathscr{E})$ is an unoriented weighted graph with *vertices* $\mathscr{V}$ and *weighted edges* $\mathscr{E}$. In the setting of electrical networks, the weights correspond to the conductances. We say that $x, y \in \mathscr{V}$ are *neighbors* if $\mathscr{E}(x, y) \neq 0$ and denote it by $x \sim y$. We say that there is a *loop* in $x \in \mathscr{V}$ if $\mathscr{E}(x, x) \neq 0$. The set of *neighbors* of $x \in \mathscr{E}$ is denoted by

$$\mathscr{N}_G(x) := \{y \in \mathscr{E} \mid x \sim y\}.$$

The *degree* of $x \in V$ is by definition

$$\deg_G(x) := |\mathscr{N}_G(x)|,$$

the number of neighbors of x. A graph is *locally finite* if $|\mathscr{N}_G(x)|$ is finite for all $x \in V$. We also need a weight on the vertices

$$m : \mathscr{V} \to (0, \infty).$$

Finally, as we are dealing with magnetic fields, we fix a phase

$$\theta : \mathscr{V} \times \mathscr{V} \to [-\pi, \pi], \text{ such that } \theta(x, y) = -\theta(y, x).$$

We set $\theta_{x,y} := \theta(x, y)$. A graph is *connected*, if for all $x, y \in V$, there exists an *x-y-path*, i.e., there is a finite sequence

$$(x_1, \ldots, x_{N+1}) \in \mathscr{V}^{N+1} \text{ such that } x_1 = x,\, x_{N+1} = y \text{ and } x_n \sim x_{n+1},$$

for all $n \in \{1, \ldots, N\}$. In this case, we endow V with the metric $\rho_{\mathscr{V}}$ defined by

$$\rho_{\mathscr{V}}(x, y) := \inf\{n \in \mathbb{N} \mid \text{there exists an } x\text{-}y\text{-path of length } n\}.$$

In the sequel, we shall always consider (magnetic) graphs $G = (\mathscr{V}, \mathscr{E}, m, \theta)$, which are locally finite, connected and have no loop. A graph G is *simple* if $\mathscr{E}$ has values in $\{0, 1\}$ and $\theta = 0$.

We recall that a *tree* is a connected graph $G = (\mathscr{V}, \mathscr{E})$ such that for each edge $e \in \mathscr{V} \times \mathscr{V}$ with $\mathscr{E}(e) \neq 0$ the graph $(\tilde{\mathscr{E}}, \mathscr{V})$, with $\tilde{\mathscr{E}} := \mathscr{E} \times 1_{\{e\}^c}$, i.e., with e removed, is disconnected. Finally, we recall that a *bi-partite* graph is a graph whose vertex set can be partitioned into two subsets in such a way that no two points in the same subset are neighbors. Trees are bi-partite graphs.

We now associate a certain Hilbert space and some operators on it to a given graph $G = (\mathscr{V}, \mathscr{E}, m, \theta)$. Let $\ell^2(G, m^2) := \ell^2(\mathscr{V}, m^2; \mathbb{C})$ be the set of functions $f : \mathscr{V} \to \mathbb{C}$, such that $\|f\|^2 := \sum_{x \in \mathscr{V}} m(x)^2 |f(x)|^2$ is finite. The associated scalar product is given by $\langle f, g \rangle = \sum_{x \in \mathscr{V}} m^2(x) \overline{f(x)} g(x)$, for $f, g \in \ell^2(\mathscr{V}, m^2)$. We also denote by $\mathcal{C}_c(\mathscr{V})$ the set of functions $f : \mathscr{V} \to \mathbb{C}$, which have finite support.

We define the quadratic form:

$$\mathscr{Q}(f,f) := \mathscr{Q}_{\mathscr{E},\theta}(f,f) := \frac{1}{2} \sum_{x,y \in \mathscr{V}} \mathscr{E}(x,y) |f(x) - e^{i\theta_{x,y}} f(y)|^2 \geq 0, \text{ for } f \in \mathcal{C}_c(\mathscr{V}). \tag{5.1.1}$$

It is closable and there exists a unique self-adjoint operator $\Delta_{\mathscr{E},\theta}$, such that

$$\mathscr{Q}_{\mathscr{E},\theta}(f,f) = \langle f, \Delta_{\mathscr{E},\theta} f \rangle, \text{ for } f \in \mathcal{C}_c(\mathscr{V})$$

and $\mathcal{D}(\Delta_{\mathscr{E},\theta}^{1/2}) = \mathcal{D}(\mathscr{Q}_{\mathscr{E},\theta})$, where the latter is the completion of $\mathcal{C}_c(\mathscr{V})$ under $\|\cdot\|^2 + \mathscr{Q}_{\mathscr{E},\theta}(\cdot,\cdot)$. This operator is the *Friedrichs extension* associated with the form $\mathscr{Q}_{\mathscr{E},\theta}$. It acts as follows:

$$\Delta_{\mathscr{E},\theta} f(x) := \frac{1}{m^2(x)} \sum_{y \in \mathscr{V}} \mathscr{E}(x,y)(f(x) - e^{i\theta_{x,y}} f(y)), \text{ for } f \in \mathcal{C}_c(\mathscr{V}). \tag{5.1.2}$$

When $m = 1$, it is essentially self-adjoint on $\mathcal{C}_c(\mathscr{V})$ (see Section 5.2 for further discussion). There exist other definitions for the discrete Laplacian. The one we study here is sometimes called the "physical Laplacian".

In $\ell^2(\mathscr{V}, m^2)$, we define the *weighted degree* by

$$d_G(x) := \frac{1}{m^2(x)} \sum_{y \in \mathscr{V}} \mathscr{E}(x,y).$$

Given a function $V : \mathscr{V} \to \mathbb{C}$, we denote by $V(Q)$ the operator of multiplication by V. It is elementary that $\mathcal{D}(d_G^{1/2}(Q)) \subset \mathcal{D}(\Delta_{\mathscr{E},\theta}^{1/2})$. Indeed, one has:

$$\begin{aligned}\langle f, \Delta_{\mathscr{E},\theta} f \rangle &= \frac{1}{2} \sum_{x \in \mathscr{V}} \sum_{y \sim x} \mathscr{E}(x,y) |f(x) - e^{i\theta_{x,y}} f(y)|^2 \\ &\leq \sum_{x \in \mathscr{V}} \sum_{y \sim x} \mathscr{E}(x,y)(|f(x)|^2 + |f(y)|^2) = 2\langle f, d_G(Q) f \rangle,\end{aligned} \tag{5.1.3}$$

for $f \in \mathcal{C}_c(\mathscr{V})$. This inequality also gives a necessary condition for the absence of essential spectrum for $\Delta_{\mathscr{E},\theta}$. We mention also that, in general, the constant 2 cannot be improved.

The boundedness of the Laplacian is an easy question. We refer to [KeLe12, KeLeWo11] for more discussions in the setting of Dirichlet forms and ℓ^p spaces:

Proposition 5.1.1. *Let $G = (\mathscr{V}, \mathscr{E}, m, \theta)$ be a weighted graph. The operator $\Delta_{\mathscr{E},\theta}$ is bounded if and only if $d_G(Q)$ is bounded.*

Proof. First, (5.1.3) gives one direction. On the other hand, $\langle \mathbf{1}_{\{x\}}, \Delta_{\mathscr{E},\theta} \mathbf{1}_{\{x\}} \rangle = d_G(x)$, for all $x \in \mathscr{V}$. □

One can also study the so-called (magnetic) *adjacency matrix*:

$$(\mathcal{A}_{\mathscr{E},\theta} f)(x) := \sum_{y \sim x} \mathscr{E}(x,y) e^{\mathrm{i}\theta_{x,y}} f(y), \text{ with } f \in \mathcal{C}_c(\mathscr{V}). \tag{5.1.4}$$

Unlike the physical Laplacian, $\mathcal{A}_{\mathscr{E},\theta}$ is not necessary essentially self-adjoint when $m = 1$, $\mathscr{E} \in \{0, 1\}$, and $\theta = 0$ (see Section 5.3). When $\mathscr{E}$ takes integer values, $\mathcal{A}_{\mathscr{E},\theta}$ is bounded if and only if $\deg_G$ and $\mathscr{E}$ are bounded, see [Go10].

5.2 Essential self-adjointness

Essential self-adjointness of the discrete Laplacian was proved in many situations by Jørgensen (see [Jo08] and references therein). In [Jo08], he says that every discrete Laplacian is essentially self-adjoint on simple graphs. The proof of [Jo08] was incomplete (see [JoPe]). It was fixed later in [JoPe]. In the meantime, [Wo07] proves this fact. An alternative proof can be found in [We10] where one uses the maximum principle. Similar ideas are found in [KeLe12], where one generalizes this fact to some weighted graphs by studying Dirichlet forms. Then come the works of [To10, Ma09] for weighted graphs which are metrically complete, see also [CoToTr11] for the non-metrically complete case. Finally for the magnetic case, we mention the works [CoToTr11b, Mi11, Mi11b]. We point out that in the older work of [Ao89] ones gives some characterization of possible self-adjoint extensions of a weighted discrete Laplacian in the limit point/circle spirit in the case of trees.

We now improve a self-adjointness criteria given in [KeLe12] and extend it in two directions: we allow magnetic operators and potentials that are unbounded from below. The result comes from [Go11].

Proposition 5.2.1. *Let $G = (\mathscr{V}, \mathscr{E}, m, \theta)$ be a weighted graph, $V : \mathscr{V} \to \mathbb{R}$ and $\gamma > 0$. Take $\lambda \in \mathbb{R}$ so that*

$$\{x \in \mathscr{V}, \lambda + d_G(x) + V(x) = 0\} = \emptyset. \tag{5.2.1}$$

Suppose that, for any $(x_n)_{n\in\mathbb{N}} \in \mathscr{V}^{\mathbb{N}}$, such that the weight $\mathscr{E}(x_n, x_{n+1}) > 0$ for all $n \in \mathbb{N}$, the property

$$\sum_{n\in\mathbb{N}} m^2(x_n) a_n^2 = \infty, \text{ where } a_n := \prod_{i=0}^{n-1} \left(\frac{\gamma}{d_G(x_i)} + \left| 1 + \frac{\lambda + V(x_i)}{d_G(x_i)} \right| \right) \tag{5.2.2}$$

holds true. Then, the operator $H := \Delta_{\mathscr{E},\theta} + V(Q)$ is essentially self-adjoint on $\mathcal{C}_c(\mathscr{V})$.

First, note it is always possible to find a λ fulfilling (5.2.1), as $\mathscr{V}$ is countable. Our technique relies on an improvement of [Wo07, Theorem 1.3.1].

Proof. Let $f \in \mathcal{D}(H^*) \setminus \{0\}$ such that $H^* f + (\gamma \mathrm{i} + \lambda) f = 0$ or $H^* f + (-\gamma \mathrm{i} + \lambda) f = 0$. We get easily:

$$|f(x)| \leq \frac{1}{m^2(x)} \sum_{y \in \mathscr{V}} \frac{\mathscr{E}(x,y)}{\gamma + |\lambda + d_G(x) + V(x)|} |f(y)|.$$

We derive:

$$\max_{y\sim x} |f(y)| \geq \left(\frac{\gamma}{d_G(x)} + \left| 1 + \frac{\lambda + V(x)}{d_G(x)} \right| \right) |f(x)|, \text{ for all } x, y \in \mathscr{V}, \text{ so that } \mathscr{E}(x,y) \neq 0. \tag{5.2.3}$$

Now, since $f \neq 0$, there is $x_0 \in \mathscr{V}$ such that $f(x_0) \neq 0$. Therefore, inductively, we obtain a sequence $(x_n)_{n\in\mathbb{N}} \in \mathscr{V}^{\mathbb{N}}$ such that $\mathscr{E}(x_n, x_{n+1}) > 0$, for all $n \in \mathbb{N}$, and so that (5.2.3) holds for $y = x_{n+1}$ and $x = x_n$. Hence, we get

$$\sum_{n=0}^{N} m^2(x_n)|f(x_n)|^2 \geq \sum_{n=0}^{N} m^2(x_n) \prod_{i=0}^{n-1} \left(\frac{\gamma}{d_G(x_i)} + \left| 1 + \frac{\lambda + V(x_i)}{d_G(x_i)} \right| \right)^2 |f(x_0)|^2.$$

By letting N go to infinity and remembering (5.2.2), we obtain a contradiction of the fact that $f \in \ell^2(\mathscr{V}, m^2)$. We conclude with the help of [ReSi79, Theorem X.1]. □

In [KeLe12], the hypothesis is stronger, i.e., they take $a_n = 1$, do not consider magnetic fields, and consider potentials that are bounded from below. We provide two examples which were not covered.

Corollary 5.2.2. *Let $G = (\mathscr{V}, \mathscr{E}, m, \theta)$ be a weighted graph and $V : \mathscr{V} \to \mathbb{R}$ such that $V(x) \geq -d_G(x)/2$, for all $x \in \mathscr{V}$. Suppose that, for any $(x_n)_{n\in\mathbb{N}} \in \mathscr{V}^{\mathbb{N}}$, such that the weight $\mathscr{E}(x_n, x_{n+1}) > 0$ for all $n \in \mathbb{N}$,*

$$\sum_{n\in\mathbb{N}} m^2(x_n) = \infty$$

holds true. Then, the operator $H := \Delta_{\mathscr{E},\theta} + V(Q)$ is essentially self-adjoint on $\mathcal{C}_c(\mathscr{V})$.

Corollary 5.2.3. *Let $G = (\mathscr{V}, \mathscr{E}, m, \theta)$ be a weighted graph, $V : \mathscr{V} \to \mathbb{R}$, and $\gamma > 0$. Suppose that, for any $(x_n)_{n\in\mathbb{N}} \in \mathscr{V}^{\mathbb{N}}$, such that the weight $\mathscr{E}(x_n, x_{n+1}) > 0$ for all $n \in \mathbb{N}$,*

$$\sum_{n\in\mathbb{N}} m^2(x_n) \prod_{i=0}^{n-1} \left(\frac{\gamma}{d_G(x_i)} \right) = \infty$$

holds true. Then, the operator $H := \Delta_{\mathscr{E},\theta} + V(Q)$ is essentially self-adjoint on $\mathcal{C}_c(\mathscr{V})$.

We stress that in the latter, we make no hypothesis on the growth of V.

We now present other criteria, based on commutators techniques. There are given in [GoSc11] (see also [Go10]). We point out that one can consider potentials that tend to $-\infty$.

Proposition 5.2.4. *Let $G = (\mathscr{V}, \mathscr{E})$ be a locally finite graph and $V : \mathscr{V} \to \mathbb{R}$ be a potential. Then, the following assertions hold true:*

(a) Let $x_0 \in \mathscr{V}$, set $b_i := \sup\{\sum_{x,y} \mathscr{E}(x,y) \mid \rho_{\mathscr{V}}(x_0, x) = i$ and $\rho_{\mathscr{V}}(x_0, y) = i+1\}$, and take $V : \mathscr{V} \to \mathbb{R}$. If $\sum_{i\in\mathbb{N}} 1/b_i = +\infty$, then $\mathcal{A}_G + V(Q)$ and $\Delta_G + V(Q)$ is essentially self-adjoint on $\mathcal{C}_c(\mathscr{V})$.

(b) Suppose that $\sup_x \max_{y\sim x} |\deg_G(x) - \deg_G(y)| < \infty$, $\sup_{x\in\mathscr{V}} |V(x)/\deg_G(x)| < \infty$, and $\mathscr{E}$ is bounded, then $\mathcal{A}_G + V(Q)$ is essentially self-adjoint on $\mathcal{C}_c(\mathscr{V})$.

(c) Suppose that $\deg_G$ is bounded, $\sup_x \max_{y\sim x} |\mathscr{E}(x) - \mathscr{E}(y)| < \infty$, where we used the notation $\mathscr{E}(x) := \max_{y\sim x} \mathscr{E}(x,y)$, and that $\sup_{x\in\mathscr{V}} |V(x)/\mathscr{E}(x)| < \infty$, then $\mathcal{A}_G + V(Q)$ is essentially self-adjoint on $\mathcal{C}_c(\mathscr{V})$.

(d) Suppose there is a compact set $K \subset \mathscr{V}$, such that $\sum_{y\sim x} \mathscr{E}^2(x,y)\deg_G(y) \leq V^2(x)$ for all $x \notin K$. Then $\mathcal{A}_G + V(Q)$ is essentially self-adjoint on $\mathcal{C}_c(\mathscr{V})$.

(e) Suppose there is a compact set $K \subset \mathscr{V}$, such that $\sum_{y\sim x} \mathscr{E}^2(x,y)\big(1 + \deg_G(y)\big) \leq V^2(x)$ for all $x \notin K$, then $\Delta_G + V(Q)$ is essentially self-adjoint on $\mathcal{C}_c(\mathscr{V})$.

The first point is a Carleman-type condition, see for instance [Be68, Page 504] for the case of Jacobi matrices. We stress that this result holds true without any hypothesis of size or of sign on the potential part. In particular, the Schrödinger operators could be unbounded from below and from above, see [Go10] for instance. Unlike in [Be68], we rely on an commutator approach, see [Wo08, Wo12] for similar techniques. The points (b) and (c) follow by application of the Nelson commutator Theorem. The two last ones are an application of Wüst's Theorem by considering $\mathcal{A}$ and Δ as perturbation of the potential.

5.3 Deficiency indices

In quantum physics, proving that a symmetric operator is self-adjoint is a central problem. In contrast with (5.1.2), even in the case of a locally finite tree G, $\mathcal{A}_G$ is not necessarily essentially self-adjoint on $\mathcal{C}_c(\mathscr{V})$. The first examples are due independently to [MoOm85, Mü87]. In order to characterize all the possible extensions, one studies the so-called deficiency indices.

For simplicity, we shall present the results of this section in the setting of a simple locally finite graph, i.e., $\mathscr{E} \in \{0,1\}$, $m = 1$, and $\theta = 0$. Here we are also interested in the *discrete Schrödinger operators* $\mathcal{A}_G + V(Q)$ and $\Delta_G + V(Q)$ with *potential* $V := \mathscr{V} \to \mathbb{R}$. The operators are defined as the closures of $\mathcal{A}_G + V(Q)$ and of $\Delta_G + V(Q)$ on $\mathcal{C}_c(\mathscr{V})$, respectively. They are symmetric and therefore closable. We denote with the same symbol their closure. Note that Δ_G, up to sign, is actually a discrete Schrödinger operator formed with the help of $\mathcal{A}_G$:

$$\Delta_G = V(Q) - \mathcal{A}_G, \text{ where } V(x) := \sum_{y \sim x} \mathscr{E}(x, y). \tag{5.3.1}$$

In the sequel, we investigate the number of possible self-adjoint extensions of discrete Schrödinger operators by computing their deficiency indices. Given a closed and densely defined symmetric operator T acting on a complex Hilbert space, the deficiency indices of T are defined by $\eta_\pm(T) := \dim\ker(T^* \mp \mathrm{i}) \in \mathbb{N} \cup \{+\infty\}$. We recall some well-known facts. The operator T possesses a self-adjoint extension if and only if $\eta_+(T) = \eta_-(T)$. If this is the case, we denote the common value by $\eta(T)$. T is self-adjoint if and only if $\eta(T) = 0$. Moreover, if $\eta(T)$ is finite, the self-adjoint extensions can be explicitly parametrized by the unitary group $U(n)$ in dimension $n = \eta(T)$. Using the Krein formula, it follows that the absolutely continuous spectrum of all self-adjoint extensions is the same.

Since the operator $\mathcal{A}_G + V(Q)$ commutes with the complex conjugation, its deficiency indices are equal, e.g., [ReSi79, Theorem X.3]. We denote by $\eta(G)$ the common value, when $V = 0$. This means that $\mathcal{A}_G + V(Q)$ possesses a self-adjoint extension. Remark that $\eta(\mathcal{A}_G + V(Q)) = 0$ (resp. $\eta(\Delta_G + V(Q)) = 0$) if and only if $\mathcal{A}_G + V(Q)$ (resp. $\Delta_G + V(Q)$) is essentially self-adjoint on $\mathcal{C}_c(\mathscr{V})$.

Concentrate for a moment on the case of the adjacency matrix acting on trees. Keep in mind, it is no gentle perturbation of the Laplacian. In [MoOm85, Mü87], adjacency matrices for simple trees with positive deficiency indices are constructed. In fact, it follows from the proof that the deficiency indices are infinite in both references. In fact we prove:

Theorem 5.3.1. *Let $G = (\mathscr{V}, \mathscr{E})$ be a simple locally finite tree and let $V : \mathscr{V} \to \mathbb{R}$ be a potential. Then one has:*

$$\eta(\mathcal{A}_G + V(Q)) \in \{0, +\infty\} \text{ and } \eta(\Delta_G + V(Q)) \in \{0, +\infty\}. \tag{5.3.2}$$

In particular, one obtains $\eta(G) \in \{0, +\infty\}$.

This can be generalized to a family of graphs obtained recursively. We refer to [GoSc11] for their construction.

We now point out that the self-adjointness of the adjacency matrix, acting on a simple locally finite tree G, is linked with the growth of the offspring, i.e., of the number of sons. When the latter grows up to linearly, one has $\eta(G) = 0$. On the other hand, if the growth is "exponential", we obtain that $\eta(G) = \infty$. Using some invariant spaces, we prove the following sharp result:

Proposition 5.3.2. *Let $\alpha > 0$ and G be a tree with offspring $\lfloor n^\alpha \rfloor$ per individual at generation n. Then, one obtains:*

$$\eta(G) = \begin{cases} 0, & \text{if } \alpha \le 2, \\ +\infty, & \text{if } \alpha > 2. \end{cases}$$

Moreover we prove some generic results for random trees and their deterministic Schrödinger operators. We obtain:

Proposition 5.3.3. *Let $G = (\mathscr{V}, \mathscr{E})$ be a random tree with independent and identically distributed (i.i.d.) offspring. Suppose that the offspring distribution has finite expectation. Then for almost all trees, the Schrödinger operators $\mathcal{A}_G + V(Q)$ and $\Delta_G + V(Q)$ are essentially self-adjoint on $\mathcal{C}_c(\mathscr{V})$, for all potentials $V : \mathscr{V} \to \mathbb{R}$. In particular, almost surely, one gets $\eta(G) = 0$.*

We now discuss the possibility to obtain finite and non-zero deficiency indices for the adjacency matrix acting on a general simple locally finite graph. In [MoWo89, Section 3], one finds:

Theorem 5.3.4. *For all $n \in \mathbb{N} \cup \{\infty\}$, there is a simple graph G, such that $\eta(\mathcal{A}_G) = n$.*

Their proof is unfortunately incomplete. However, the statement is correct, we give a proof. Using standard perturbation theory, e.g., [GoSc11, Proposition A.1], one sees that the validity of Theorem 5.3.4 is equivalent to the existence of a simple graph G for which

$$\eta(\mathcal{A}_G) = 1. \tag{5.3.3}$$

In [MoWo89], instead of pointing a simple graph such that (5.3.3) holds, they relied on a tree. More precisely, they refer to the works of [MoOm85, Mü87].

Keeping that in mind and strongly motivated by some other examples, we had proposed a drastically different scenario and had conjectured in [GoSc11] that that for any simple graph, one has $\eta(\mathcal{A}_G) \in \{0, \infty\}$.

We now turn to the proof of Theorem 5.3.4 and therefore disprove our conjecture. We rely on the decomposition of anti-trees, see [BrKe12, Theorem 4.1].

Let S_n, $n \in \mathbb{N}$, be nonempty, finite and pairwise disjoint sets. We set $s_n := |S_n|$, $\mathscr{V} := \cup_{n\in\mathbb{N}} S_n$ and $|x| := n$ for $x \in S_n$. Set also $\mathscr{E}(x, y) = 1$, if $\big||x| - |y|\big| = 1$, and $\mathscr{E}(x, y) = 0$ otherwise. We define:

$$P := \bigoplus_{n\in\mathbb{N}} P_n, \text{ where } P_n f(x) := \frac{1}{s_n} \mathbf{1}_{S_n}(x) \sum_{y\in S_n} f(y),$$

for all $f \in \ell^2(\mathscr{V})$. Note that $P = P^2 = P^*$ and $\operatorname{rank} P\mathbf{1}_{S_n} = 1$ for all $n \in \mathbb{N}$. Given $f \in \ell^2(\mathscr{V})$ such that $f = Pf$, i.e., f is radially symmetric, we set $\tilde{f}(|x|) := f(x)$, for all $x \in \mathscr{V}$. Note that

$$\begin{aligned} P\ell^2(\mathscr{V}) &= \{f \in \ell^2(\mathscr{V}), \tilde{f}(|\cdot|) := f(\cdot) \text{ and } \sum_{n\in\mathbb{N}} s_n |\tilde{f}(n)|^2 < \infty\} \\ &\simeq \ell^2(\mathbb{N}, (s_n)_{n\in\mathbb{N}}), \end{aligned}$$

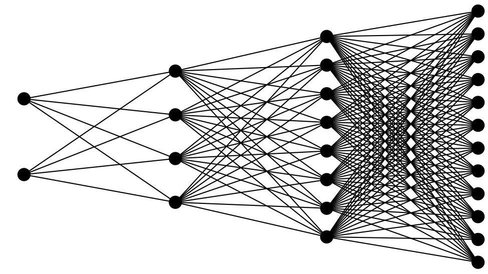


Figure 5.1: An antitree with $s_0 = 2, s_1 = 4, s_2 = 8$, and $s_4 = 12$

where $(s_n)_{n\in\mathbb{N}}$ is now a sequence of weights. The key remark of [BrKe12, Theorem 4.1] is that

$$\mathcal{A}_G = P\mathcal{A}_G P \text{ and } \widetilde{\mathcal{A}_G Pf}(|x|) = s_{|x|-1}\widetilde{Pf}(|x|-1) + s_{|x|+1}\widetilde{Pf}(|x|+1),$$

for all $f \in \mathcal{C}_c(\mathscr{V})$ with the convention that $s_{-1} = 0$. Using the unitary transformation $U\colon \ell^2(\mathbb{N}) \to \ell^2(\mathbb{N}, s_n)$ given by $U\tilde{f}(n) = \sqrt{s_n}\tilde{f}(n)$, we see that $\mathcal{A}_G$ is unitarily equivalent to the direct sum of 0 and of a Jacobi matrix acting on $\ell^2(\mathbb{N})$, with 0 on the diagonal and the sequence $(\sqrt{s_n}\sqrt{s_{n+1}})_{n\in\mathbb{N}}$ on the off-diagonal. Finally using [Be68, Page 504 and 507], we derive that: Given $\alpha > 0$ and $s_n := \lfloor n^\alpha \rfloor$,

$$\eta(\mathcal{A}_G) = \begin{cases} 0, & \text{if } \alpha \le 1, \\ 1, & \text{if } \alpha > 1. \end{cases}$$

5.4 Semi-boundedness

The study of random walk on graph is intimately linked with the study of the heat equation associated with a discrete Laplace operator, see for instance [Chu97, MoWo89]. In some recent papers [We10, Wo07], one works in the general context of locally finite graph and consider a non-negative discrete Laplacian, see also [KeLe12, KeLe09] for generalizations to Dirichlet forms. A key feature to obtain a Markov semi-group and to hope to apply these techniques is the boundedness from below (or from above) of a certain self-adjoint operator. In this note, we are interested in some self-adjoint realization of the adjacency matrix on locally finite graphs. We give some optimal conditions to ensure that the operator is unbounded from above and from below. For simplicity, we stick to the locally finite setting, $\mathscr{E} \in \mathbb{N}$, $m = 1$, and $\theta = 0$.

We study the unboundedness of the self-adjoint realizations of the adjacency matrix. It is well-known that the operator $\mathcal{A}_G$ is bounded if $\deg_G$ and $\mathscr{E}(\cdot,\cdot)$ are bounded. The reciprocal is true since $\mathscr{E}$ is integer valued. The first statement is easy:

Proposition 5.4.1. *Let $G = (\mathscr{V}, \mathscr{E})$ be a locally finite graph. Let $\hat{\mathcal{A}}_G$ be a self-adjoint realization of the $\mathcal{A}_G$. If the weight $\mathscr{E}$ is unbounded, then $\hat{\mathcal{A}}_G$ is unbounded from above and from below.*

We now deal with bounded weights $\mathscr{E}$. We say that $\mathscr{E}$ is *bounded from below* is $\inf_{x,y} \mathscr{E}(x,y) > 0$. We will restrict to this case. Suppose also that $\deg_G$ is unbounded. Let $\kappa_d(G)$ be the filter generated by $\{x \in \mathscr{V}, \deg_G(x) \ge n\}$, with $n \in \mathbb{N}$. We introduce the *lower local complexity* of a graph G by:

$$C_{\mathrm{loc}}(G) := \liminf_{x \to \kappa_d(G)} \frac{N_G(x)}{d_G^2(x)}, \text{ where } N_G(x) := |\{x - \text{triangles}\}|, \tag{5.4.1}$$
$$:= \inf \bigcap \left\{ \overline{\left\{ \frac{N_G(x)}{d_G^2(x)}, x \in \mathscr{V} \text{ and } \deg_G(x) \geq n \right\}}, n \in \mathbb{N} \right\}.$$

Here $x \to \kappa_d(G)$ means converging to infinity along the filter $\kappa_d(G)$. Recall that G has no loop and beware that the $x-$triangle given by (x, y, z, x) is different from the one given by (x, z, y, x). In other words a $x-$triangle is oriented.

We introduce also the refined quantity, the *sub-lower local complexity* of a graph G:

$$C_{\mathrm{loc}}^{\mathrm{sub}}(G) := \inf_{\{G' \subset G, \sup d_{G'} = \infty\}} C_{\mathrm{loc}}(G'), \tag{5.4.2}$$

where the inclusion of weighted graph is understood in the following sense:

$$G' = (\mathscr{V}', \mathscr{E}') \subset G \text{ if } \mathscr{V}' \subset \mathscr{V} \text{ and } \mathscr{E}' := \mathscr{E}|_{\mathscr{V}' \times \mathscr{V}'}. \tag{5.4.3}$$

This means we can remove vertices but not edges. We conserve the induced weight. Easily, one gets:

$$0 \leq C_{\mathrm{loc}}^{\mathrm{sub}}(G) \leq C_{\mathrm{loc}}(G) \leq 1. \tag{5.4.4}$$

The sub-lower local complexity gives an optimal condition to ensure the unboundedness, from above and from below, of the self-adjoint realizations of the adjacency matrix. We give the main result:

Theorem 5.4.2. *Let $G = (\mathscr{V}, \mathscr{E})$ be a locally finite graph such that $\deg_G$ is unbounded. Let $\hat{\mathcal{A}}_G$ be a self-adjoint realization of the $\mathcal{A}_G$. Suppose that $\mathscr{E}$ is bounded. Then, one has:*

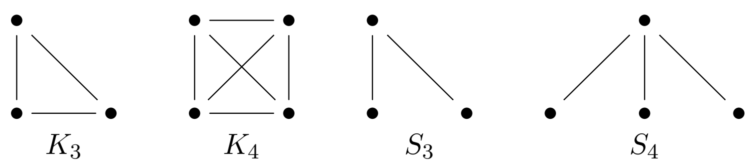
(a) $\hat{\mathcal{A}}_G$ is unbounded from above.

(b) If $C_{\mathrm{loc}}^{\mathrm{sub}}(G) = 0$ and $\mathscr{E}$ is bounded from below. Then $\hat{\mathcal{A}}_G$ is unbounded from below.

(c) For all $\varepsilon > 0$, there is a connected simple graph G such that $C_{\mathrm{loc}}(G) \in (0, \varepsilon)$, $\mathcal{A}_G$ is essentially self-adjoint on $\mathcal{C}_c(\mathscr{V})$ and is bounded from below.

By contrast, for any locally finite graph, Δ_G is a non-negative operator, i.e. $\langle f, \Delta_G f \rangle \geq 0$, for all $f \in \mathcal{C}_c(\mathscr{V})$. The two first points come rather easily. The main difficulty is to prove the optimality given in the last point.

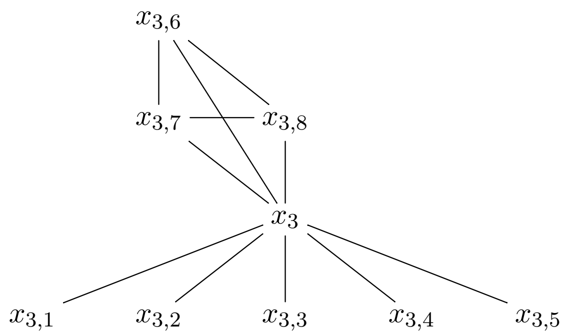
Example 5.4.3. *Consider G a simple graph. If a graph G has a subgraph, in the sense of* (5.4.3)*, being $\cup_{n \geq 0} S_{u_n}$ for some sequence $(u_n)_{n \in \mathbb{N}}$ that tends to infinity, then $C_{\mathrm{loc}}^{\mathrm{sub}}(G) = 0$. Here, $S_n = (\mathscr{V}_n, \mathscr{E}_n)$ denotes the* star graph *of order n, i.e., $|\mathscr{V}_n| = n$ and there is $x_\circ \in \mathscr{V}_n$ so that $\mathscr{E}(x, x_\circ) = 1$ for all $x \neq x_\circ$ and $\mathscr{E}(x, y) = 0$ for all $x \neq x_\circ$ and $y \neq x_\circ$.*



(5.4.5)

We recall the definition of $K_n := (\mathscr{V}_n, \mathscr{E}_n)$ the *complete graph* of n elements: $\mathscr{V}_n$ is a set of n elements and $\mathscr{E}(a,b) = 1$ for all $a, b \in \mathscr{V}_n$, so that $a \neq b$. One has $N_{K_n}(x)/deg^2_{K_n}(x) = (n-1)(n-2)/n^2$, for all $x \in \mathscr{V}_n$. Therefore, one can hope to increase the lower local complexity by having a lot of complete graphs as sub-graph in the sense of (5.4.3). More precisely, it is possible that $C_{\rm loc}(G)$ is positive, whereas $C^{\rm sub}_{\rm loc}(G) = 0$. For instance, one has:

Example 5.4.4. *For all $\alpha \in \mathbb{N}^*$, there is a simple graph G such that $0 = C^{\rm sub}_{\rm loc}(G) < C_{\rm loc}(G) = 1/(1+\alpha)^2$. Now we construct the graph $S_{m+1}K_n = (\mathscr{V}_{m,n}, \mathscr{E}_{m,n})$ as follows. Take $\mathscr{V}_{m,n} := \{x_n, x_{n,1}, \dots, x_{n,m+n}\}$. Set $\mathscr{E}_{m,n}(x_n, x_{n,j}) = 1$, for all $j = 1, \dots, m+n$, $\mathscr{E}_{m,n}(x_{n,j}, x_{n,k}) = 0$, for all $j, k = 1, \dots, m$, and $\mathscr{E}_{m,n}(x_{n,j}, x_{n,k}) = 1$, for all $j, k = m+1, \dots, m+n$, with $j \neq k$. Set $G_\circ := (\mathscr{V}_\circ, \mathscr{E}_\circ)$ as $\cup_{n\in\mathbb{N}^*} S_{\alpha n+1}K_n$. Finally, consider $G := (\mathscr{V}, \mathscr{E})$, with $\mathscr{V} := \mathscr{V}_\circ$ and $\mathscr{E}(x,y) := \mathscr{E}_\circ(x,y) + \sum_{n\in\mathbb{N}^*} \delta_{\{x_n\}}(x)\delta_{\{x_{n+1}\}}(y)$ for all $x, y \in \mathscr{V}$, where δ is the Kronecker delta.*



(5.4.6)

We mention also that the (sub-)lower local complexity does not imply the essential self-adjointness of the adjacency matrix. We point out that we know no example of a simple graph having the properties that the sub-lower local complexity is non-zero and that a self-adjoint realization of the adjacency matrix is unbounded from below.

5.5 Asymptotic eigenvalue distribution

The uncertainty principle is a central point in quantum physics. It can be expressed by the following Hardy inequality:

$$\left(\frac{n-2}{2}\right)^2 \int_{\mathbb{R}^n} \left|\frac{1}{|x|} f(x)\right|^2 dx \leq \int_{\mathbb{R}^n} |\nabla f|^2\, dx = \langle f, -\Delta_{\mathbb{R}^n} f\rangle, \text{ where } n \geq 3, \tag{5.5.1}$$

and $f \in \mathcal{C}^\infty_c(\mathbb{R}^n)$. Roughly speaking, the Laplacian controls some local singularities of a potential. Here, we investigate which potentials a discrete Laplacian is able to control. Obviously, since the value of a potential on a vertex has to be finite, we will not focus on local singularities. However, unlike in the continuous case, we will control potentials that blow up at infinity.

We are interested in lower bounds for the Laplacian with the help of the weighted degree. In the case of non-magnetic Laplacians, one standard approach is to use isoperimetric inequalities. The classical version gives estimates on the bottom of the spectrum. This is not adapted to our situation. We rely on a modified version. Given a subset $W \subset \mathscr{V}$, let

$$\partial W := \{x \in W, \text{ there is } y \sim x \text{ such that } y \notin W\}.$$

We define the following isoperimetric constant associated to (the weighted degree of) G by

$$\alpha(G) := \inf_{W \subset \mathscr{V}, \sharp W < \infty} \frac{\langle \mathbf{1}_{\partial W}, d_G(Q)\mathbf{1}_{\partial W}\rangle}{\langle \mathbf{1}_W, d_G(Q)\mathbf{1}_W\rangle},$$

where $\mathbf{1}_X$ denotes the characteristic function of X. By [KeLe09, page 14, line -4] (see also [Do84, DoKe86, Ke10] and references therein), we obtain:

$$\left(1-\sqrt{1-\alpha^2(G)}\right)\langle f, d_G(Q)f\rangle \le \langle f, \Delta_{\mathscr{E},0} f\rangle \le \left(1+\sqrt{1-\alpha^2(G)}\right)\langle f, d_G(Q)f\rangle, \tag{5.5.2}$$

for all $f \in \mathcal{C}_c(\mathscr{V})$. So, if $\alpha(G)>0$, (5.1.3) is improved and $\mathcal{D}(\Delta_{\mathscr{E},0}^{1/2}) = \mathcal{D}(d_G^{1/2}(Q))$. In particular, one sees that the essential spectrum $\sigma_{\rm ess}(d_G(Q))$ is empty if and only if $\sigma_{\rm ess}(\Delta_{\mathscr{E},0})$ is.

We point out that a converse is also true. Namely, if there is $a>0$ so that $a\langle f, \Delta_{\mathscr{E},0} f\rangle \ge \langle f, d_G(Q)f\rangle$, for all $f\in\mathcal{C}_c(\mathscr{V})$, then $\alpha(G)>0$.

Assume that $\alpha(G)>0$. Supposing that $\sigma_{\rm ess}(\Delta_{\mathscr{E},0})=\emptyset$ (or equivalently that $\lim_{|x|\to\infty} d_G(x) = +\infty$), the inequality (5.5.2) and the min-max principle provide the bound

$$\left(1-\sqrt{1-\alpha^2(G)}\right) \le \liminf_{\lambda\to\infty} \frac{\mathscr{N}_\lambda(\Delta_{\mathscr{E},0})}{\mathscr{N}_\lambda(d_G(Q))} \le \limsup_{\lambda\to\infty} \frac{\mathscr{N}_\lambda(\Delta_{\mathscr{E},0})}{\mathscr{N}_\lambda(d_G(Q))} \le \left(1+\sqrt{1-\alpha^2(G)}\right),$$

where

$$\mathscr{N}_\lambda(A) := \dim \operatorname{Ran} \mathbf{1}_{(-\infty,\lambda]}(A),$$

for a self-adjoint operator A. This estimate has to be refined so as to give the asymptotic of eigenvalues and to deal with magnetic fields. Moreover, (5.5.2) is not stable by small perturbation for the question of the equality of the form-domain. For instance, take a simple graph G_1, such that $\alpha(G_1)>0$ and the (simple) half-line graph G_2. Note that $\alpha(G_2)=0$. Now connect the disjoint union of G_1 and G_2 by one edge to obtain a new graph G. One sees easily that $\alpha(G)=0$ and $\mathcal{D}(\Delta_G^{1/2}) = \mathcal{D}(d_G^{1/2}(Q))$. This is why we seek a minoration by $ad_G(Q)-b$ for some $a,b>0$.

On the other hand, given $m_0:\mathscr{V}\to(0,\infty)$, we know that the Laplacian acting in $\ell^2(\mathscr{V},m^2)$ is unitarily equivalent to a Schrödinger operator acting in $\ell^2(\mathscr{V},m_0^2)$. This has already been noticed before, e.g., [CoToTr11, HaKe11]. By extracting some positivity, we obtain our analog of the Hardy inequality:

Proposition 5.5.1. *Let $G=(\mathscr{V},\mathscr{E},m_0,\theta)$ be a locally finite graph. Given $m:\mathscr{V}\to(0,\infty)$, one has:*

$$\langle f, V_m(Q)f\rangle \le \langle f, \Delta_{\mathscr{E},\theta} f\rangle, \text{ for } f\in\mathcal{C}_c(\mathscr{V}), \tag{5.5.3}$$

where

$$V_m(x) := d_G(x) - W_m(x), \text{ with } W_m(x) := \frac{1}{m_0^2(x)} \sum_{y\in\mathscr{V}} \mathscr{E}(x,y)\frac{m(y)}{m(x)}\frac{m_0(x)}{m_0(y)}. \tag{5.5.4}$$

Moreover, if G is bi-partite, we get:

$$\langle f, \Delta_{\mathscr{E},\theta} f\rangle \le \langle f, (d_G(Q)+W_m(Q))f\rangle, \text{ for } f\in\mathcal{C}_c(\mathscr{V}).$$

Note that by choosing $m=m_0$, we recover that $\Delta_{\mathscr{E},\theta}\ge 0$. Moreover, V_m is independent of the magnetic field. We stress that the inequality (5.5.3) is in some cases trivial. One has to find a favorable situation in order to exploit it. This is the case for some perturbations of weighted trees. We present our main result:

Theorem 5.5.2. *Let $G_\circ=(\mathscr{V},\mathscr{E}_\circ,m,\theta_\circ)$ be a weighted tree. Assume that there is $\varepsilon_0\in(0,1)$, so that*

$$C_0 := \sup_{x\in\mathscr{V}} \max_{y\in\mathscr{V}} d_{G_\circ}^{\varepsilon_0-1}(x)\mathscr{E}_\circ(x,y)m^{-2}(x) < \infty. \tag{5.5.5}$$

Let $G = (\mathscr{V}, \mathscr{E}, m, \theta)$ be a perturbed graph and $V : \mathscr{V} \to \mathbb{R}$ be a potential, satisfying:

$$|V(x)| + \Lambda(x) = o(1 + d_{G_\circ}(x)), \text{ as } |x| \to \infty, \tag{5.5.6}$$

where $\Lambda(x) := \frac{1}{m^2(x)} \sum_{y\sim x} |\mathscr{E}(x,y) - \tilde{\mathscr{E}}(x,y)|$. Then, the following properties hold:

(a) The quadratic form associated to $\Delta_{\mathscr{E},\theta} + V(Q)$ is bounded from below by some constant $-C$. We denote by H the associated Friedrichs extension.

(b) For all $\varepsilon > 0$, there is $c_\varepsilon \geq 0$, so that

$$(1-\varepsilon)\langle f, d_{G_\circ}(Q) f\rangle - c_\varepsilon \|f\|^2 \leq \langle f, Hf\rangle \leq (1+\varepsilon)\langle f, d_{G_\circ}(Q)f\rangle + c_\varepsilon\|f\|^2, \tag{5.5.7}$$

for $f \in \mathcal{C}_c(\mathscr{V})$. We have $\mathcal{D}((H+C)^{1/2}) = \mathcal{D}((d_{G_\circ}(Q)^{1/2})$.

(c) The essential spectrum of H is equal to the one of $\Delta_{\mathscr{E}_\circ,\theta_\circ}$.

(d) The essential spectrum of H is empty if and only if $\lim_{|x|\to\infty} d_{G_\circ}(x) = +\infty$. In this case we obtain:

$$\lim_{N\to\infty} \frac{\lambda_N(H)}{\lambda_N(d_{G_\circ}(Q))} = 1, \tag{5.5.8}$$

where λ_N denotes the N-th eigenvalue counted with multiplicity.

Note that we improve on the bound (5.1.3). We point out that Hypothesis (5.5.5) is fulfilled by simple trees, i.e., when $\mathscr{E} = m_0 = 1$. Since G_0 is a tree, we recall that $\Delta_{\mathscr{E}_\circ,\theta_\circ}$ is unitarily equivalent to $\Delta_{\mathscr{E}_\circ,0}$. However, G is a priori not a tree (recall that Zorn's Lemma ensures that every simple graph has a maximal subtree). Therefore it is interesting to observe that there is no hypothesis on θ. We indicate that the inequality (5.5.7) is valid for a larger class of perturbations.

We point out that the first part of d), namely the absence of the essential spectrum, has been studied in many works, e.g., [Ke10, KeLe09, KeLe12, KeLeWo11]. They generalize some ideas of [DoKe86, Fu96]. Their approach is based on some isoperimetric estimates and on the Persson's Lemma. The latter characterizes the infimum of the essential spectrum.

The asymptotic of eigenvalues is a novelty and was not considered in the literature before. Here one should keep in mind that our approach is different from the one used in the continuous setting. Whereas one usually relies on the Dirichlet-Neumann bracketing technique, by cutting the space into boxes, it is hard to believe that such an approach would be efficient here. Indeed, cutting the graph gives a perturbation which is of the same size as the operator.

We stress that one can prescribe any asymptotic of eigenvalues by choosing a proper tree G (and in fact d_G). We mention that the spectral asymptotic estimates obtained in [DoMa06] are for some operators with non-empty essential spectrum. They study graphs which are equipped with a free action of a discrete group and establish a bound on the $\operatorname{tr} e^{-t\Delta_{\mathscr{E},\theta}}$, where the trace is adapted to a fundamental domain.

We turn to the question of the form-domain. We stress that we do not suppose that the isoperimetric constant is non-zero. To our knowledge, this is the first time that the form-domain of the unbounded discrete Laplacian on a simple tree is identified. It is remarkable that the form-domain coincides with that of $d_G(Q)$, a multiplication operator. A useful consequence is the stability of the essential spectrum, obtained in c). This is also new. On the other hand, we stress that there are simple bi-partite graphs, such that the form-domain of the Laplacian is different from that of $d_G(Q)$. In this case, (5.5.7) is not fulfilled.

Having the same form-domain does not necessarily ensure that the domains are also equal. In [Go11], we construct a simple tree which is such an example. However, under some further hypotheses on the graph, we can ensure that the domain of the magnetic Laplacian is equal to that of $d_G(Q)$. Moreover, there is a simple tree T, which has 0 as associated isoperimetric constant and such that the domain of the Laplacian is the same as that of the weighted degree. Besides that, one obtains that $\sigma(\Delta_T) = \sigma_{\mathrm{ac}}(\Delta_T) = [0, \infty)$.

Partial proof of Theorem 5.5.2. We start with a remark about bi-partite graphs:

Proposition 5.5.3. *Given a bi-partite graph $G = (\mathscr{V}, \mathscr{E}, m, \theta)$ and a function $V : \mathscr{V} \to [0, \infty)$, the following assertions are equivalent:*

$$\langle f, (d_G(Q) - V(Q))f\rangle \leq \langle f, \Delta_{\mathscr{E},\theta} f\rangle, \quad \text{for } f \in \mathcal{C}_c(\mathscr{V}), \tag{5.5.9}$$

$$\langle f, \Delta_{\mathscr{E},\theta} f\rangle \leq \langle f, (d_G(Q) + V(Q))f\rangle, \quad \text{for } f \in \mathcal{C}_c(\mathscr{V}), \tag{5.5.10}$$

$$|\langle f, \mathcal{A}_{\mathscr{E},\theta} f\rangle| \leq \langle f, V(Q) f\rangle, \quad \text{for } f \in \mathcal{C}_c(\mathscr{V}), \tag{5.5.11}$$

where $\mathcal{A}_{\mathscr{E},\theta}$ is the magnetic adjacency matrix defined by

$$(\mathcal{A}_{\mathscr{E},\theta} f)(x) := \frac{1}{m^2(x)} \sum_{y \in \mathscr{V}} \mathscr{E}(x, y) e^{\mathrm{i}\theta_{x,y}} f(y), \tag{5.5.12}$$

for $f \in \mathcal{C}_c(\mathscr{V})$ and $x \in \mathscr{V}$.

Proof. Let $x_0 \in \mathscr{V}$. Given $x \in \mathscr{V}$, by definition of connectedness, there is a sequence $x_1, \ldots, x_n$ of elements of $\mathscr{V}$, so that $\mathscr{E}(x_i, x_{i+1}) \neq 0$, for $i = 0, \ldots, n-1$ and $x_n = x$. The minimal possible n is the *unweighted length* between x_0 and x. We denote it by $\ell(x)$. Set $Uf(x) := (-1)^{\ell(x)} f(x)$. Note that $U^2 = \mathrm{Id}$ and $U^{-1} = U^* = U$. Notice now that

$$U^{-1} \mathcal{A}_{\mathscr{E},\theta} U = -\mathcal{A}_{\mathscr{E},\theta} \text{ and } \Delta_{\mathscr{E},\theta} = d_G(Q) - \mathcal{A}_{\mathscr{E},\theta}.$$

We start with (5.5.9) and rewrite it as follows: $\langle f, \mathcal{A}_{\mathscr{E},\theta} f\rangle \leq \langle f, V(Q) f\rangle$, for $f \in \mathcal{C}_c(\mathscr{V})$. Applying this to Uf, we infer immediately (5.5.11). We start now from (5.5.11). We get:

$$\langle f, \Delta_{\mathscr{E},\theta}\, f\rangle = \langle f, (d_G(Q) - \mathcal{A}_{\mathscr{E},\theta}) f\rangle \geq \langle f, (d_G(Q) - V(Q)) f\rangle$$

for $f \in \mathcal{C}_c(\mathscr{V})$. In the same way, (5.5.10) is equivalent to (5.5.11). □

We now focus on the weighted tree G_0. First It is convenient to choose a root in the tree. Due to its structure, one can take any point of $\mathscr{V}$. We denote it by ϵ. We define inductively the *sphere* S_n by

$$S_{-1} = \emptyset, S_0 := \{\epsilon\}, \text{ and } S_{n+1} := \mathscr{N}_G(S_n) \setminus S_{n-1}.$$

Given $n \in \mathbb{N}$, $x \in S_n$, and $y \in \mathscr{N}_G(x)$, one sees that $y \in S_{n-1} \cup S_{n+1}$. We write $x \sim> y$ and say that x is a *son* of y, if $y \in S_{n-1}$, while we write $x <\sim y$ and say that x is a *father* of y, if $y \in S_{n+1}$. Notice that ϵ has no father. Given $x \neq \epsilon$, note that there is a unique $y \in \mathscr{V}$ with $x \sim> y$, i.e., everyone apart from ϵ has one and only one father. We denote the father of x by $\overleftarrow{x}$.

We focus on the left hand side of (5.5.7) for $G_\circ$ and $V = 0$, i.e., for $H = \Delta_{\mathscr{E}_\circ, \theta_\circ}$. Set $K := \{x \in \mathscr{V}, d_{G_\circ}(x) \leq 1\}$ and $\tilde{\mathscr{V}} := \mathscr{V} \setminus K$. Note that the induced graph $\tilde{G}_\circ$ of $G_\circ$ w.r.t. $\tilde{\mathscr{V}} = \cup_{n \in \mathbb{N}} \tilde{\mathscr{V}}_n$ is a forest of disjoint and maximal subtrees $\tilde{G}_n := (\tilde{\mathscr{V}}_n, \mathscr{E}_n, m|_{\tilde{\mathscr{V}}_n}, \theta_\circ|_{\tilde{\mathscr{E}}_n})$, where $\tilde{\mathscr{E}}_n := \mathscr{E}_\circ|_{\tilde{\mathscr{V}}_n \times \tilde{\mathscr{V}}_n}$. For each $\tilde{G}_n$ of $\tilde{G}_\circ$, we define:

$$\tilde{m}(\epsilon_{\mathscr{V}_n}) := 1 \text{ and } \tilde{m}(x) := \eta\, \tilde{m}(\overleftarrow{x}) \frac{m(x)}{m(\overleftarrow{x})} d_{G_\circ}^{-\varepsilon_0/2}(x), \text{ for all } x \in \tilde{\mathscr{V}}_n.$$

With this definition and $V_{\tilde{m}}$ as in (5.5.4), we obtain:

$$\begin{aligned}\frac{V_{\tilde{m}}(x)}{d_{\tilde{G}}(x)} &= 1 - \frac{1}{d_G(x)m^2(x)}\left(\mathscr{E}(\overleftarrow{x}, x)\frac{\tilde{m}(\overleftarrow{x})}{\tilde{m}(x)}\frac{m(x)}{m(\overleftarrow{x})} + \sum_{y\sim>x}\mathscr{E}(y,x)\frac{\tilde{m}(y)}{\tilde{m}(x)}\frac{m(x)}{m(y)}\right)\\ &= 1 - \frac{1}{\eta}\frac{1}{d_G^{(1-\varepsilon_0/2)}(x)m^2(x)}\mathscr{E}(\overleftarrow{x}, x) - \frac{\eta}{d_G(x)m^2(x)}\sum_{y\sim>x}\mathscr{E}(y,x)d_G^{-\varepsilon_0/2}(y)\\ &\geq 1 - \eta - \frac{1}{\eta}d_G^{-\varepsilon_0/2}(x)C_0, \end{aligned} \tag{5.5.13}$$

for all $x \in \tilde{\mathscr{V}}_n$ and where C_0 is given by (5.5.5). Consider $f \in \mathcal{C}_c(\mathscr{V})$. We apply Proposition 5.5.1 to $\tilde{G}_\circ$. Since $\mathscr{E} \geq 0$ we derive that there is a constant $C(\eta) > 0$, so that:

$$\begin{aligned}\langle f, \Delta_{\mathscr{E}_\circ,\theta_\circ} f\rangle &\geq \langle f|_{\tilde{\mathscr{V}}}, \Delta_{\mathscr{E}_\circ,\theta_\circ}(f|_{\tilde{\mathscr{V}}})\rangle \geq \langle f|_{\tilde{\mathscr{V}}}, V_{\tilde{m}}(Q)(f|_{\tilde{\mathscr{V}}})\rangle\\ &\geq \langle d_{\tilde{G}}^{1/2}(Q)f|_{\tilde{\mathscr{V}}}, (1-\eta-C_0/d_{\tilde{G}}^{\varepsilon_0/2}(Q)\eta)d_{\tilde{G}}^{1/2}(Q)f|_{\tilde{\mathscr{V}}}\rangle\\ &\geq (1-2\eta)\langle f|_{\tilde{\mathscr{V}}}, d_{\tilde{G}}(Q)f|_{\tilde{\mathscr{V}}}\rangle - C(\eta)\|f|_{\tilde{\mathscr{V}}}\|^2\\ &\geq (1-2\eta)\langle f, d_{G_\circ}(Q)f\rangle - (C_\eta + 1)\|f\|^2. \end{aligned} \tag{5.5.14}$$

This gives (5.5.7) for $G_\circ$ and $V = 0$, where the second inequality is obtained by applying Proposition 5.5.3.

Next, the equality of the domains of the forms follow immediately and so the essential spectrum of $\Delta_{\mathscr{E}_\circ,\theta_\circ}$ is empty if and only if $\lim_{|x|\to\infty} d_{G_\circ}(x) = +\infty$. Finally, we use twice the min-max principle. This yields:

$$1-\varepsilon \leq \liminf_{N\to\infty}\frac{\lambda_N(\Delta_{\mathscr{E},\theta})}{\lambda_N(d_{G_\circ}(Q))} \leq \limsup_{N\to\infty}\frac{\lambda_N(\Delta_{\mathscr{E},\theta})}{\lambda_N(d_{G_\circ}(Q))} \leq 1+\varepsilon.$$

By letting ε go to zero we obtain the asymptotic (5.5.8) for $\Delta_{\mathscr{E}_\circ,\theta_\circ}$. We finish with $H = \Delta_{\mathscr{E},\theta} + V(Q)$ by perturbing $\Delta_{\mathscr{E}_\circ,\theta_\circ}$ (see [Go11]). □

Chapter 6

Other topics

6.1 1-dimensional discrete Dirac operator

We study properties of relativistic (massive or not) charged particles with spin-1/2. We follow the Dirac formalism, see [Di82]. Unlike in [BoGo10], we shall focus on the 1-dimensional discrete version of the problem. We stick to the case of $\mathbb{Z}$ for simplicity. The mass of the particle is given by $m \geq 0$. For simplicity, we re-normalize the speed of light and the reduced Planck constant by 1. The Dirac discrete operator, acting on $\ell^2(\mathbb{Z}, \mathbb{C}^2)$, is defined by

$$D_m := \begin{pmatrix} m & d \\ d^* & -m \end{pmatrix},$$

where $d := \mathrm{Id} - \tau$ and τ is the right shift, defined by $\tau f(n) = f(n+1)$, for all $f \in \ell^2(\mathbb{Z}, \mathbb{C})$. The operator D_m is self-adjoint. Moreover, notice that

$$D_m^2 = \begin{pmatrix} \Delta + m^2 & 0 \\ 0 & \Delta + m^2 \end{pmatrix},$$

where $\Delta f(n) := 2f(n) - f(n+1) - f(n-1)$. This yields that $\sigma(D_m^2) = [m^2, 4 + m^2]$. To remove the square above D_m, we define the symmetry S on $\ell^2(\mathbb{Z}, \mathbb{C})$ by $Sf(n) = f(-n)$ and the unitary operator on $\ell^2(\mathbb{Z}, \mathbb{C}^2)$

$$U := \begin{pmatrix} 0 & \mathrm{i}S \\ -\mathrm{i}S & 0 \end{pmatrix}. \tag{6.1.1}$$

Clearly $U = U^* = U^{-1}$. Thus, $UD_mU = -D_m$. We infer that the spectrum of D_m is purely absolutely continuous (ac) and that

$$\sigma(D_m) = \sigma_{\mathrm{ac}}(D_m) = [-\sqrt{m^2+4}, -m] \cup [m, \sqrt{m^2+4}].$$

We shall now perturb the operator by an electrical potential $V = (V_1, V_2)^t \in \ell^\infty(\mathbb{Z}, \mathbb{R}^2)$. We set

$$H := D_m + \begin{pmatrix} V_1(Q) & 0 \\ 0 & V_2(Q) \end{pmatrix}. \tag{6.1.2}$$

Clearly, the essential spectrum of H is the same as the one of D_m if V tends to 0 at infinity. We turn to refined questions. The singularly continuous spectrum, quantum transport, and localization have been studied before [CaOl12, PrOl12, CaOlPr11, PrOl08, OlPr05, OlPr05b]. The question of the purely ac spectrum seems not to have been answered before.

We recall the following standard result for the Laplacian (the non-relativistic setting).

Theorem 6.1.1. *Take $V \in \ell^\infty(\mathbb{Z}, \mathbb{R})$ and $\nu \in \mathbb{Z}_+^*$ such that:*

$$\lim_{n\to\pm\infty} V(n) = 0, \qquad (6.1.3)$$
$$V_{|\mathbb{Z}_+} - \tau^\nu V_{|\mathbb{Z}_+} \in \ell^1(\mathbb{Z}_+, \mathbb{R}),$$

then the spectrum of $\Delta + V(Q)$ is purely absolutely continuous on $(0, 4)$.

In the case of $\mathbb{Z}^+$ and for $\nu = 1$, the result has been essentially proved in [We67] (in fact in the quoted reference, one focuses only on the continuous setting). The proof for the discrete setting can be found in [DoNe86, Si96]. For $\nu > 1$, it seems that it was first done in [St94]. Note that for instance, one covers potentials like $V(n) = (-1)^n W(n)$, where W is decay to 0. We refer to [GoNe01] and to [KaLa11] for recent results in this direction.

An amusing and easy remark is the difference between $\mathbb{N}$ and $\mathbb{Z}$. In the latter, the decay hypothesis is asked only to the right part of the potential. This reflects the fact that the particle can always escape to the right even if the left part of the potential should have led to some singularity continuous spectrum in a half-line setting.

Partial proof. We start by proving Theorem 6.1.1 with $\mathbb{N}$ instead of $\mathbb{Z}$. Apart from Proposition 6.1.3, our presentation is very close to the one of [FrHaSp06]. We start with the truncated case. Set:

$$\alpha_n := \left\langle \delta_n, \left(\Delta^{(n)} + V_{|\mathbb{N}_n}(Q) - \lambda\right)^{-1} \delta_n \right\rangle \in \mathbb{H},$$

where $\Delta^{(n)}$ is the Laplacian on $\mathbb{N}_n := [n, \infty) \cap \mathbb{Z}$. We have $\alpha_n = \Phi_n(\alpha_{n+1})$ with

$$\Phi_n(z) = -\left(\lambda - V(n) - (1 + z)^{-1}\right)^{-1}.$$

Note that Φ_n is a (hyperbolic) contraction of Poincaré half-plane $\mathbb{H}$. This is not a strict contraction. However, $\Phi_n \circ \Phi_{n+1}$ has two key properties. First, $\Phi_n \circ \Phi_{n+1}$ is strict contraction. Secondly, there is a fixed hyperbolic ball $B \subset \mathbb{H}$, depending on $\mathrm{Im}(z)$ and on $\|V\|_\infty$, such that $\Phi_n \circ \Phi_{n+1}(\mathbb{H}) \subset B$, e.g., [FrHaSp06][Proposition 2.2]. We infer:

Proposition 6.1.2. *Take $V \in \ell^\infty(\mathbb{N}, \mathbb{R})$, then for all $\lambda \in \mathbb{H}$ and $(\zeta_n)_n \in \mathbb{H}^\mathbb{N}$ we have*

$$d_\mathbb{H}\text{--}\lim_{n\to\infty} \Phi_0 \circ \cdots \circ \Phi_n(\zeta_n) = \alpha_0.$$

Now unlike in [FrHaSp06][Lemma 4.5] or in [FrHaSp09][Proposition 3.4] we use the fixed point of $\Phi_n \circ \cdots \circ \Phi_{n+\nu-1}$. We obtain:

Proposition 6.1.3. *Take $x \in (0, 4)$, $V \in \ell^\infty(\mathbb{N}, \mathbb{R})$, and $\nu \in \mathbb{Z}_+^*$ with $\lim_{n\to+\infty} V(n) = 0$ and $V - \tau^\nu V \in \ell^1(\mathbb{N}, \mathbb{R})$. Then there exist $x_1, x_2 \in \mathbb{R}$ such that $x \in (x_1, x_2)$ and $M_1, \varepsilon > 0$ so that*

$$d_\mathbb{H}(\alpha_0, \mathrm{i}) \le M_1$$

for all $\lambda \in K_{x_1,x_2,\varepsilon} := (x_1, x_2) + \mathrm{i}(0, \varepsilon)$.

Proof. We study the fixed points of $\Phi_n \circ \cdots \circ \Phi_{n+\nu}$ in a neighbourhood of

$$\omega_{\infty,x} := (x, \ldots, x).$$

The fixed points of $\varphi_x := -(x - (1 + z)^{-1})^{-1}$ are

$$-\frac{1}{2} \pm \frac{1}{2}\mathrm{i}\sqrt{\frac{4}{x} - 1},$$

The rest remains the same. □

Finally Proposition 2.3.5 concludes the proof of Theorem 6.1.1 where $\mathbb{Z}$ is replaced by $\mathbb{N}$.

We turn to the case of the line and reduce the problem to the case of $\mathbb{N}$ because

$$\left|\left\langle \delta_0, \left(\Delta^{(\mathbb{Z})} + V(Q) - \lambda\right)^{-1} \delta_0 \right\rangle\right| = \left|\left(\lambda - V(0) - (1+\alpha_\lambda)^{-1} - (1+\alpha'_\lambda)^{-1}\right)^{-1}\right| \leq \frac{1}{\Im(-(1+\alpha_\lambda)^{-1})}.$$

where

$$\alpha_\lambda := \left\langle \delta_1, \left(\Delta^{(\mathbb{N}^*)} + V_{|_{\mathbb{N}_1}}(Q) - \lambda\right)^{-1} \delta_1 \right\rangle \in \mathbb{H}$$
$$\alpha'_\lambda := \left\langle \delta_{-1}, \left(\Delta^{(-\mathbb{N}^*)} + V_{|_{-\mathbb{N}^*}}(Q) - \lambda\right)^{-1} \delta_{-1} \right\rangle \in \mathbb{H},$$

with $\Delta^{(\mathbb{N}^*)}$ and $\Delta^{(-\mathbb{N}^*)}$ the Laplacian on $\mathbb{N}^*$ and $-\mathbb{N}^*$ respectively. This gives Theorem 6.1.1. □

We now turn to the main result.

Theorem 6.1.4. *Take $V \in \ell^\infty(\mathbb{Z}, \mathbb{R}^2)$ and $\nu \in \mathbb{Z}_+^*$ with:*

$$\lim_{n\to\pm\infty} V(n) = 0,$$

$$V_{|_{\mathbb{Z}_+}} - \tau^\nu V_{|_{\mathbb{Z}_+}} \in \ell^1(\mathbb{Z}_+, \mathbb{R}^2),$$

then the spectrum of H is purely absolutely continuous on $\left(-\sqrt{m^2+4}, -m\right) \cup \left(m, \sqrt{m^2+4}\right)$.

As in [DoEs00, BoGo10], we perform a spin-up/down decomposition. We reduce the study of H to a non-self-adjoint Laplacian like operator which depends on the spectral parameter. This approach seems to be new in the discrete setting. Then, we adapt the iterative process to the non-self-adjoint Laplacian like operator.

6.2 Chessboards

On a chessboard, a knight moves by two squares in one direction and by one square in the other one (like a L). A classical challenge is the so-called *knight tour*. The knight is placed on the empty board and, moving according to the rules of chess, must visit each square exactly once. A knight's tour is called a *closed tour* if the knight ends on a square attacking the square from which it began. If the latter is not satisfied and the knight has visited each square exactly once, we call it an *open tour*.

Some early solutions were given by Euler, see [Eu59] and also by De Moivre (we refer to Mark R. Keen for historical remarks, see [Ke]). The problem was recently considered for various types of chessboards: as a cylinder [Wa00], a torus [Wa97], a sphere [Ca02], the exterior of the cube [QiWa06], the interior of the cube [De07],... It represents also an active field of research in computer science, e.g., [Pa97] (see references therein). Here, we shall focus on rectangular boards.

In 1991, Schwenk considered the question of the closed knight tour problem in a 2-dimensional rectangular chessboard. He provided a necessary and sufficient condition on the size of the board in order to have a closed knight tour. He obtained:

Theorem 6.2.1 (Schwenk)**.** *Let $1 \leq m \leq n$. The $m \times n$ chessboard has* no *closed knight tour if and only if one of the following assumption holds:*

1	**30**	**33**	**16**	**3**	**24**
32	**17**	**2**	**23**	**34**	**15**
29	**36**	**31**	**14**	**25**	**4**
18	**9**	**6**	**35**	**22**	**13**
7	**28**	**11**	**20**	**5**	**26**
10	**19**	**8**	**27**	**12**	**21**

Figure 6.1: A 6×6 closed tour

(a) m *and* n *are both odd,*

(b) $m \in \{1, 2, 4\}$*,*

(c) $m = 3$ *and* $n \in \{4, 6, 8\}$*.*

We refer to [Sc91] (see also [Wa04]) for a proof. When conditions (a),(b), and (c) are not fulfilled, he reduced the problem to studying a finite number of elementary boards. On each of them, he exhibited a closed tour and then explained how to "glue" the elementary boards together, in order to make one closed tour for the union out of the disjoint ones given by the elementary blocks. We explain the latter on an example. Say we want a closed tour for a 12×6 board. Write, side by side, two copies of Figure 6.1. Delete the connection between 21 and 22 for the left board and the connection between 28 and 29 for the right one. Then link 21 with 28 and 22 with 29. The Hamiltonian cycle goes as follows:

$$1[L] \to 2[L] \to \ldots \to 21[L] \to 28[R] \to 27[R] \to \ldots \to 1[R] \to$$
$$\to 36[R] \to \ldots \to 29[R] \to 22[L] \to 23[L] \to \cdots \to 36[L] \to 1[L],$$

where $[L]$ and $[R]$ stand for left and right, respectively.

We turn to the question for higher dimensions. In dimension 3 or above, a knight moves by two steps along one coordinate and by one step along a different one. Stewart [St71] and DeMaio [De07] constructed some examples of 3-dimensional knight tours. Then, in 2011, in [DeMa11], DeMaio and Mathew extended Theorem 6.2.1 by classifying all the 3-dimensional rectangular chessboards which admit a knight tour.

Theorem 6.2.2 (DeMaio and Mathew)**.** *Let* $2 \le m \le n \le p$*. The* $m \times n \times p$ *chessboard has* no *closed knight tour if and only if one of the following assumption holds:*

(a) m*,* n*, and* p *are all odd,*

(b) $m = n = 2$*,*

(c) $m = 2$ *and* $n = p = 3$*.*

The strategy is the same as in Theorem 6.2.1.

We now extend the previous results to higher dimensional boards. We rely strongly on the structure of the solutions for the case $n = 3$ to treat the case $n \ge 4$. We proceed by induction.

Before giving the main statement, we explain the key idea with Figure 6.1. We first extract two *cross-patterns* (cp). We represent them up to some rotation, see Figure 6.2. Note they are with disjoint support.

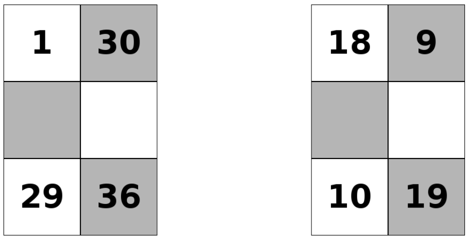


Figure 6.2: Two cross-patterns

We construct a tour for a $6 \times 6 \times 2$ board first. We work with coordinates. The tour given in 6.1 is given by $(a^i)_{i \in [\![1,36]\!]}$, with $a^1 := (1,6)$, $a^2 := (3,5)$, ... We take two copies of the tour given in 6.1 and denote them by $(a^i, 1)_{i \in [\![1,36]\!]}$ and $(a^i, 2)_{i \in [\![1,36]\!]}$ for the first and second copy, respectively. We can construct a tour as follows:

$$(2,4,1) \to (2,6,2) \to (3,4,2) \to \ldots \to (1,4,2) \to (1,6,1) \to \ldots \to (2,4,1).$$

We point out that we use coordinates in matrix way. To enhance the idea we rewrite it abusively by

$$(\text{“36”}, 1) \to (\text{“30”}, 2) \to (\text{“31”}, 2) \to \ldots \to (\text{“29”}, 2) \to (\text{“1”}, 1) \to \ldots \to (\text{“36”}, 1).$$

We explain how to treat a $6 \times 6 \times k$ board for $k \geq 3$. As the proof is the same, we write the case $k = 3$. We use the two cp as follows:

$$\begin{aligned} (\text{“36”}, 1) &\to (\text{“30”}, 2) \to (\text{“31”}, 2) \to \ldots \to (\text{“9”}, 2) \to \\ &\to (\text{“19”}, 3) \to (\text{“20”}, 3) \to \ldots \to (\text{“18”}, 3) \to \\ &\to (\text{“10”}, 2) \to (\text{“11”}, 2) \to \ldots \to (\text{“29”}, 2) \to \\ &\to (\text{“1”}, 1) \to \ldots \to (\text{“36”}, 1). \end{aligned} \tag{6.2.1}$$

Note that we have used only one cp on the first copy and one on last one. Two of them are still free. We can therefore repeat the procedure and add inductively further dimensions. For instance, we can go from a tour for a $6 \times 6 \times k$ board to one for a $6 \times 6 \times k \times l$ board, with $k, l \geq 2$. One takes l copies of the tour. By noticing that there are two cp on the initial tour, we proceed as in (6.2.1) for the tour. Thus, we will get a tour for the $6 \times 6 \times k \times l$ board, which contains in turn two cp. To prove all these facts, one can use coordinates.

The strategy is now clear. We shall study the structure of the elementary boards, which are obtained in [DeMa11] and look for specific patterns into them. Then, we shall conclude by induction on the dimension. We obtain:

Theorem 6.2.3. *Let $2 \leq n_1 \leq n_2 \leq \ldots \leq n_k$, with $k \geq 3$. The $n_1 \times \ldots \times n_k$ chessboard has* no *closed knight tour if and only if one of the following assumption holds:*

(a) For all i, n_i is odd,

(b) $n_{k-1} = 2$,

(c) $n_k = 3$.

Note that the hypotheses are the same as the ones given in Theorem 6.2.2 when $k = 3$. In the same paper they asked about higher dimensional tours, This question was also asked by DeMaio [De07] and Watkins [Wa04b]. We mention that a conjecture for this theorem was given in [Ku12].

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