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Commutateurs, analyse spectrale et applications aux opérateurs de Schrödinger discrets

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Résumé : L'objet de cette thèse est l'étude spectrale et dynamique de systèmes de la mécanique quantique en utilisant des techniques de commutateurs. Deux parmi les trois articles présentés traitent l'opérateur de Schrödinger discret sur un réseau.

Dans le premier article, un principe d'absorption limite est établi pour le Laplacien discret multidimensionnel perturbé par la somme d'un potentiel de type Wigner-von Neumann et d'un potentiel de type longue portée. Ce résultat implique notamment l'absolue continuité du spectre de cet Hamiltonien à certaines énergies.

Dans le second article, nous considérons à nouveau l'opérateur de Schrödinger discret multidimensionnel dont le potential est de type longue portée. Il est démontré que les fonctions propres correspondant à des valeurs propres de l'Hamiltonien décroissent sous-exponentiellement lorsque ces dernières ne sont pas un seuil. En dimension un, il est démontré de surcroît que ces fonctions propres décroissent exponentiellement. Une conséquence de ceci est l'absence de valeurs propres dans la partie centrale du spectre délimité aux extrémités par des seuils.

Le troisième article étudie des propriétés dynamiques d'Hamiltoniens vérifiants des hypothèses minimales dans la théorie des commutateurs. En se basant sur une estimation des vitesses minimales d'une part et une version améliorée du théorème du RAGE d'autre part, nous dérivons deux estimations de propagation pour cette famille d'Hamiltoniens. Ces estimations indiquent que les états du système se comportent dynamiquement de façon très similaire aux états de diffusion. Toutefois, ceci n'écarte pas la possibilité de spectre singulier continu.

Mots-clés : Théorie spectrale, estimation de propagation, commutateurs, théorie de Mourre, opérateurs de Schrödinger discrets

Abstract : This thesis deals with the analysis of spectral and dynamical properties of quantum mechanical systems using techniques of operator commutators. Two of the three research papers that are presented deal exclusively with the discrete Schrödinger operators on the lattice.

The first article proves a limiting absorption principle for the multi-dimensional discrete Laplacian perturbed by the sum of a Wigner-von Neumann potential and long-range potential. This result notably implies the absolute continuity of the spectrum of this Hamiltonian at certain energies.

The second article proves that eigenfunctions corresponding to non-threshold eigenvalues of multidimensional discrete Schrödinger operators decay sub-exponentially. In one dimension, it is further proven that these eigenfunctions decay exponentially. A consequence of this is the absence of eigenvalues when the middle portion of the spectrum does not contain any thresholds.

The third article investigates dynamical properties of Hamiltonians under very minimal assumptions in the theory of commutators. Based on minimal escape velocities and an improved version of the RAGE Theorem, we derive propagation estimates for these types of Hamiltonians. These estimates indicate that the states of the system behave dynamically very much like scattering states. Nonetheless, the existence of singularly continuous states cannot be disproved.

Key words : Spectral theory, propagation estimates, commutators, Mourre theory, discrete Schrödinger operators

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Marc-Adrien Mandich

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INTRODUCTION

Notation: For Hilbert spaces $\mathcal{F}$ and $\mathcal{G}$, let $\mathcal{B}(\mathcal{F},\mathcal{G})$ and $\mathcal{K}(\mathcal{F},\mathcal{G})$ respectively be the set of bounded linear operators and compact linear operators from $\mathcal{F}$ into $\mathcal{G}$. If $\mathcal{F}=\mathcal{G}$, then we set $\mathcal{B}(\mathcal{F})=\mathcal{B}(\mathcal{F},\mathcal{G})$ and $\mathcal{K}(\mathcal{F})=\mathcal{K}(\mathcal{F},\mathcal{G})$. The Hilbert space by default will be denoted $\mathcal{H}$ and it will be assumed to be separable and over the complex numbers. For an arbitrary self-adjoint operator T on $\mathcal{H}$ we denote by $\mathcal{D}(T)$ its domain and $\sigma(T)$ its spectrum. The two specific Hilbert spaces we will be working with are $L^2(\mathbb{R}^\nu)$ and $\ell^2(\mathbb{Z}^\nu)$, where ν is the dimension. More notation will be added as we go along.

1 Generalities about Schrödinger operators

1.1 The continuous and discrete Schrödinger operators

Quantum mechanics is an important branch of physics concerned with the theoretical and experimental study of atoms and subatomic particles. A quantum mechanical system consists of one or several subatomic particles interacting between themselves and with the surrounding environment. Because of the interactions, the configuration of the system changes. We say that system evolves through various *states*. The states of the system are represented by unit vectors belonging to a Hilbert space. The observable physical quantities of the system, such as position of the particles, their momentum, spin or energy, are represented by self-adjoint linear operators acting on the Hilbert space.

Unlike the everyday world, where the macroscopic systems that surround us appear to have a definite position, a definite momentum and a definite energy, all at a definite time of occurrence, quantum systems are probabilistic in nature. This means that when making an experiment, there are several possible outcomes for a given measurement. In theory, all of these outcomes are associated a probability – or likeliness – of occurrence.

In mathematical physics, one of the simplest systems is that of a single particle that is free to travel in ν dimensions. The particle could be an electron for example. At any given time t, the position of the particle is given by coordinates in $\mathbb{R}^\nu$. The Hilbert space for the associated position states is $L^2(\mathbb{R}^\nu)$. This is the collection of functions $\psi:\mathbb{R}^\nu\mapsto\mathbb{C}$ such that

$$\|\psi\|^2 := \int_{\mathbb{R}^\nu} |\psi(x)|^2 d^\nu x < +\infty, \quad x=(x_1,...,x_\nu)\in\mathbb{R}^\nu.$$

A state describing the system at time t is a function $\psi\in L^2(\mathbb{R}^\nu)$ with $\|\psi\|=1$. This function is just a probability distribution for position. This means that the probability of finding the particle at time t in a region Ω of space is given by

$$\int_\Omega |\psi(x,t)|^2 d^\nu x.$$

If at time t the system is in a state $\psi(x,t)$, then we expect the particle to be in a neighborhood of the point with coordinates

$$\int_{\mathbb{R}^\nu} x|\psi(x,t)|^2 d^\nu x.$$

This quantity is called the expectation value of the position of the particle in the state $\psi(x)$ at time t. If the state of the particle is known in position space, we can infer the state of the particle in momentum space, thanks to the Fourier transform. It is given by

$$\hat{\psi}(p,t) = \frac{1}{(2\pi)^{\nu/2}} \int_{\mathbb{R}^\nu} \psi(x,t) e^{-\mathrm{i}x\cdot p} d^\nu x, \quad p = (p_1, ..., p_\nu) \in \mathbb{R}^\nu.$$

The expectation value of the momentum of the particle in this state is then

$$\int_{\mathbb{R}^\nu} p|\hat{\psi}(p,t)|^2 d^\nu p.$$

Another observable of central importance is energy. The kinetic energy is given by $|p|^2/2m$, where m is the mass of the particle. In the mathematical physics literature, it is standard to set the non-relativistic kinetic energy operator to be $H_0 := |p|^2 = |p_1|^2 + ... + |p_\nu|^2$. This is an operator of multiplication in momentum space. In other words, it is diagonalized in momentum space. By applying the inverse Fourier transform, we see that $H_0 = -\Delta := -\sum_{i=1}^{\nu} \partial^2/\partial x_i^2$. As many problems are initially formulated in position space, this is the form that is often used. In addition to kinetic energy, the particle may have potential energy $V(x)$ depending on its position. Here V is a function from $\mathbb{R}^\nu$ to $\mathbb{R}$. For this reason, we denote the full energy operator for the particle $H := H_0 + V$ in position space. It is typically called the *Hamiltonian* for the system. Under suitable conditions on the potential V, H is a self-adjoint operator on $\mathcal{H}^2(\mathbb{R}^\nu)$, the Sobolev space corresponding to the operator domain of H_0. By the Kato-Rellich Theorem for instance, this is the case if V is real-valued and H_0-bounded with relative bound strictly less than 1. For more details about self-adjointness, we refer to [Si3] and references therein for a concise review. The set of all possible energies the system can take is called the spectrum of H and it is denoted by $\sigma(H)$. If the particle is free, that is, in the absence of any potential energy, it is well-known that $\sigma(H) = \sigma(H_0) = [0, +\infty)$. In particular, the kinetic energy may be arbitrarily large. This follows easily from the Spectral Theorem.

The thesis is more geared towards a discretized version of the latter example. It consists in discretizing position. We can imagine the electron is now hopping from one lattice site to another, instead of moving in a continuous space. The lattice is composed of regularly spaced out sites. The Hilbert space for the position states is then $\ell^2(\mathbb{Z}^\nu)$. This is the collection of functions $\psi : \mathbb{Z}^\nu \mapsto \mathbb{C}$ such that

$$\|\psi\|^2 := \sum_{n\in\mathbb{Z}^\nu} |\psi(n)|^2 < +\infty, \quad n = (n_1, ..., n_\nu) \in \mathbb{Z}^\nu.$$

If the particle is in the quantum state ψ at time t, then the probability of finding it at site n is simply $|\psi(n,t)|^2$. By the Fourier transform, the state of the particle in momentum space $L^2([-\pi,\pi]^\nu, d^\nu p)$ is given by

$$\hat{\psi}(p,t) := \sum_{n\in\mathbb{Z}^\nu} \psi(n,t) e^{\mathrm{i}n\cdot p}, \quad p = (p_1, ..., p_\nu) \in [-\pi,\pi]^\nu.$$

The kinetic energy operator is diagonalized in momentum space. It is given by

$$H_0 := \sum_{i=1}^{\nu} 2 - 2\cos(p_i). \tag{1}$$

In position space, it acts on a state $\psi \in \ell^2(\mathbb{Z}^\nu)$ in this way:

$$(H_0\psi)(n) = (\Delta\psi)(n) = \sum_{|n-m|=1} \psi(n) - \psi(m). \tag{2}$$

Here $|n-m| := \sum_{i=1}^{\nu} |n_i - m_i|$ for all $n = (n_1, ..., n_\nu)$ and $m = (m_1, ..., m_\nu)$ belonging to $\mathbb{Z}^\nu$. The spectrum of the kinetic energy operator is $\sigma(H_0) = [0, 4\nu]$, since it corresponds to the range of the function given in (1). If the particle has potential energy $V(n)$ depending on position, then the Hamiltonian is $H = H_0 + V$. If V is real-valued and bounded for example, then H is a bounded self-adjoint operator on $\ell^2(\mathbb{Z}^\nu)$. This model has important applications in Solid State Physics, notably for the so-called tight-binding approximation. The lattice $\mathbb{Z}^\nu$ represents regularly spaced out atoms composing a crystal and the electron is hopping from one atom to another. In this model, the interatomic motion of the free electron is slowed down by the atoms, so that the kinetic energy has an a priori upper bound which does not exist in the continuous case.

1.2 The spectral decomposition of the Hamiltonian

As mentioned previously, the spectrum of $H = H_0 + V$ is the set of energies the system can have. Mathematically, the spectrum of H is defined as the collection of $z \in \mathbb{C}$ such that either $(H - z)$ is not invertible or $(H - z)^{-1}$ is not bounded. When the potential energy is non-zero, the spectrum of H is typically different than that of H_0. One of the main goals of Spectral Theory is to characterize the differences between the spectra of H_0 and $H_0 + V$. To recall a first well-known result, we need a definition.

Definition 1.1. *Let T be a self-adjoint operator on a Hilbert space $\mathcal{H}$. The discrete spectrum of T is defined to be*

$$\sigma_{\mathrm{d}}(T) := \{\lambda \in \sigma(T) : 0 < \dim\ker(T - \lambda) < +\infty \text{ and } \lambda \text{ is isolated in } \sigma(T)\}.$$

The essential spectrum of T is defined to be $\sigma_{\mathrm{ess}}(T) := \sigma(T) \setminus \sigma_{\mathrm{d}}(T)$.

We now recall Weyl's Theorem on relative compactness, applied to continuous Schrödinger operators:

Theorem 1.2 (Weyl's Theorem)**.** *Let H_0 be the self-adjoint realization of the Laplace operator $-\Delta$ in $L^2(\mathbb{R}^\nu)$. Let $V : \mathbb{R}^\nu \mapsto \mathbb{R}$ be a bounded function that goes to zero at infinity, and consider $H = H_0 + V$. Then V is H_0-form relatively compact, and so $\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ess}}(H_0)$.*

The corresponding result holds in the discrete case as well. The only major difference is that in the discrete case, V is H_0-relatively compact if and only if it is compact. This powerful result says that a relatively compact perturbation of H_0 may produce only eigenvalues of finite multiplicity located in $(-\infty, 0)$ in the continuous case and $(-\infty, 0) \cup (4\nu, +\infty)$ in the discrete case. In the first (resp. second) case, these eigenvalues may accumulate only at energy 0 (resp. 0 and 4ν).

Not all energies are of the same nature. The above discussion shows that $\sigma(H)$ is a disjoint union of $\sigma_{\mathrm{d}}(H)$ and $\sigma_{\mathrm{ess}}(H)$. But there is also another significant way of differentiating the energies, which we now describe. Let f belong to a Hilbert space $\mathcal{H}$. By the Spectral Theorem, to f is associated a unique Borel measure on the real line, μ_f, such that

$$\langle f, e^{-\mathrm{i}tH} f\rangle = \int_{\mathbb{R}} e^{-\mathrm{i}tx} d\mu_f(x), \quad \text{for all } t \in \mathbb{R}.$$

This is equivalent to saying that $\mu_f(\Sigma) = \langle f, E_\Sigma(H) f\rangle$ for all Borel sets $\Sigma \subset \mathbb{R}$. Here $E_\Sigma(H)$ is the spectral projection of H onto Σ. By the Lebesgue Decompostion Theorem,

$$\mu_f = (\mu_f)_{\mathrm{ac}} + (\mu_f)_{\mathrm{sc}} + (\mu_f)_{\mathrm{pp}},$$

where $(\mu_f)_{\mathrm{ac}}$ and $(\mu_f)_{\mathrm{sc}}$ are measures respectively absolutely continuous and singularly continuous with respect to the Lebesgue measure, and $(\mu_f)_{\mathrm{pp}}$ is a pure point measure. We can now refine the spectrum of H in terms of the support of measures:

Definition 1.3. *Let* $\sigma_\sharp(H) := \overline{\bigcup_{f\in\mathcal{H}} \mathrm{supp}\ (\mu_f)_\sharp}$*, where* $\sharp$ *stands for* ac*,* sc*, or* pp*. This defines the absolutely continuous, singularly continuous and point spectrum of* H*.*

It can be shown that $\sigma_{\mathrm{pp}}(H)$ is the closure of the collection of eigenvalues of H. Furthermore, we have that $\sigma(H)$ is a union of $\sigma_{\mathrm{ac}}(H)$, $\sigma_{\mathrm{sc}}(H)$ and $\sigma_{\mathrm{pp}}(H)$, however this union is not necessarily disjoint. For instance, there are many examples of H where singularly continuous or point spectrum is embedded in the absolutely continuous spectrum. If we further let $\mathcal{H}_{\mathrm{ac}}$ (resp. $\mathcal{H}_{\mathrm{sc}}$ and $\mathcal{H}_{\mathrm{pp}}$) be the closure of the linear span of vectors of the form $(H-z)^{-1}f$, where $z \in \mathbb{C}\setminus\mathbb{R}$ and $f \in \mathcal{H}$ is such that its spectral measure is purely absolutely continuous (resp. purely singularly continuous and pure point), then we have the following decomposition:

$$\mathcal{H} = \mathcal{H}_{\mathrm{ac}} \oplus \mathcal{H}_{\mathrm{sc}} \oplus \mathcal{H}_{\mathrm{pp}}, \quad \text{and} \quad \mathcal{H}_{\mathrm{c}} = \mathcal{H}_{\mathrm{ac}} \oplus \mathcal{H}_{\mathrm{sc}}.$$

We denote by $P_{\mathrm{ac}}(H)$, $P_{\mathrm{c}}(H)$ and $P_{\mathrm{pp}}(H)$ the orthogonal projections onto $\mathcal{H}_{\mathrm{ac}}$, $\mathcal{H}_{\mathrm{c}}$ and $\mathcal{H}_{\mathrm{pp}}$ respectively. An important task of Spectral Theory is to characterize the three components of the spectrum according to the potential. In the absence of a potential, the spectrum of H_0 is purely absolutely continuous for both the continuous and discrete Schrödinger operator. In the next section, we give a meaningful physical interpretation of this spectral decomposition.

1.3 Dynamical properties of the spectrum

The time-dependent Schrödinger equation describes the evolution of a non-relativistic system with time. For a single particle in $\mathbb{R}^\nu$, it reads

$$\mathrm{i}\frac{\partial}{\partial t}\psi(x,t) = H\psi(x,t) = \big[-\Delta + V(x)\big]\psi(x,t), \quad \psi(x,0) := f \in L^2(\mathbb{R}^\nu).$$

Assuming H to be self-adjoint, this equation has a unique solution for the given initial condition ψ. The solution is the wave function $\psi(x,t) = e^{-\mathrm{i}tH} f$.

Theorem 1.4 (Dynamics of continuous Schrödinger operators)**.** *Assume* $H = -\Delta + V$ *is self-adjoint on* $L^2(\mathbb{R}^\nu)$*.*

1. *If* $f \in \mathcal{H}_{\mathrm{pp}}$*, then*

$$\lim_{R\to+\infty} \sup_{t\geqslant 0} \int_{\mathbb{R}^\nu\setminus[-R,R]^\nu} |e^{-\mathrm{i}tH} f(x)|^2 d^\nu x = 0. \tag{3}$$

2. *If $f \in \mathcal{H}_{\rm c}$, then for all $R \geqslant 0$,*

$$\lim_{T\to+\infty} \frac{1}{T}\int_0^T \left(\int_{[-R,R]^\nu} |e^{-{\rm i}tH} f(x)|^2 d^\nu x\right) dt = 0. \tag{4}$$

3. *If $f \in \mathcal{H}_{\rm ac}$, then for all $R \geqslant 0$,*

$$\lim_{t\to+\infty} \int_{[-R,R]^\nu} |e^{-{\rm i}tH} f(x)|^2 d^\nu x = 0. \tag{5}$$

Estimate (3) says that states $f \in \mathcal{H}_{\rm pp}$ do not escape at infinity with time. For this reason these are called *bound states*. On the other hand, estimate (4) says that states $f \in \mathcal{H}_{\rm c}$ propagate to infinity averagely in time. If further $f \in \mathcal{H}_{\rm ac}$ then estimate (5) improves (4). We should mention that (4) is a consequence of the RAGE Theorem, while estimate (5) follows from the Riemann-Lebesgue Lemma, which we quote for convenience:

Theorem 1.5 (RAGE)**.** *If H is a self-adjoint operator on a Hilbert space $\mathcal{H}$, then for any $f \in \mathcal{H}$ and any $W \in \mathcal{B}(\mathcal{H})$ that is H-relatively compact,*

$$\lim_{T\to\pm\infty} \frac{1}{T}\int_0^T \|We^{-{\rm i}tH} P_{\rm c}(H) f\|^2 dt = 0. \tag{6}$$

The RAGE Theorem is attributed to Ruelle [Ru], Amrein and Georgescu [AG] and Enss [E]. The version cited here can be found in [CFKS, Theorem 5.8] for example. In [GM], we remark that this result can be improved, namely, under the same assumptions we have

$$\lim_{T\to\pm\infty} \sup_{\substack{f\in\mathcal{H}\\ \|f\|\leqslant 1}} \frac{1}{T}\int_0^T \|We^{-{\rm i}tH} P_{\rm c}(H) f\|^2 dt = 0. \tag{7}$$

Here we have included the supremum, which we have not found in the literature, see [CFKS, Theoerm 5.8] and [GM, Appendix B] for more details.

Theorem 1.6 (Riemann-Lebesgue Lemma)**.** *If H is a self-adjoint operator on a Hilbert space $\mathcal{H}$, then for any $f \in \mathcal{H}$ and any $W \in \mathcal{B}(\mathcal{H})$ that is H-relatively compact,*

$$\lim_{t\to\pm\infty} \|We^{-{\rm i}tH} P_{\rm ac}(H) f\| = 0. \tag{8}$$

Although estimate (6) characterizes states $f \in \mathcal{H}_{\rm sc}$, it is not specific to these states. Let us provide another dynamical property of these states. Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$. Let $\Omega \subset \mathbb{R}^\nu$ be a set of finite Lebesgue measure. We define the indicator function of the set Ω to be

$$(\mathbf{1}_\Omega \psi)(x) = \begin{cases} \psi(x), & \text{if } x \in \Omega \\ 0, & \text{if } x \notin \Omega. \end{cases}$$

The probability that the particle with initial state f be found in a region of space Ω after time t is $\|\mathbf{1}_\Omega e^{-{\rm i}tH} f\|^2$. Then the total time the particle with initial state f spends in the region of space Ω is given by

$$J(\Omega, f) := \int_0^{+\infty} \|\mathbf{1}_\Omega e^{-{\rm i}tH} f\|^2 dt.$$

We call $J(\Omega, f)$ the total *time of sojourn* of the initial state f in the region Ω.

Theorem 1.7. *If there exists a sequence of regions* $\{\Omega_n\}$, *with* $|\Omega_n| < +\infty$, *such that* $\operatorname*{s-lim}_{n\to+\infty} \mathbf{1}_{\Omega_n} = \mathbf{1}$ *and* $J(\Omega_n, f) < +\infty$ *for all* n, *then* $f \in \mathcal{H}_{\text{ac}}$. *If* $f \in \mathcal{H}_{\text{sc}}$, *then there exists at least one finite region of space* Ω *such that* $J(\Omega, f) = +\infty$.

This means that if $f \in \mathcal{H}_{\text{sc}}$, then the probability $\|\mathbf{1}_\Omega e^{-\mathrm{i}tH} f\|^2$ decays sufficiently slowly that it is not integrable for large times. This is a result due to Sinha [Sin].

1.4 Analytical properties of the spectrum

If the Hamiltonian is diagonalizable, then we may infer information about its spectrum. In many situations however, we do not know how to do this and so we rely on practical analytical tools to infer information about the quality of the spectrum. Perhaps the simplest and best known result in this regard is the Theorem of de la Vallée Poussin:

Theorem 1.8. *Let* H *be a self-adjoint operator on a Hilbert space* $\mathcal{H}$. *For* $f \in \mathcal{H}$, *let* μ_f *be the associated spectral measure. For Lebesgue almost every* $\lambda \in \mathbb{R}$, *the following limit exists in* $\mathbb{C}$, *is finite and non-zero:*

$$\lim_{\epsilon \downarrow 0} \langle f, (H - \lambda - \mathrm{i}\epsilon)^{-1} f \rangle = \lim_{\epsilon \downarrow 0} \int_{\mathbb{R}} (x - \lambda - \mathrm{i}\epsilon)^{-1} d\mu_f(x).$$

The absolutely continuous part of the measure μ_f *is given by*

$$d(\mu_f)_{\text{ac}}(x) = \pi^{-1} \lim_{\epsilon \downarrow 0} \operatorname{Im} \langle f, (H - \lambda - \mathrm{i}\epsilon)^{-1} f \rangle dx = \lim_{\epsilon \downarrow 0} \frac{\epsilon}{\pi} \int_{\mathbb{R}} \frac{1}{(x-\lambda)^2 + \epsilon^2} d\mu_f(x).$$

As for the singular part of the measure, $(\mu_f)_{\text{sc}} + (\mu_f)_{\text{pp}}$, *it is concentrated on the set*

$$\big\{\lambda \in \mathbb{R} : \lim_{\epsilon \downarrow 0} \operatorname{Im} \langle f, (H - \lambda - \mathrm{i}\epsilon)^{-1} f \rangle = +\infty \big\}.$$

This is yet another powerful way of characterizing the absolutely continuous and singular parts of the spectrum. One of the aims of this thesis is to prove the absence of singularly continuous spectrum for some discrete Schrödinger operators. The estimate that really underlies our approach is the following. It is a direct consequence of the above Theorem:

Corollary 1.9. *Let* $(\lambda_1, \lambda_2) \subset \mathbb{R}$ *be an open interval, and let* $f \in \mathcal{H}$. *If*

$$\sup_{\epsilon > 0} \sup_{\lambda \in (\lambda_1, \lambda_2)} \big| \operatorname{Im} \langle f, (H - \lambda - \mathrm{i}\epsilon)^{-1} f \rangle \big| \leqslant c(f) < +\infty, \tag{9}$$

then the spectral measure $\Sigma \mapsto \langle f, E_\Sigma(H) f \rangle$ *is purely absolutely continuous with respect to the Lebesgue measure on* (λ_1, λ_2).

A resolvent estimate like (9) is often called a limiting absorption principle (LAP) for H.

2 Positive Commutator Techniques

Given two observables A and B on a Hilbert space $\mathcal{H}$, their commutator is defined to be the operator $[A, B] := AB - BA$. Rigorous domain considerations will be specified later. Commutators arise naturally in quantum mechanics and play a central role. As a matter of fact, the Heisenberg picture is formulated in terms of a commutator:

$$\frac{d}{dt}A(t) = \mathrm{i}[H, A(t)] + \left(\frac{\partial A}{\partial t}\right)_H.$$

Here H is the Hamiltonian of the system and $A(t)$ is an observable. Commutators also appear in the formulation of the uncertainty principle:

$$\sigma_A \sigma_B \geqslant \frac{1}{2}\left|\langle [A, B]\rangle\right|.$$

Here σ_A and σ_B are the standard deviations for observables A and B. This inequality gives a fundamental limit to the precision with which the expectation values of A and B can be known simultaneously for a given state.

It turns out that commutator techniques give insight into the spectral decomposition of a system. In the mathematical physics community, a first result in this direction was obtained by Putnam in [P].

Proposition 2.1. *Let $H \in \mathcal{B}(\mathcal{H})$ be a self-adjoint operator. If there are $A, C \in \mathcal{B}(\mathcal{H})$, with A self-adjoint and C injective such that $[H, \mathrm{i}A] = C^*C$, then for all $f \in \mathcal{D}((C^*)^{-1})$,*

$$\sup_{\epsilon > 0} \sup_{\lambda \in \mathbb{R}} \left|\mathrm{Im}\langle f, (H - \lambda - \mathrm{i}\epsilon)^{-1} f\rangle\right| \leqslant 4\|A\| \cdot \|(C^*)^{-1} f\|^2 = c(f) < +\infty.$$

In particular the spectrum of H is purely absolutely continuous.

This Proposition establishes a clear link between the commutator and the LAP (boundary values of the resolvent), which is so valuable to characterize the spectral decomposition, as seen in the previous section. The problem with this result however is that practical applications are limited, partly because the result does not allow H to have eigenvalues, partly because many important Hamiltonians H are unbounded, and partly because A is typically unbounded, see e.g. [Go, Proposition 3.2.1].

2.1 Commutators as derivatives: regularity

We work in an abstract and more general setting. Consider two self-adjoint (possibly unbounded) operators T and A acting in some complex separable Hilbert space $\mathcal{H}$. The goal is to study the spectral properties of T with A as auxiliary. We define the commutator of T and A in the form version:

$$\langle f, [T, A]g\rangle := \langle Tf, Ag\rangle - \langle Af, Tg\rangle.$$

This definition makes sense provided $f, g \in \mathcal{D}(T) \cap \mathcal{D}(A)$. Typically we wish the r.h.s. extends to a closed operator. For instance, if $\mathcal{D}(T) \cap \mathcal{D}(A)$ is dense in $\mathcal{D}(T)$ and if there is $c > 0$ such that for all $f, g \in \mathcal{D}(T) \cap \mathcal{D}(A)$,

$$\langle f, [T, A]g\rangle \leqslant c\|(T + \mathrm{i})f\| \cdot \|(T + \mathrm{i})g\|,$$

then by the Riesz lemma the closure of $[T, A]$ belongs to $\mathcal{B}(\mathcal{D}(T), \mathcal{D}(T)^*)$. In any case, the closure is denoted $[T, A]_\circ$. In principle, two levels of assumptions are expected:

1. the first commutator of T with A, $[T, A]_\circ$, belongs to $\mathcal{B}(\mathcal{D}(T), \mathcal{D}(T)^*)$.

2. the second commutator of T with A, $[[T, A]_\circ, A]_\circ$, belongs to $\mathcal{B}(\mathcal{D}(T), \mathcal{D}(T)^*)$.

Looking back with more than thirty years of Mourre theory, one can say that assumption (1) is minimal, whereas (2) is plentiful. A lot of the work in abstract Mourre theory has been to formulate refined assumptions that fit somewhere in between these two. This will be explained in greater detail in Section 2.3.

Let us get into the rigorous details of regularity. Consider the map

$$\mathbb{R} \ni t \mapsto e^{\mathrm{i}tA}(T + \mathrm{i})^{-1}e^{-\mathrm{i}tA} \in \mathcal{B}(\mathcal{H}). \tag{10}$$

If this map is of class $\mathcal{C}^k(\mathbb{R})$ for some $k \in \mathbb{N}$, with $\mathcal{B}(\mathcal{H})$ endowed with the strong operator topology, then we say that $T \in \mathcal{C}^k(A)$. If $T \in \mathcal{C}^1(A)$, then the derivative of the map (10) at $t = 0$ is denoted by $[T, \mathrm{i}A]_\circ$ and belongs to $\mathcal{B}(\mathcal{H})$. If however we endow $\mathcal{B}(\mathcal{H})$ with the operator norm topology, then we say that $T \in \mathcal{C}^{k,\mathrm{u}}(A)$. Finally, we say that $T \in \mathcal{C}^{1,1}(A)$ if

$$\int_0^1 \left\| \left[[(T + \mathrm{i})^{-1}, e^{\mathrm{i}tA}]_\circ, e^{\mathrm{i}tA} \right]_\circ \right\| t^{-2} dt < +\infty.$$

It turns out that

$$... \subset \mathcal{C}^3(A) \subset \mathcal{C}^2(A) \subset \mathcal{C}^{1,1}(A) \subset \mathcal{C}^{1,\mathrm{u}}(A) \subset \mathcal{C}^1(A). \tag{11}$$

We note that if $T \in \mathcal{C}^1(A)$ then (1) holds; whereas if $T \in \mathcal{C}^2(A)$ then (2) holds. A good part of this thesis deals with bounded T; in this case we may simply take T instead of $(T + \mathrm{i})^{-1}$ in the above definitions. Importantly, for $T \in \mathcal{B}(\mathcal{H})$, there is a simpler criterion to verify the $\mathcal{C}^1(A)$ regularity, see [ABG, Lemma 6.2.9] and [ABG, Theorem 6.2.10].

Let us take a moment to explain how these abstract definitions relate to the concrete problems of Schrödinger operators.

Example 2.2 (Continuous Schrödinger operators)**.** *Let H_0 be the self-adjoint realization of the Laplace operator $-\Delta$ in $L^2(\mathbb{R}^\nu)$. Let Q be the operator of multiplication by $x = (x_1, ..., x_\nu) \in \mathbb{R}^\nu$, and let $P := -\mathrm{i}\nabla$. Set*

$$H := H_0 + V_{\mathrm{sr}}(Q) + V_{\mathrm{lr}}(Q),$$

where $V_{\mathrm{sr}}(x)$ and $V_{\mathrm{lr}}(x)$ are real-valued functions that belong to $L^\infty(\mathbb{R}^\nu)$. Thus $V_{\mathrm{sr}}(Q)$ and $V_{\mathrm{lr}}(Q)$ are bounded self-adjoint operators on $L^2(\mathbb{R}^\nu)$ and they are respectively the short- and long-range perturbations. Thus H is a self-adjoint operator. For the long-range perturbation, further assume that $x \cdot \nabla V_{\mathrm{lr}}(x)$ is a well-defined function. Suppose that $\lim V_{\mathrm{sr}}(x) = \lim V_{\mathrm{lr}}(x) = 0$ as $\|x\| \to +\infty$. Thus $V_{\mathrm{sr}}(Q) + V_{\mathrm{lr}}(Q)$ is a H_0-form relatively compact operator. In particular, $\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ess}}(H_0) = [0, +\infty)$.

Let

$$A := (Q \cdot P + P \cdot Q)/2. \tag{12}$$

It is self-adjoint and essentially self-adjoint on the Schwartz space $\mathcal{S}(\mathbb{R}^\nu)$. It is called the generator of dilations and is the standard conjugate operator to H. Table 1 displays continuous Schrödinger operators belonging to each of the classes introduced in (11). The idea is clear: stronger decaying bounds on the potential imply stronger regularity.

In addition, if $\langle x\rangle V_{\rm sr}(x)$ and $x\cdot\nabla V_{\rm lr}(x)$ are	Then H belongs to
$L^\infty(\mathbb{R}^\nu)$	$\mathcal{C}^1(A)$
$L^\infty(\mathbb{R}^\nu)$ and $o(1)$	$\mathcal{C}^{1,\rm u}(A)$
$L^\infty(\mathbb{R}^\nu)$ and $o(\langle x\rangle^{-\epsilon})$, for some $\epsilon>0$	$\mathcal{C}^{1,1}(A)$
$L^\infty(\mathbb{R}^\nu)$ and $O(\langle x\rangle^{-1})$	$\mathcal{C}^2(A)$

Table 1: Regularity of Hamiltonian H w.r.t. a bound on the decay of the potential at infinity

The corresponding example for the discrete Schrödinger operators is the following. Note that in this case, short-range potentials are long-range.

Example 2.3 (Discrete Schrödinger operators)**.** *Let $\mathcal{H}=\ell^2(\mathbb{Z}^\nu)$. Let $H_0=\Delta$ be the discrete Schrödinger operator on $\mathbb{Z}^d$ given by (2). Set*

$$H=H_0+V,$$

where $V:\mathbb{Z}^d\to\mathbb{R}$ is a bounded function. Thus V and H are bounded self-adjoint operators on $\mathcal{H}$. Suppose that $\lim V(n)=0$ as $|n|\to+\infty$. Then V is compact and in particular, $\sigma_{\rm ess}(H)=\sigma_{\rm ess}(H_0)=[0,4\nu]$. To define the conjugate operator A, we need some notation. Let $S=(S_1,...,S_\nu)$, where, for $1\leqslant i\leqslant\nu$, S_i is the shift operator given by

$$(S_i\psi)(n):=\psi(n_1,...,n_i-1,...,n_\nu),\quad \textit{for all } n\in\mathbb{Z}^\nu \textit{ and } \psi\in\mathcal{H}.$$

Let $N=(N_1,...,N_\nu)$, where, for $1\leqslant i\leqslant\nu$, N_i is the position operator given by

$$(N_i\psi)(n):=n_i\psi(n),\quad \textit{with domain}\quad \mathcal{D}(N_i):=\Big\{\psi\in\mathcal{H}:\sum_{n\in\mathbb{Z}^\nu}|n_i\psi(n)|^2<+\infty\Big\}.$$

The conjugate operator, denoted by A, is the closure of the following operator

$$A_0:=\frac{\mathrm{i}}{2}\sum_{i=1}^{\nu}(S_i-S_i^*)N_i+N_i(S_i-S_i^*),\quad \textit{with domain}\quad \mathcal{D}(A_0):=\ell_0(\mathbb{Z}^\nu),\tag{13}$$

the sequences with compact support. The operator A is self-adjoint, see [BS] and [GGo]. Let τ_iV be the shifted potential acting as follows:

$$[(\tau_iV)\psi](n):=V(n_1,...,n_i-1,...,n_\nu)\psi(n),\quad \textit{for all } \psi\in\mathcal{H}.$$

Table 3 displays discrete Schrödinger operators belonging to the classes introduced in (11).

We refine the above definitions. Let $\mathcal{G}$ and $\mathcal{H}$ be Hilbert spaces verifying the following continuous and dense embeddings $\mathcal{G}\subset\mathcal{H}=\mathcal{H}^*\subset\mathcal{G}^*$, where we have identified $\mathcal{H}$ with its antidual $\mathcal{H}^*$ by the Riesz isomorphism Theorem. Let A be a self-adjoint operator on $\mathcal{H}$, and suppose that the semi-group $\{e^{\mathrm{i}tA}\}_{t\in\mathbb{R}}$ stabilizes $\mathcal{G}$. Then by duality it stabilizes $\mathcal{G}^*$. Let $T\in\mathcal{B}(\mathcal{G},\mathcal{G}^*)$ be a self-adjoint operator on $\mathcal{H}$ and consider the map

$$\mathbb{R}\ni t\mapsto e^{-\mathrm{i}tA}Te^{\mathrm{i}tA}\in\mathcal{B}(\mathcal{G},\mathcal{G}^*).\tag{14}$$

In addition, if for all $1 \leqslant i \leqslant \nu$, $n_i(V - \tau_i V)(n)$ is	Then H belongs to
$O(1)$	$\mathcal{C}^1(A)$
$o(1)$	$\mathcal{C}^{1,\mathrm{u}}(A)$
$o(\langle n \rangle^{-\epsilon})$ for some $\epsilon > 0$	$\mathcal{C}^{1,1}(A)$
$o(\langle n \rangle^{-1})$	$\mathcal{C}^2(A)$

Table 2: Regularity of Hamiltonian H w.r.t. a bound on the decay of the potential at infinity

If this map is of class $\mathcal{C}^k(\mathbb{R}; \mathcal{B}(\mathcal{G}, \mathcal{G}^*))$, with $\mathcal{B}(\mathcal{G}, \mathcal{G}^*)$ endowed with the strong operator topology, we say that $T \in \mathcal{C}^k(A; \mathcal{G}, \mathcal{G}^*)$; whereas if the map is of class $\mathcal{C}^k(\mathbb{R}; \mathcal{B}(\mathcal{G}, \mathcal{G}^*))$, with $\mathcal{B}(\mathcal{G}, \mathcal{G}^*)$ endowed with the norm operator topology, we say that $T \in \mathcal{C}^{k,\mathrm{u}}(A; \mathcal{G}, \mathcal{G}^*)$. If $T \in \mathcal{C}^1(A; \mathcal{G}, \mathcal{G}^*)$, then the derivative of map (14) at $t = 0$ is denoted by $[T, \mathrm{i}A]_\circ$ and belongs to $\mathcal{B}(\mathcal{G}, \mathcal{G}^*)$. Moreover, by [ABG, Proposition 5.1.6], for all $\sharp \in \{k; k,\mathrm{u}\}$, $T \in \mathcal{C}^\sharp(A; \mathcal{G}, \mathcal{G}^*)$ if and only if $(T + \mathrm{i})^{-1} \in \mathcal{C}^\sharp(A; \mathcal{G}^*, \mathcal{G})$. This notably implies that $\mathcal{C}^\sharp(A; \mathcal{G}, \mathcal{G}^*) \subset \mathcal{C}^\sharp(A)$.

To finish this Section, we recall one very useful result for unbounded T :

Proposition 2.4. *[ABG, p. 258] Let T and A be self-adjoint operators in a Hilbert space $\mathcal{H}$ and denote $\mathcal{H}^1 := \mathcal{D}(\langle T \rangle^{1/2})$, the form domain of T, and $\mathcal{H}^{-1} := (\mathcal{H}^1)^*$. Suppose that $e^{\mathrm{i}tA}\mathcal{H}^1 \subset \mathcal{H}^1$. Then the following are equivalent:*

1. *$T \in \mathcal{C}^1(A; \mathcal{H}^1, \mathcal{H}^{-1})$*
2. *The form $[T, \mathrm{i}A]$ defined on $\mathcal{D}(T) \cap \mathcal{D}(A)$ extends to an operator in $\mathcal{B}(\mathcal{H}^1, \mathcal{H}^{-1})$.*

Remark 2.1. *The form $[T, \mathrm{i}A]$ is defined for $\psi, \phi \in \mathcal{D}(T) \cap \mathcal{D}(A)$ as follows :*

$$\langle \psi, [T, \mathrm{i}A]\phi \rangle := \langle T^*\psi, \mathrm{i}A\phi \rangle - \langle A^*\psi, \mathrm{i}T\phi \rangle = \langle T\psi, \mathrm{i}A\phi \rangle - \langle A\psi, \mathrm{i}T\phi \rangle.$$

The last equality holds because T and A are assumed to be self-adjoint.

2.2 Localizing commutators in energy: Mourre's estimate

In the beginning of the eighties, E. Mourre realized that localizing $[H, \mathrm{i}A]$ in energy would generalize the idea of Putnam to unbounded operators, see Proposition 2.1. In the seminal paper [M], the absence of singularly continuous spectrum was proved for 3-body Schrödinger operators with the help of positive commutators methods and their scattering properties were studied. The results were generalized to the N-body case in [PSS]. Today, Mourre's commutator theory is a fundamental tool to study the stationary scattering theory of general self-adjoint operators. An excellent and thorough work in this field is [ABG].

Let H and A be self-adjoint operators in a Hilbert space $\mathcal{H}$. Suppose that $H \in \mathcal{C}^1(A)$. We say that the *Mourre estimate* holds for H with respect to A on a bounded interval $\mathcal{I} \subset \mathbb{R}$ if there is $c > 0$ and a compact operator K such that

$$E_\mathcal{I}(H)[H, \mathrm{i}A]_\circ E_\mathcal{I}(H) \geqslant cE_\mathcal{I}(H) + K, \tag{15}$$

in the form sense on $\mathcal{H} \times \mathcal{H}$. Since $E_\mathcal{I}(H)$ belongs to $\mathcal{B}(\mathcal{H}, \mathcal{D}(\mathcal{H}))$, it also belongs to $\mathcal{B}(\mathcal{D}(\mathcal{H})^*, \mathcal{H})$ by duality, and so we see that the $\mathcal{C}^1(A)$ hypothesis ensures that the l.h.s. of (15) is a bounded operator.

If the Mourre estimate holds over some interval $\mathcal{I}$ with $K = 0$, then we say that the estimate is *strict*, in which case it can be shown that H has no eigenvalues in the interval $\mathcal{I}$. This is a consequence of the Virial Theorem, see [ABG, Proposition 7.2.10]. If the Mourre estimate holds on $\mathcal{I}$, but is not strict, then the best we can say is that the number of eigenvalues of H in $\mathcal{I}$ is finite, including multiplicities, see [ABG, Corollary 7.2.11]. This is still good enough to conclude that for every $\lambda \in \mathcal{I}$ that is not an eigenvalue of $\mathcal{H}$, there is an interval $\mathcal{I}_\lambda$ containing λ (perhaps much smaller than $\mathcal{I}$) such that the strict Mourre estimate holds for H on $\mathcal{I}_\lambda$. This is because $\|E_{\mathcal{I}'}(H)KE_{\mathcal{I}'}(H)\| \to 0$ as $|\mathcal{I}'| \to 0$ for all $\mathcal{I}'$ void of eigenvalues. So when we localize in energy away from eigenvalues, we may assume without loss of generality that a strict Mourre estimate holds.

To distinguish between the strict and non strict Mourre estimates, we introduce notation.

Definition 2.5 (The sets $\mu^A(T)$ and $\tilde{\mu}^A(T)$)**.** *For a self-adjoint operator T acting on $\mathcal{H}$, let $\mu^A(T)$ be the set of reals for which there is neighborhood where the strict Mourre estimate holds for T with respect to A. Let $\tilde{\mu}^A(T)$ be the set of reals for which there is neighborhood where the Mourre estimate holds for T with respect to A.*

Let us examine the Mourre estimate for our two ongoing examples.

Example 2.6 (Continuous Schrödinger operators)**.** *Let $\mathcal{H}^2(\mathbb{R}^\nu)$ be the Sobolev space corresponding to the domain of the self-adjoint realization H_0 of the Laplacian $-\Delta$, and $\mathcal{H}^1 = \mathcal{H}^1(\mathbb{R}^\nu)$ its form domain. Let $A := (Q \cdot P + P \cdot Q)/2$ be the generator of dilations. The relation*

$$(e^{\mathrm{i}tA}\psi)(x) = e^{t\nu/2}\psi(e^t x), \quad \text{for all } \psi \in L^2(\mathbb{R}^\nu),\ x \in \mathbb{R}^\nu,\ t \in \mathbb{R},$$

implies that $\{e^{\mathrm{i}tA}\}_{t\in\mathbb{R}}$ stabilizes $\mathcal{H}^2(\mathbb{R}^\nu)$, and thus $\mathcal{H}^\theta(\mathbb{R}^\nu)$ for all $\theta \in [-2, 2]$ by duality and interpolation. A straightforward computation gives

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

in the sense of operators in $\mathcal{B}(\mathcal{H}^1, \mathcal{H}^{-1})$, thereby implying that $H_0 \in \mathcal{C}^1(A; \mathcal{H}^1, \mathcal{H}^{-1})$ by Proposition 2.4. An easy induction yields $H_0 \in \mathcal{C}^k(A; \mathcal{H}^1, \mathcal{H}^{-1})$ for all $k \in \mathbb{N}$. The strict Mourre estimate therefore holds for H_0 with respect to A on all intervals $\mathcal{I}$ verifying $\overline{\mathcal{I}} \subset (0, +\infty)$. In particular, $\mu^A(H_0) = (0, +\infty)$.

Example 2.7 (Discrete Schrödinger operators)**.** *Let $\mathcal{H} = \ell^2(\mathbb{Z}^\nu)$, and $H_0 = \Delta$, the discrete Schrödinger operator. A calculation shows that*

$$[H_0, \mathrm{i}A]_\circ = \sum_{i=1}^{\nu} \Delta_i(4 - \Delta_i) \tag{16}$$

as operators in $\mathcal{B}(\mathcal{H})$. Here $\Delta_i := 2 - S_i - S_i^*$. In particular, $H_0 \in \mathcal{C}^1(A)$. An easy induction shows that $H_0 \in \mathcal{C}^k(A)$ for all $k \in \mathbb{N}$. In dimension one, we see that $\mu^A(H_0) = (0, 4)$ because the function $x \mapsto x(4 - x)$ is strictly positive above $(0, 4)$. In higher dimensions, we have, by (16) and [ABG, Theorem 8.3.6] that

$$\mu^A(H_0) = [0, 4\nu] \setminus \{4k : k = 0, ..., \nu\}. \tag{17}$$

In the previous examples, we explained the Mourre estimate for the free operator H_0. If we want to consider a potential in addition, then we have a general result, the proof of which follows from the definitions. For a self-adjoint operator H, let $\mathcal{H}^1$ denote its form domain.

Proposition 2.8. *Let $V \in \mathcal{K}(\mathcal{H}^1, \mathcal{H}^{-1}) \cap \mathcal{C}^{1,\mathrm{u}}(A; \mathcal{H}^1, \mathcal{H}^{-1})$. Then $[V, \mathrm{i}A]_\circ \in \mathcal{K}(\mathcal{H}^1, \mathcal{H}^{-1})$.*

We can immediately apply this result.

Example 2.9 (Continuous Schrödinger operators)**.** *Let $H = -\Delta + V_{\mathrm{sr}}(Q) + V_{\mathrm{lr}}(Q)$, with both components of the potential being bounded real-valued functions. Suppose that $|V_{\mathrm{sr}}(x)| \to 0$ and $|V_{\mathrm{lr}}(x)| \to 0$ as $\|x\| \to +\infty$, so that the potential is H_0-form relatively compact. If also $x \cdot \nabla V_{\mathrm{lr}}(x) \in L^\infty(\mathbb{R}^\nu)$, $\langle x \rangle V_{\mathrm{sr}}(x) \to 0$ and $x \cdot \nabla V_{\mathrm{lr}}(x) \to 0$ as $\|x\| \to +\infty$, then the Mourre estimate holds for H on every bounded interval $\mathcal{I}$ with $\overline{\mathcal{I}} \subset (0, +\infty)$.*

Example 2.10 (Discrete Schrödinger operators)**.** *Let $H = \Delta + V$, where V is a bounded real-valued potential. If $V(n) \to 0$ as $\|n\| \to +\infty$, then $V \in \mathcal{K}(\mathcal{H})$. If for all $1 \leqslant i \leqslant \nu$, $n_i(V - \tau_i V)(n) \to 0$ as $\|n\| \to +\infty$, then the Mourre estimate holds for H on every bounded interval $\mathcal{I}$ with $\overline{\mathcal{I}} \subset [0, 4\nu] \setminus \{4k : k = 0, ..., \nu\}$.*

If the potential does not belong the $\mathcal{C}^{1,\mathrm{u}}(A)$ class, then the Mourre estimate may still hold, but it becomes a case by case analysis. We have examples of this for the discrete Schrödinger operators:

Example 2.11 (Discrete Wigner-von Neumann operator 1)**.** *Let $\mathcal{H} = \ell^2(\mathbb{Z}^\nu)$. Let $q \in \mathbb{R}$ and $k \in (0, \pi) \cup (\pi, 2\pi)$. Let W be a Wigner-von Neumann potential defined by*

$$(Wu)(n) := \frac{q \sin(k(n_1 + ... + n_d))}{|n|} u(n), \quad \textit{for all } n \in \mathbb{Z}^\nu \textit{ and } u \in \mathcal{H}. \tag{18}$$

Note that $W \in \mathcal{K}(\mathcal{H}) \cap \mathcal{C}^1(A)$. Consider also a $V \in \mathcal{K}(\mathcal{H}) \cap \mathcal{C}^{1,\mathrm{u}}(A)$, and let $H := \Delta + W + V$. We define the sets

$$m(H) := \begin{cases} (0, 4) \setminus \{E_\pm(k)\} & \textit{for } \nu = 1, \\ (0, E(k)) \cup (4\nu - E(k), 4\nu) & \textit{for } \nu \geqslant 2, \end{cases} \tag{19}$$

where

$$E_\pm(k) := 2 \pm 2\cos(k/2) \quad \textit{and} \quad E(k) := \begin{cases} 4 - 4\cos(k/2) & \textit{for } k \in (0, \pi) \\ 4 + 4\cos(k/2) & \textit{for } k \in (\pi, 2\pi). \end{cases}$$

Then it is proved in [Ma1, Propositions 3.5 and 4.5] that $m(H) \subset \tilde{\mu}^A(H)$.

Example 2.12 (Discrete Wigner-von Neumann operator 2)**.** *Let $\mathcal{H} = \ell^2(\mathbb{Z}^\nu)$. Let $q = (q_i)_{i=1}^\nu \in \mathbb{R}^\nu$ and $k = (k_i)_{i=1}^\nu \in ((0, \pi) \cup (\pi, 2\pi))^\nu$. Consider this variant of the Wigner-von Neumann potential:*

$$(W'u)(n) := \left(\prod_{i=1}^{\nu} \frac{q_i \sin(k_i n_i)}{n_i} \right) u(n), \quad \textit{for all } n \in \mathbb{Z}^\nu \textit{ and } u \in \mathcal{H}. \tag{20}$$

Note that $W' \in \mathcal{K}(\mathcal{H}) \cap \mathcal{C}^1(A)$. Consider also a $V \in \mathcal{K}(\mathcal{H}) \cap \mathcal{C}^{1,\mathrm{u}}(A)$, and let $H' := \Delta + W' + V$. We define the sets

$$m(H') := \begin{cases} (0,4) \setminus \{E_\pm(k)\} & \text{for } \nu = 1, \\ (0, E'(k)) \cup (4\nu - E'(k), 4\nu) & \text{for } \nu \geqslant 2, \end{cases} \tag{21}$$

where $E_\pm(k)$ are as in the previous example, and $E'(k) := \min\{\ell(k_i) : 1 \leqslant i \leqslant \nu\}$, with

$$\ell(k_i) := \begin{cases} 2 - 2\cos(k_i/2), & k_i \in (0, 2\pi/3] \\ 2 + 2\cos(k_i), & k_i \in (2\pi/3, \pi) \cup (\pi, 4\pi/3] \\ 2 + 2\cos(k_i/2), & k_i \in (4\pi/3, 2\pi). \end{cases}$$

Then it is proved in [Ma1, Propositions 3.5 and 4.6] that $m(H') \subset \tilde{\mu}^A(H')$.

Remark 2.2. *It is proved in [Ma1, Propositions 3.3 and 4.2] that W and W' of the previous two examples do not belong to $\mathcal{C}^{1,\mathrm{u}}(A)$.*

At this point, one may wonder what the Mourre estimate is good for. In the next section, we shall see that it plays a key role in proving the absence of singularly continuous spectrum with the method of commutators.

2.3 Mourre theory: absence of singularly continuous spectrum

There is a simple argument using only the $\mathcal{C}^1(A)$ hypothesis and the Mourre estimate that shows that the time expectation value of A basically grows linearly with time. Precisely, let us suppose that the strict Mourre estimate holds for H on the bounded interval $\mathcal{I}$. If $f = \varphi(H)g$ is a unit vector with $g \in \mathcal{D}(A)$ and $\varphi \in \mathcal{C}_c^\infty(\mathcal{I})$, then there are $c, C > 0$ such that

$$ct \leqslant \langle e^{-\mathrm{i}tH} f, A e^{-\mathrm{i}tH} f \rangle - \langle f, Af \rangle \leqslant Ct, \quad \text{for all } t \geqslant 0.$$

This argument is detailed for instance in [GM, Appendix A]. This means that the transport of the particle is ballistic with respect to A. From a dynamical point of view, this behavior suggests purely absolutely continuous spectrum. In [M], using a method of differential inequalities and assuming the strict Mourre estimate for H on the interval $\mathcal{I}$ together with a second-commutator hypothesis, $H \in \mathcal{C}^2(A)$ in the setting of [ABG], the author proves a limiting absorption principle (LAP) on any compact sub-interval $\mathcal{I}'$ of $\mathcal{I}$:

$$\sup_{\lambda \in \mathcal{I}', \epsilon > 0} \| \langle A \rangle^{-s} (H - \lambda - \mathrm{i}\epsilon)^{-1} \langle A \rangle^{-s} \| < +\infty, \tag{22}$$

for all $s > 1/2$. Here $\langle A \rangle := \sqrt{1 + A^2}$. This yields the following Kato-type propagation estimate:

$$\sup_{\substack{\psi \in \mathcal{H} \\ \|\psi\| \leqslant 1}} \int_{-\infty}^{+\infty} \| \langle A \rangle^{-s} e^{-\mathrm{i}tH} E_{\mathcal{I}'}(H) \psi \|^2 dt < +\infty, \tag{23}$$

which in turn implies the absence of singularly continuous spectrum on $\mathcal{I}'$, e.g. [RS4, Section XIII.7]. The main improvement of this result is done in [ABG]. The same LAP is derived assuming only $H \in \mathcal{C}^{1,1}(A)$ and the Mourre estimate. It is further shown that this class is optimal in the general abstract framework. Indeed, in [ABG, Appendix 7.B], there is an example of $H \in \mathcal{C}^{1,\mathrm{u}}(A)$ for which no LAP holds.

The aim of Mourre theory can therefore be summarized as follows: Prove a resolvent estimate (LAP) for H over some interval $\mathcal{I}$, which in turn yields robust dynamical properties for H at these energies (propagation estimates), as well as the the absence of singularly continuous spectrum for H on $\mathcal{I}$.

Moving forward, it is relevant to restrict our attention to H belonging to a class somewhere between $\mathcal{C}^{1,1}(A)$ and $\mathcal{C}^{1}(A)$. Natural questions that arise are the following:

1. Are there propagation estimates, like (23) for instance, that hold?
2. Is the absence of singularly continuous spectrum of H still valid?
3. What more about the point spectrum of H can be said?

These questions are all the more justified given the following known results concerning continuous Schrödinger operators. When $\nu = 1$, Kiselev proved in [Ki] that the continuous Schrödinger operator $H = -\Delta + V$ on $\mathbb{R}$ has no singularly continuous spectrum whenever $V = O(|x|^{-1})$. The decay assumption is optimal, since it is further proved that for any positive function h which grows to infinity, there is a potential V such that $V = O(h(|x|)|x|^{-1})$ and $H = -\Delta + V$ has some singularly continuous spectrum. Naboko [Nab] and Simon [Si] have also shown, that for this same function h, one can also construct a potential V such that $V = O(h(|x|)|x|^{-1})$ as well and $H = -\Delta + V$ has dense point spectrum. In ν dimensions, if $V(x) = V_1(x) + V_2(x)$ where $|x||V_1(x)| \to 0$ and $|(x \cdot \nabla)V_2(x)| \to 0$ as $|x| \to +\infty$, then $-\Delta + V$ has no eigenvalues in $[0, +\infty)$. This was proved by Kato [Ka] when $V_2 = 0$, and the full result is attributed to Agmon [A] and Simon [Si2], but we refer also to [FH] and [CFKS, Section 4.4].

Finally, we underline that the LAP has been derived for several specific systems where the Hamiltonian H belongs to a regularity class as low as $\mathcal{C}^1(A)$, and sometimes even lower (see for example [DMR], [GJ2], [JM] and [Ma1] to name a few). In all these cases, a strong propagation estimate of type (23) and absence of singularly continuous spectrum hold.

3 LAP for the discrete Wigner-von Neumann operator

We present the results of [Ma1]. A LAP for the discrete Wigner-von Neumann operators presented in Examples 2.11 and 2.12 is proved. We recall that $H = \Delta + W + V$ and $H = \Delta + W + V$, where W and W' are some Wigner-von Neumann type potentials and V is a long-range perturbation. However, slightly stronger conditions on the additional perturbation $V \in \mathcal{K}(\mathcal{H}) \cap \mathcal{C}^{1,\mathrm{u}}(A)$ are required here. Specifically, we suppose that there is $\rho > 0$ such that

$$\langle n \rangle^{\rho} |V(n)| = O(1), \tag{24}$$

$$\langle n \rangle^{\rho} |n_i| |(V - \tau_i V)(n)| = O(1), \quad \text{for all } 1 \leqslant i \leqslant \nu. \tag{25}$$

Recall that $m(H)$ and $m(H')$ are given by (19) and (21) respectively. Let $P_{\mathrm{pp}}(H)$ and $P_{\mathrm{c}}(H)$ respectively denote the spectral projectors onto the pure point subspace of H and its complement. We prove:

Theorem 3.1. *We have that $m(H) \subset \tilde{\mu}^A(H)$. For all $E \in m(H)$ there is an open interval $\mathcal{I}$ containing E such that for all $s > 1/2$ and all compact intervals $\mathcal{I}' \subset \mathcal{I}$, the reduced LAP for H holds with respect to $(\mathcal{I}', s, A)$, that is,*

$$\sup_{x \in \mathcal{I}', y \neq 0} \| \langle A \rangle^{-s} (H - x - \mathrm{i}y)^{-1} P_{\mathrm{c}}(H) \langle A \rangle^{-s} \| < +\infty. \tag{26}$$

Notably, the spectrum of H is purely absolutely continuous on Σ' when $P_{\mathrm{pp}}(H) = 0$ on $\mathcal{I}'$.

This is actually a slightly improved version of the original result of [Ma1]. The improvement relies on [Ma2, Theorem 1.5], which allows to remove the abstract assumption $\ker(H - E) \subset \mathcal{D}(A)$ that appears in [Ma1, Theorem 1.1]. The corresponding result also holds for H'.

The proof follows the approach of [GJ2], where the corresponding LAP is proved in the continuous operator case. The LAP for the continuous Wigner-von Neumann operator had been proved previously in [DMR], but using different techniques and did not include the long-range perturbation V.

The Wigner-von Neumann operator has two interesting aspects. First, when the long-range perturbation V is chosen suitably, the Schrödinger operator H has an eigenvalue embedded in its absolutely continuous spectrum, see [RS4, Section XIII.13, Example 1] and [Ma2, Proposition 1.6]. Second, the regularity of the Wigner-von Neumann potential is only $\mathcal{C}^1(A)$, and yet we are able to get a Mourre estimate and a LAP using commutator methods. Without a doubt, the oscillations of the potential play a key role in this. With regard to second point, we mention that at the heart of the proof of the LAP (26) is a *weighted Mourre estimate*. This idea originates from Gérard's proof of the abstract LAP using energy estimates [G]. In [GJ2] and our proof, this weighted Mourre estimate is the starting point of the proof, rather than an intermediary estimate. This allows to overcome the low regularity of H. However, and unfortunately, the LAP (26) does not come with any information about the continuity of the boundary values, as it is the case when the operator is of class $\mathcal{C}^{1,1}(A)$. This is because we use an approach to Mourre theory that proves the LAP by contradiction, see [GJ1].

4 The Mourre estimate and decay of eigenfunctions

This topic deals with the link between the point spectrum of the discrete Schrödinger operator $H = \Delta + V$ and the Mourre estimate. The method we use is entirely based on ideas of Froese and Herbst in [FH]. They essentially show that under a first commutator hypothesis, $V \in \mathcal{C}^1(A)$ in the setting of [ABG], if ψ is an eigenfunction of the continuous Schrödinger operator $H = -\Delta + V$ with eigenvalue E, then $\exp(\alpha \|x\|)\psi \in L^2(\mathbb{R}^\nu)$ for all $\alpha \in [0, \sqrt{\tau - E})$, where τ is the nearest *threshold* above E. By a threshold, we mean a real for which the Mourre estimate does not hold over any interval containing this value. A consequence is that if V has slightly better decay, for instance $|(x \cdot \nabla)V(x)| \to 0$, then H does not have any positive eigenvalues, see e.g. [CFKS, Theorem 4.19].

We now present the results of [Ma2]. Let $\mathcal{H} = \ell^2(\mathbb{Z}^\nu)$. Let $V : \mathbb{Z}^\nu \mapsto \mathbb{R}$ be a bounded function. Let us identify two hypotheses that will be needed:
Hypothesis 1: The potential V satisfies

$$|n_i(V - \tau_i V)(n)| = O(1), \quad \text{for all } 1 \leqslant i \leqslant \nu. \tag{27}$$

Hypothesis 2: V is compact, i.e.

$$V(n) \to 0, \quad \text{as } |n| \to +\infty. \tag{28}$$

Note that the first hypothesis sets us right in the $\mathcal{C}^1(A)$ class. The best result we have is in one dimension:

Theorem 4.1. *Assume Hypotheses 1 and 2, and $\nu = 1$. If $H\psi = E\psi$ with $\psi \in \mathcal{H}$, then if*

$$\theta_E := \begin{cases} \sup\left\{2 + (E-2)/\cosh\alpha : \alpha \geqslant 0 \text{ and } \exp(\alpha|n|)\psi \in \mathcal{H}\right\}, & \text{for } E < 2 \\ \inf\left\{2 + (E-2)/\cosh\alpha : \alpha \geqslant 0 \text{ and } \exp(\alpha|n|)\psi \in \mathcal{H}\right\}, & \text{for } E > 2, \end{cases}$$

one has that either $\theta_E \in \mathbb{R} \setminus \tilde{\mu}^A(H)$ or $\theta_E = 2$. If $E = 2$, the statement is that either $\exp(\alpha|n|)\psi \in \mathcal{H}$ for all $\alpha \geqslant 0$ or $2 \in \mathbb{R} \setminus \tilde{\mu}^A(H)$. Moreover, if $\exp(\alpha|n|)\psi \in \mathcal{H}$ for all $\alpha \geqslant 0$, then $\psi = 0$.

So if E is both an eigenvalue and a threshold, this result does not provide any information. However, if E is an eigenvalue but not a threshold, the corresponding eigenfunction decays at a rate at least of $\cosh^{-1}\left((E-2)/(\theta_E - 2)\right)$. As in the continuous operator setting, we deduce the absence of eigenvalues:

Theorem 4.2. *Let $\nu = 1$. Suppose that V satisfies $\lim_{|n|\to+\infty} |n||V(n) - V(n-1)| = 0$ and $\lim_{|n|\to+\infty} |V(n)| = 0$. Then $H := \Delta + V$ has no eigenvalues in $(0, 4)$.*

At this point, we recall Remling's optimal result [R], that if $\lim_{|n|\to+\infty} |n||V(n)| = 0$, then the spectrum of the one-dimensional discrete operator $\Delta + V$ is purely absolutely continuous on $(0, 4)$. Of course, Remling's result is stronger than that of Theorem 4.2, but the assumptions are also stronger.

In the multi-dimensional discrete operator case, we prove:

Theorem 4.3. *Let $\nu \geqslant 1$. Suppose that Hypothesis 1 holds for the potential V. If $H\psi = E\psi$ with $\psi \in \mathcal{H}$ and $E \in \tilde{\mu}^A(H)$, then $\exp(\alpha(1 + |n|^2)^{\gamma/2})\psi \in \mathcal{H}$ for all $(\alpha, \gamma) \in [0, \infty) \times [0, 2/3)$.*

Although Theorem 4.3 does not yield exponential decay of eigenfunctions at non-threshold energies as in the continuous operator case, the result is still useful for applications in Mourre theory. Let us note that in a general abstract framework, it is proved in [FMS] that if the second commutator of H and A exists and other domain conditions hold, then $\psi \in \mathcal{D}(A)$. This general result is optimal and improves that of [Ca] and [CGH]. Here, we see that for the discrete Schrödinger operators, minimal hypotheses yield much stronger results.

It appears that the method of Froese and Herbst adapts quite well for the one-dimensional discrete operator; however, there seems to be a non-trivial difference between the dimensions $\nu \geqslant 2$ and $\nu = 1$ in the discrete setting as far as the method is concerned. The exponential decay of eigenfunctions at non-threshold energies in higher dimensions therefore remains an open question because our proof does not attain it. Yet an indication it may occur comes from the Combes-Thomas method, see [Ma2, Theorem 1.1] and references therein. The latter method proves the exponential decay of eigenfunctions corresponding to eigenvalues outside the essential spectrum of H.

On the one hand, if E belongs to the discrete spectrum of H, then for any interval Σ containing E and located outside the essential spectrum of H, $E_\Sigma(H)$ is simply a finite rank eigenprojection and so the Mourre estimate holds by default, both sides of (15) being compact operators. So under Hypothesis 1 only, the corresponding eigenfunction decays sub-exponentially according to Theorem 4.3. In this case, the Combes-Thomas method is clearly superior. On the other hand, the Mourre estimate typically holds above the essential spectrum of H. So Theorem 4.3 is able to characterize the decay of eigenfunctions for non-threshold eigenvalues embedded in the essential spectrum, if *any* exist. We emphasize the last point, because to our knowledge there is no example of a Schrödinger operator with a non-threshold embedded eigenvalue. What is certainly known however is the existence of operators with a threshold embedded eigenvalue, the Wigner-von Neumann operator being the classical illustration of it, as discussed in the previous Section.

We give two applications of Theorem 4.3. First, it can be used to show that an eigenvalue embedded in the essential spectrum of H is a threshold. An example of this is depicted in [Ma2, Proposition 1.6]. It is interesting to note that in this example the eigenfunction does not belong to the domain of A. The second application consists in improving [Ma1, Theorem 1.1] and [GM, Theorem 4.4] by suppressing the abstract condition $\ker(H-E) \subset \mathcal{D}(A)$.

5 Propagation estimates for the $\mathcal{C}^{1,\mathrm{u}}(A)$ class

We present the results of [GM]. The goal is to obtain propagation estimates for Hamiltonians belonging to the $\mathcal{C}^{1,\mathrm{u}}(A)$ class and infer information about the nature of the spectrum. The first result shows that when the Mourre estimate holds over an interval $\mathcal{I}$, the Fourier transform of the spectral measures of H go to zero at infinity whenever $\mathcal{I}$ is void of eigenvalues.

Theorem 5.1. *Let H and A be self-adjoint operators in a separable Hilbert space $\mathcal{H}$ with $H \in \mathcal{C}^{1,\mathrm{u}}(A)$. Assume that $\mathcal{I} \subset \mathbb{R}$ is a compact interval for which $\lambda \in \tilde{\mu}^A(H)$ for all $\lambda \in \mathcal{I}$. Suppose moreover that $\ker(H-\lambda) \subset \mathcal{D}(A)$ for all $\lambda \in \mathcal{I}$. Then for all $\psi \in \mathcal{H}$ and all $s > 0$,*

$$\lim_{t \to +\infty} \| \langle A \rangle^{-s} e^{-\mathrm{i}tH} P_{\mathrm{c}}(H) E_{\mathcal{I}}(H) \psi \| = 0. \tag{29}$$

Moreover, if W is H-relatively compact, then

$$\lim_{t \to +\infty} \| W e^{-\mathrm{i}tH} P_{\mathrm{c}}(H) E_{\mathcal{I}}(H) \psi \| = 0. \tag{30}$$

In particular, if H has no eigenvalues in $\mathcal{I}$, then the Fourier transform of the spectral measure $\Sigma \mapsto \langle \psi, E_{\mathcal{I} \cap \Sigma}(H) \psi \rangle$ tends to zero at infinity.

The proof of this result is an application of the minimal escape velocities obtained in [Ri], itself a continuation of [HSS]. Note that (23) implies (29). Indeed, the integrand of (23) is a real-valued $L^1(\mathbb{R})$ function with bounded derivative (hence uniformly continuous on $\mathbb{R}$). Such a function must go to zero at infinity. We should mention also that it is an open question to know if (23) is true when $H \in \mathcal{C}^{1,\mathrm{u}}(A)$. While (30) is a consequence of the Riemann-Lebesgue Lemma (8) when $\psi = P_{\mathrm{ac}}(H)\psi$, our result is new. However, it is not strong enough to imply the absence of singularly continuous spectrum for H. Indeed, there exist measures whose Fourier transform goes to zero at infinity, and yet their support is a set of Hausdorff dimension zero, see [B].

Note that the estimates (29) and (30) cannot hold uniformly on the unit sphere of states in $\mathcal{H}$. We now present a second propagation estimate, and this one however will be uniform. It is based on an improved version of the RAGE Theorem, see (7). Let us go deeper in the hypotheses. Let H_0 be a self-adjoint operator on $\mathcal{H}$, with domain $\mathcal{D}(H_0)$. We use standard notation and set $\mathcal{H}^2 := \mathcal{D}(H_0)$ and $\mathcal{H}^1 := \mathcal{D}(\langle H_0 \rangle^{1/2})$, the form domain of H_0. Also, $\mathcal{H}^{-2} := \mathcal{D}(H_0)^*$, and $\mathcal{H}^{-1} := \mathcal{D}(\langle H_0 \rangle^{1/2})^*$. The following continuous and dense embeddings hold:

$$\mathcal{H}^2 \subset \mathcal{H}^1 \subset \mathcal{H} = \mathcal{H}^* \subset \mathcal{H}^{-1} \subset \mathcal{H}^{-2}. \tag{31}$$

These are Hilbert spaces with the appropriate graph norms. We split the assumptions into two groups: spectral and regularity assumptions. We start with the former.
Spectral Assumptions:

- A1 : H_0 is a semi-bounded operator.
- A2 : V defines a symmetric quadratic form on $\mathcal{H}^1$.
- A3 : $V \in \mathcal{K}(\mathcal{H}^1, \mathcal{H}^{-1})$.

Importantly, these assumptions allow us to define the perturbed Hamiltonian H. Indeed, A1 - A3 imply, by the KLMN Theorem, e.g. [RS2, Theorem X.17], that $H := H_0 + V$ in the form sense is a semi-bounded self-adjoint operator with domain $\mathcal{D}(\langle H \rangle^{1/2}) = \mathcal{H}^1$. Furthermore, we have by Weyl's Theorem that $\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ess}}(H_0)$.

Under these few assumptions, both the (improved) RAGE Theorem (7) and the Riemann-Lebesgue Lemma (8) hold. We continue with the assumptions concerning this operator.
Regularity Assumptions: There is a self-adjoint operator A on $\mathcal{H}$ such that

- A4 : $e^{\mathrm{i}tA}\mathcal{H}^1 \subset \mathcal{H}^1$ for all $t \in \mathbb{R}$.
- A5 : $H_0 \in \mathcal{C}^2(A; \mathcal{H}^1, \mathcal{H}^{-1})$.
- A6 : $V \in \mathcal{C}^{1,\mathrm{u}}(A; \mathcal{H}^1, \mathcal{H}^{-1})$.

We refer to Section 2.1 for a description of the regularity classes. While A4 and A5 are standard assumptions to apply Mourre theory, A6 is significantly weaker. It causes H to have no more than the $\mathcal{C}^{1,\mathrm{u}}(A; \mathcal{H}^1, \mathcal{H}^{-1})$ regularity, in which case the LAP may fail to hold. Assumption A3 together with the $\mathcal{C}^{1,\mathrm{u}}(A)$ regularity implies that $\tilde{\mu}^A(H) = \tilde{\mu}^A(H_0)$, by [GM, Lemma 3.3] or [ABG, Theorem 7.2.9]. The uniform estimate derived in [GM] is:

Theorem 5.2. *Suppose A1 through A6. Let $\lambda \in \tilde{\mu}^A(H)$ be such that $\ker(H - \lambda) \subset \mathcal{D}(A)$. Then there exists a bounded open interval $\mathcal{I}$ containing λ such that for all $s > 1/2$,*

$$\lim_{T \to \pm\infty} \sup_{\substack{\psi \in \mathcal{H} \\ \|\psi\| \leqslant 1}} \frac{1}{T} \int_0^T \| \langle A \rangle^{-s} P_{\mathrm{c}}(H) E_{\mathcal{I}}(H) e^{-\mathrm{i}tH} \psi \|^2 \, dt = 0. \tag{32}$$

This formula is to be compared with (7), (23) and (29). The parallel between (32) and the RAGE formula (7) raises an important concern however. The novelty of the propagation estimate (32) depends critically on the non-compactness of the operator $\langle A\rangle^{-s}E_{\mathcal{I}}(H)$. This issue is discussed in [GM, Section 7], where we study several examples including continuous and discrete Schrödinger operators. In all of these examples, it appears that $\langle A\rangle^{-s}E_{\mathcal{I}}(H)$ is compact in dimension one, but not in higher dimensions. Theorem 5.2 therefore appears to be a new result for multi-dimensional Hamiltonians. Interestingly, our proof of this Theorem is very similar to the derivation of the weighted Mourre estimate which is used in the proof of a LAP for Hamiltonians with oscillating potentials belonging to the $\mathcal{C}^1(A)$ class, see [G], [GJ2] and [Ma1].

The various propagation estimates discussed in the Introduction are listed in Table 3 according to the regularity of the potential V. Sufficient regularity for the free operator H_0 is implicit. In this table, question marks indicate open problems.

V is of class	RAGE formula	R.-L. formula	Prop. estimates (29) and (30)	Prop. estimate (32)	Kato - type Prop. estimate	LAP
$\mathcal{C}^1(A)$	✓	✓	?	?	?	?
$\mathcal{C}^{1,\mathrm{u}}(A)$	✓	✓	✓	✓	?	?
$\mathcal{C}^{1,1}(A)$	✓	✓	✓	✓	✓	✓
$\mathcal{C}^2(A)$	✓	✓	✓	✓	✓	✓

Table 3: The estimates for H depending on the regularity of the potential V

In this article we also provide a criterion to check the $\mathcal{C}^{1,\mathrm{u}}(A;\mathcal{H}^1,\mathcal{H}^{-1})$ condition, see [GM, Proposition 2.1]. A very similar result appears in [ABG, Theorem 9.4.10].

Proposition 5.3. *Suppose that* $T\in\mathcal{B}(\mathcal{H}^1,\mathcal{H}^{-1})\cap\mathcal{C}^1(A;\mathcal{H}^1,\mathcal{H}^{-1})$. *If* $[T,\mathrm{i}A]_\circ\in\mathcal{K}(\mathcal{H}^1,\mathcal{H}^{-1})$, *then* $T\in\mathcal{C}^{1,\mathrm{u}}(A;\mathcal{H}^1,\mathcal{H}^{-1})$.

We apply the results of this Section to the continuous Schrödinger operators.

Theorem 5.4. *Let* $\mathcal{H}=L^2(\mathbb{R}^\nu)$. *Let* $H:=H_0+V_{\mathrm{sr}}(Q)+V_{\mathrm{lr}}(Q)$ *and* A *be as follows:*

1. $H_0=-\Delta$ *and* $A=(Q\cdot P+P\cdot Q)/2$,
2. $V_{\mathrm{sr}}(x)$ *and* $V_{\mathrm{lr}}(x)$ *are real-valued functions in* $L^\infty(\mathbb{R}^\nu)$,
3. $\lim V_{\mathrm{sr}}(x)=\lim V_{\mathrm{lr}}(x)=0$ *as* $\|x\|\to+\infty$,
4. $\lim\langle x\rangle V_{\mathrm{sr}}(x)=0$ *as* $\|x\|\to+\infty$, *and*
5. $x\cdot\nabla V_{\mathrm{lr}}(x)$ *exists as a function, belongs to* $L^\infty(\mathbb{R}^\nu)$, *and* $\lim x\cdot\nabla V_{\mathrm{lr}}(x)=0$ *as* $\|x\|\to+\infty$.

Then $V_{\mathrm{sr}}(Q)$ *and* $V_{\mathrm{lr}}(Q)$ *belong to* $\mathcal{C}^{1,\mathrm{u}}(A;\mathcal{H}^1,\mathcal{H}^{-1})$. *In particular* $H\in\mathcal{C}^{1,\mathrm{u}}(A)$. *Moreover,* $\tilde{\mu}^A(H)=\tilde{\mu}^A(H_0)=(0,+\infty)$. *Finally, for all* $\lambda\in(0,+\infty)$ *there is a bounded open interval* $\mathcal{I}$ *containing* λ *such that for all* $s>1/2$ *and* $\psi\in\mathcal{H}$, *the propagation estimates* (29), (30) *and* (32) *hold.*

Remark 5.1. *Notice that the condition* $\ker(H-\lambda) \subset \mathcal{D}(A)$ *that appears in the formulation of Theorems 5.1 and 5.2 is totally absent here. As mentioned previously in the Introduction, this is because under the assumptions* $\lim \langle x \rangle V_{\mathrm{sr}}(x) = \lim x \cdot \nabla V_{\mathrm{lr}}(x) = 0$ *as* $\|x\| \to +\infty$*, it is well-known that the continuous Schrödinger operator* H *does not have any eigenvalues in* $[0, +\infty)$*, see articles by Kato [Ka], Simon [Si2] and Agmon [A].*

Finally, we apply the results of this Section to the discrete Schrödinger operators.

Theorem 5.5. *Let* $\mathcal{H} = \ell^2(\mathbb{Z}^\nu)$*. Let* $H := H_0 + V$ *and* A *be as follows:*

1. $H_0 = \Delta$ *is the Laplacian* (2) *and* A *is the standard conjugate operator* (13)*,*
2. $V(n)$ *is a bounded real-valued function defined on* $\mathbb{Z}^\nu$*,*
3. $\lim V(n) = 0$ *as* $|n| \to +\infty$*, and*
4. $\lim |n_i(V - \tau_i V)(n)| = 0$ *as* $|n| \to +\infty$ *for all* $1 \leqslant i \leqslant \nu$*.*

Then V *and* H *belong to* $\mathcal{C}^{1,\mathrm{u}}(A)$*. Moreover,* $\tilde{\mu}^A(H) = \tilde{\mu}^A(H_0) = [0, 4\nu] \setminus \{4k : k = 0, ..., \nu\}$*, by* (17)*. Finally, for all* $\lambda \in \tilde{\mu}^A(H)$ *there is a bounded open interval* $\mathcal{I}$ *containing* λ *such that for all* $s > 1/2$ *and* $\psi \in \mathcal{H}$*, the propagation estimates* (29)*,* (30) *and* (32) *hold.*

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THE LIMITING ABSORPTION PRINCIPLE FOR THE DISCRETE WIGNER-VON NEUMANN OPERATOR

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Abstract. We apply weighted Mourre commutator theory to prove the limiting absorption principle for the discrete Schrödinger operator perturbed by the sum of a Wigner-von Neumann and long-range type potential. In particular, this implies a new result concerning the absolutely continuous spectrum for these operators even for the one-dimensional operator. We show that methods of classical Mourre theory based on differential inequalities and on the generator of dilation cannot apply to the aforementioned Schrödinger operators.

1. Introduction

The spectral theory of discrete Schrödinger operators has received much attention in the past few decades. The absolutely continuous spectrum is important because it allows to describe the quantum dynamics of a system. The limiting absorption principle (LAP) plays a profound role in spectral and scattering theory, in particular, it implies the existence of purely absolutely continuous spectrum. The LAP has been derived for a wide class of potentials, including the Wigner-von Neumann potential (cf. [NW], [DMR], [RT1], [RT2], [MS] and [EKT] to name a few), but only recently has the sum of a Wigner-von Neumann and long-range potential been studied in the continuous setting (cf. [GJ2]). The LAP has not been studied for the discrete Wigner-von Neumann operator. On the other hand, the absolutely continuous spectrum of the one-dimensional Wigner-von Neumann operator plus a potential $V \in \ell^p(\mathbb{Z})$ has already been studied, both in the discrete and continuous setting in [L1], [L2] and [L3], but also in [Si], [JS], [KN], [NS] and [KS] for the case $V \in \ell^1(\mathbb{Z})$ more specifically. In this paper we study the sum of a Wigner-von Neumann and long-range potential in the discrete setting which we now describe.

The configuration space is the multi-dimensional lattice $\mathbb{Z}^d$ for some integer $d \geqslant 1$. For a multi-index $n = (n_1, ..., n_d) \in \mathbb{Z}^d$ we set $|n|^2 := n_1^2 + ... + n_d^2$. Consider the Hilbert space $\mathcal{H} := \ell^2(\mathbb{Z}^d)$ of square summable sequences $u = (u(n))_{n\in\mathbb{Z}^d}$. The discrete Schrödinger operator

$$H := \Delta + W + V \tag{1.1}$$

acts on $\mathcal{H}$, where Δ is the discrete Laplacian operator defined by

$$(\Delta u)(n) := \sum_{\substack{m\in\mathbb{Z}^d \\ |n-m|=1}} (u(n) - u(m)), \quad \text{for all } n \in \mathbb{Z}^d \text{ and } u \in \mathcal{H},$$

W is the Wigner-von Neumann potential defined by

$$(Wu)(n) := \frac{q\sin(k(n_1 + ... + n_d))}{|n|} u(n), \quad \text{for all } n \in \mathbb{Z}^d \text{ and } u \in \mathcal{H}, \tag{1.2}$$

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with $q \in \mathbb{R}$ and $k \in \mathcal{T} := [0, 2\pi]\backslash\{\pi\}$, and V is a multiplication operator by a real-valued sequence $(V(n))_{n\in\mathbb{Z}^d}$:

$$(Vu)(n) := V(n)u(n), \quad \text{for all } n \in \mathbb{Z}^d \text{ and } u \in \mathcal{H}.$$

The potential V will be of long-range type, hence a compact operator, but we postpone the characterization of its exact decay properties. We will also investigate the following variation on the Wigner-von Neumann potential:

$$(1.3) \qquad (W'u)(n) := \left(\prod_{i=1}^{d} \frac{q_i \sin(k_i n_i)}{n_i}\right) u(n), \quad \text{for all } n \in \mathbb{Z}^d \text{ and } u \in \mathcal{H},$$

with $q = (q_i)_{i=1}^d \in \mathbb{R}^d$ and $k = (k_i)_{i=1}^d \in \mathcal{T}^d$. In this case, we shall denote $H' := \Delta + W' + V$. In the definitions of W and W', it is understood that $\sin(0)/0 := 1$. Using the discrete Fourier transform $\mathcal{F} : \mathcal{H} \to L^2([-\pi, \pi]^d, d\xi)$, $\xi = (\xi_1, ..., \xi_d)$, we get

$$(1.4) \quad (\mathcal{F}\Delta\mathcal{F}^{-1}f)(\xi) = f(\xi)\sum_{i=1}^{d}(2 - 2\cos(\xi_i)), \quad \text{where} \quad (\mathcal{F}u)(\xi) := \sum_{n\in\mathbb{Z}^d} u(n)e^{in\cdot\xi}(2\pi)^{-d/2}.$$

This shows that Δ is a bounded self-adjoint operator on $\mathcal{H}$, and that $\sigma(\Delta) = \sigma_{\mathrm{ac}}(\Delta) = [0, 4d]$. The operators H and H' are compact perturbations of Δ and so $\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ess}}(H') = [0, 4d]$.

The Wigner-von Neumann potential is famous for producing an eigenvalue embedded in the absolutely continuous spectrum when coupled with an appropriate perturbation V (cf. [NW], [RS4]). In the continuous setting it has been shown that the $1d$ Schrödinger operator

$$-\frac{d^2}{dx^2} + \frac{q\sin(kx)}{x} + O(x^{-2})$$

covers the interval $[0, \infty)$ with absolutely continuous spectrum and may produce exactly one eigenvalue with positive energy. In the discrete setting the $1d$ Schrödinger operator $\Delta + W$ covers the interval $(0, 4)$ with absolutely continuous spectrum due to the fact that $W \in \ell^2(\mathbb{Z})$ (cf. [DK]), and it has been shown (cf. [JS], [Si]) that there are two points located at

$$(1.5) \qquad E_\pm(k) := 2 \pm 2\cos(k/2)$$

which may be half-bound states or eigenvalues. If $V \in \ell^1(\mathbb{Z})$, the spectrum of $H := \Delta + W + V$ is purely absolutely continuous on $(0, 4)\backslash\{E_\pm(k)\}$ (cf. [JS]). The works [Si], [JS], [KN], [NS], and [KS] are concerned with the asymptotics of the generalized eigenvectors of $H := \Delta + V_P + W + V$, where V_P is periodic, W is the Wigner-von Neumann potential and $V \in \ell^1(\mathbb{Z})$.

We fix some notation. Let $S := (S_1, ..., S_d)$ where, for $1 \leqslant i \leqslant d$, S_i is the shift operator

$$(1.6) \qquad (S_i u)(n) := u(n_1, ..., n_i - 1, ..., n_d), \quad \text{for all } n \in \mathbb{Z}^d \text{ and } u \in \mathcal{H}.$$

We denote by $\tau_i V$ (resp. $\tau_i^* V$) the operator of multiplication acting by

$$[(\tau_i V)u](n) := V(n_1, ..., n_i - 1, ...n_d)u(n) \ \ (\text{resp. } [(\tau_i^* V)u](n) := V(n_1, ..., n_i + 1, ...n_d)u(n)).$$

We will also be using the bracket notation $\langle\alpha\rangle := \sqrt{1 + |\alpha|^2}$. Let us now get into the details of the potential V. All in all, we will require two conditions on V: we suppose that there exist $\rho, C > 0$ such that

$$(1.7) \qquad \langle n\rangle^\rho |V(n)| \leqslant C, \quad \text{for all } n \in \mathbb{Z}^d, \quad \text{and}$$

$$(1.8) \qquad \langle n\rangle^\rho |n_i||(V - \tau_i V)(n)| \leqslant C, \quad \text{for all } n \in \mathbb{Z}^d \text{ and } 1 \leqslant i \leqslant d.$$

These conditions can be interpreted as a discrete version of the standard long-range type potential $|\partial^\alpha V(x)| \leqslant C\langle x\rangle^{-|\alpha|-\rho}$ in the continuous case. Examples of potentials V satisfying these two conditions include $|V(n)| \leqslant C\langle n\rangle^{-1-\rho}$, the so-called short-range potential, and $V(n) = C\langle n\rangle^{-\rho}$.

The goal of this paper is to establish the LAP for H as defined in (1.1). The formulation of the LAP requires a conjugate operator which we now introduce. But first, we need the position operator $N := (N_1, ..., N_d)$, where the N_i are defined by

$$(N_i u)(n) := n_i u(n), \quad \mathcal{D}(N_i) = \Big\{u \in \mathcal{H} : \sum_{n\in\mathbb{Z}^d} |n_i u(n)|^2 < \infty\Big\}.$$

The conjugate operator to H will be the generator of dilations denoted A and is the closure of

$$A_0 := \mathrm{i}\sum_{i=1}^d \big(2^{-1}(S_i^* + S_i) - (S_i^* - S_i)N_i\big) = \mathrm{i}\sum_{i=1}^d 2^{-1}\big((S_i - S_i^*)N_i + N_i(S_i - S_i^*)\big) \tag{1.9}$$

defined on $\mathcal{D}(A_0) = \ell_0(\mathbb{Z}^d)$, the collection of sequences with compact support. The operator A is self-adjoint. We will also make use of the projectors onto the pure point spectral subspace of H and its complement, denoted P and $P^\perp := 1 - P$ respectively. We define the following sets:

$$\mu(H) = \mu(H') := (0,4)\backslash\{E_\pm(k)\} \quad \text{for} \quad d = 1, \tag{1.10}$$

$$\mu(H) := (0, E(k)) \cup (4d - E(k), 4d) \quad \text{for} \quad d \geqslant 2, \tag{1.11}$$

$$\mu(H') := (0, E'(k)) \cup (4d - E'(k), 4d) \quad \text{for} \quad d \geqslant 2. \tag{1.12}$$

Recall $E_\pm(k)$ defined by (1.5). The definitions of $E(k)$ and $E'(k)$ are respectively given in Propositions 4.5 and 4.6. We may as well already mention that the sets μ consist of points where the classical Mourre estimate holds for H and H'. The main result of the paper is the following:

Theorem 1.1. *Let $E \in \mu(H)$. Then there is an open interval $\mathcal{I}$ containing E such that H has finitely many eigenvalues in $\mathcal{I}$ and these are of finite multiplicity. Furthermore, if* $\ker(H - E) \subset D(A)$, *then $\mathcal{I}$ can be chosen so that for any $s > 1/2$ and any compact interval $\mathcal{I}' \subset \mathcal{I}$, the reduced LAP for H holds with respect to $(\mathcal{I}', s, A)$, that is to say,*

$$\sup_{x\in\mathcal{I}', y\neq 0} \|\langle A\rangle^{-s}(H - x - \mathrm{i}y)^{-1}P^\perp\langle A\rangle^{-s}\| < \infty. \tag{1.13}$$

In particular, the following local decay estimate holds:

$$\int_{\mathbb{R}} \|\langle N\rangle^{-s}e^{-\mathrm{i}tH}P^\perp\theta(H)u\|^2 dt \leqslant C\|u\|^2, \quad \textit{for any } u \in \mathcal{H}, \theta \in C_c^\infty(\mathbb{R}), \textit{ and } s > 1/2, \tag{1.14}$$

and the spectrum of H is purely absolutely continuous on $\mathcal{I}'$ whenever $P = 0$ on $\mathcal{I}'$.

The corresponding result also holds for H'. The last part of Theorem 1.1 are two well-known consequences of the LAP. The local decay estimate gives a better insight into how the initial state $\theta(H)u$ diverges to infinity.

Our result is a discrete version of the LAP for the corresponding continuous Schrödinger operator obtained by Golénia and Jecko in [GJ2], and our proof is very much inspired from theirs. The proof is based on variations of classical Mourre theory. Classical Mourre theory was proven very successful to study the point and continuous spectra of a wide class of self-adjoint operators. Standard references are the original paper by Mourre [M] and the book

[ABG] in which optimal results are obtained for a wide class of potentials. We also refer to [Sa].

In [GJ1] and [GJ2], a new approach to Mourre's theory is developed. Their approach proves the LAP without the use of differential inequalities, as it is done in Mourre's original work [M]. In the separate work of Gérard [G], he proves the LAP using traditional energy estimates and introduces weighted Mourre estimates. In [GJ2], Golénia and Jecko are able to prove the LAP under weaker conditions on the potential than what is usually assumed in [ABG] or [Sa] for example, because their starting point is not the classical Mourre estimate but rather the weighted Mourre estimate. Roughly speaking, the original Mourre theory required $[[V,A],A]$ to be bounded in a weak sense, whereas the more recent and different approaches require V to belong to a class where solely $[V,A]$ is bounded. This allows for new classes of potentials to be studied, such as the Wigner-von Neumann potential. In Propositions 3.3 and 4.2, we show that the standard Mourre commutator techniques exposed in [ABG] or [Sa] cannot be used to treat the discrete Wigner-von Neumann potential. Finally, the LAP derived in this paper is interesting because we include a long-range type potential V in addition to the Wigner-von Neumann potential and therefore provide new results including the question of the absolutely continuous spectrum.

The paper is organized as follows: In Section 2, we recall the basic notions of classical and weighted Mourre theory that we will be using. In Section 3, we study the classical Mourre theory for the one-dimensional Schrödinger operators H and H', and show that the discrete Wigner-von Neumann potential cannot be treated with the classical methods. In Section 4, we repeat our analysis for the multi-dimensional Schrödinger operators H and H', and recycle results from the one-dimensional case. In Section 5, we prove the weighted Mourre estimate that leads to the LAP. This section is done independently of the dimension. Finally in the Appendix 6, we recall essential facts about almost analytic extensions of $C^\infty(\mathbb{R})$ functions that we need to establish the weighted Mourre estimate.

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2. Preliminaries

2.1. **Regularity.** We consider two self-adjoint operators T and A acting in some complex Hilbert space $\mathcal{H}$, and for the purpose of the overview T will be bounded. Given $k \in \mathbb{N}$, we say that T is of class $\mathcal{C}^k(A)$, and write $H \in \mathcal{C}^k(A)$ if the map

$$\mathbb{R} \ni t \mapsto e^{\mathrm{i}tA} T e^{-\mathrm{i}tA} u \in \mathcal{H} \tag{2.1}$$

has the usual $C^k(\mathbb{R})$ regularity for every $u \in \mathcal{H}$. Let $\mathcal{I}$ be an open interval of $\mathbb{R}$. We say that T is locally of class $\mathcal{C}^k(A)$ on $\mathcal{I}$, and write $T \in \mathcal{C}^k_{\mathcal{I}}(A)$, if for all $\varphi \in C_c^\infty(\mathbb{R})$ with support in $\mathcal{I}$, $\varphi(T) \in \mathcal{C}^k(A)$. The form $[T,A]$ is defined on $\mathcal{D}(A) \times \mathcal{D}(A)$ by

$$\langle u, [T,A]v\rangle := \langle Tu, Av\rangle - \langle Au, Tv\rangle.$$

We recall the following result of [ABG, p. 250]:

Proposition 2.1. *Let $T \in \mathcal{B}(\mathcal{H})$, the bounded operators on $\mathcal{H}$. The following are equivalent:*

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

(2) The form $[T,A]$ extends to a bounded form on $\mathcal{H}\times\mathcal{H}$ defining a bounded operator denoted by $\mathrm{ad}^1_A(T) := [T,A]_\circ$.
(3) T preserves $\mathcal{D}(A)$ and the operator $TA - AT$, defined on $\mathcal{D}(A)$, extends to a bounded operator.

Consequently, $T \in \mathcal{C}^k(A)$ if and only if the iterated commutators $\mathrm{ad}^p_A(T) := [\mathrm{ad}^{p-1}_A(T), A]_\circ$ are bounded for $1 \leqslant p \leqslant k$. We recall a general Lemma which can found in [GGM, section 2]:

Lemma 2.2. *The class $\mathcal{C}^1(A)$ is a $*$-algebra, that is, for $T_1, T_2 \in \mathcal{C}^1(A)$ we have:*
(1) $T_1 + T_2 \in \mathcal{C}^1(A)$ and $[T_1 + T_2, A]_\circ = [T_1, A]_\circ + [T_2, A]_\circ$.
(2) $T_1T_2 \in \mathcal{C}^1(A)$ and $[T_1T_2, A]_\circ = T_1[T_2, A]_\circ + [T_1, A]_\circ T_2$.
(3) $T_1^* \in \mathcal{C}^1(A)$ and $[T_1^*, A]_\circ = [T_1, A]_\circ^*$.

Finally we will also need the following result from [GJ1]:

Proposition 2.3. *For $u, v \in \mathcal{D}(A)$, the rank one operator $|u\rangle\langle v| : w \to \langle v, w\rangle u$ is of class $\mathcal{C}^1(A)$.*

2.2. **The scale of the different classes.** Let us introduce other classes inside $\mathcal{C}^1(A)$. We say that $T \in \mathcal{C}^{1,\mathrm{u}}(A)$ if the map

$$\mathbb{R} \ni t \mapsto e^{\mathrm{i}tA} T e^{-\mathrm{i}tA} \in \mathcal{B}(\mathcal{H}) \tag{2.2}$$

has the $C^1(\mathbb{R})$ regularity. Note the difference with definition (2.1). We say that $T \in \mathcal{C}^{1,1}(A)$ if

$$\int_0^1 \|[[T, e^{\mathrm{i}tA}]_\circ, e^{\mathrm{i}tA}]_\circ\| t^{-2} dt < \infty.$$

Finally we say that $T \in \mathcal{C}^{1+0}(A)$ if $T \in \mathcal{C}^1(A)$ and

$$\int_{-1}^1 \|e^{\mathrm{i}tA}[T, A]_\circ e^{-\mathrm{i}tA}\| |t|^{-1} dt < \infty.$$

It turns out that

$$\mathcal{C}^2(A) \subset \mathcal{C}^{1+0}(A) \subset \mathcal{C}^{1,1}(A) \subset \mathcal{C}^{1,\mathrm{u}}(A) \subset \mathcal{C}^1(A). \tag{2.3}$$

The local classes are defined in the obvious way: $T \in \mathcal{C}^{[\cdot]}_{\mathcal{I}}(A)$ if, for all $\varphi \in C_c^\infty(\mathcal{I})$, $\varphi(T) \in \mathcal{C}^{[\cdot]}(A)$.

In [Sa], the LAP is obtained on compact sub-intervals of $\mathcal{I}$ when the Schrödinger operator belongs to $\mathcal{C}^{1+0}_{\mathcal{I}}(A)$, while in [ABG, section 7.B], it is obtained for Schrödinger operators belonging to $\mathcal{C}^{1,1}(A)$ and this class is shown to be optimal among the global classes in the framework.

2.3. **The Mourre estimate and the LAP.** Let $\mathcal{I}, \mathcal{J}$ be open intervals with $\overline{\mathcal{I}} \subset \mathcal{J}$, and assume $T \in \mathcal{C}^1_{\mathcal{J}}(A)$. We say that the *Mourre estimate* holds for T on $\mathcal{I}$ if there exist a finite $c > 0$ and a compact operator K such that

$$E_{\mathcal{I}}(T)[T, \mathrm{i}A]_\circ E_{\mathcal{I}}(T) \geqslant c \cdot E_{\mathcal{I}}(T) + K \tag{2.4}$$

in the form sense on $\mathcal{D}(A) \times \mathcal{D}(A)$. We say that the *strict Mourre estimate* holds for T on $\mathcal{I}$ if (2.4) holds with $K = 0$. Assuming $\overline{\mathcal{I}} \subset \mathcal{J}$ and $T \in \mathcal{C}^1_{\mathcal{J}}(A)$, there are finitely many eigenvalues of T in $\mathcal{I}$ and they are of finite multiplicity when $K \neq 0$; whereas T has no eigenvalues in $\mathcal{I}$ when $K = 0$. This is a direct consequence of the Virial Theorem ([Sa], [ABG, Proposition 7.2.10]).

Let $\mathcal{I}(E;\varepsilon)$ be the open interval of radius $\varepsilon > 0$ centered at $E \in \mathbb{R}$. When the strict Mourre estimate holds for T on some interval containing E, it is natural to consider the following function $\varrho_T^A : \mathbb{R} \to (-\infty, +\infty]$:

$$\varrho_T^A(E) := \sup \left\{a \in \mathbb{R} : \exists \varepsilon > 0 \text{ such that } E_{\mathcal{I}(E;\varepsilon)}(T)[T, \mathrm{i}A]_\circ E_{\mathcal{I}(E;\varepsilon)}(T) \geqslant a \cdot E_{\mathcal{I}(E;\varepsilon)}(T)\right\}.$$

It is known for example that ϱ_T^A is lower semicontinuous and $\varrho_T^A(E) < \infty$ if and only if $E \in \sigma(T)$. For more properties of this function, see [ABG, chapter 7].

Variations of classical Mourre theory make use of a *weighted Mourre estimate* (cf. [G], [GJ2]):

$$E_{\mathcal{I}}(T)[T, \mathrm{i}\varphi(A)]_\circ E_{\mathcal{I}}(T) \geqslant E_{\mathcal{I}}(T)\langle A\rangle^{-s}(c + K)\langle A\rangle^{-s}E_{\mathcal{I}}(T) \tag{2.5}$$

where $0 < c < \infty$, $s > 1/2$ and φ is some function in $B_b(\mathbb{R})$, the bounded Borel functions. Recall that P is the orthogonal projection onto the pure point spectral subspace of H, and $P^\perp := 1 - P$. We now quote the essential criterion established in [GJ2] that we will need to prove the LAP for H as defined in (1.1).

Theorem 2.4. [GJ2] *Let $\mathcal{I}$ be an open interval, and assume that $P^\perp\theta(T) \in \mathcal{C}^1(A)$ for all $\theta \in C_c^\infty(\mathcal{I})$. Assume the existence of an $s_0 \in (1/2, 1]$ with the following property : for any $s \in (1/2, s_0]$, there exist a finite $c > 0$ and a compact operator K such that for all $R \geqslant 1$, there exists $\psi_R \in B_b(\mathbb{R})$ so that the following projected weighted Mourre estimate*

$$P^\perp E_{\mathcal{I}}(T)[T, \mathrm{i}\varphi_R(A/R)]_\circ E_{\mathcal{I}}(T)P^\perp \geqslant P^\perp E_{\mathcal{I}}(T)\langle A/R\rangle^{-s}(c + K)\langle A/R\rangle^{-s}E_{\mathcal{I}}(T)P^\perp \tag{2.6}$$

holds. Then for all $s > 1/2$ and compact $\mathcal{I}'$ with $\overline{\mathcal{I}'} \subset \mathcal{I}$, the reduced LAP (1.13) for T holds with respect to $(\mathcal{I}', s, A)$.

3. The One-Dimensional Case

We begin with the study of the one-dimensional operator. We write the Laplacian in terms of the shift operators defined in (1.6) : $\Delta = 2 - (S^* + S)$. Note that $[S, \Delta]_\circ = [S^*, \Delta]_\circ = 0$. Recall that A is the conjugate operator to H introduced in (1.9). It is the closure of the operator

$$A_0 := -\mathrm{i}\left(2^{-1}(S^* + S) + N(S^* - S)\right) = \mathrm{i}\left(2^{-1}(S^* + S) - (S^* - S)N\right) \tag{3.1}$$

on the domain $\mathcal{D}(A_0) := \ell_0(\mathbb{Z})$. The domain of A has been shown explicitly to be $\mathcal{D}(A) = \mathcal{D}(N(S^* - S))$ and this operator has been shown to be self-adjoint (cf. [GGo]). Moreover A is unitarily equivalent to the self-adjoint realization of the operator

$$A_{\mathcal{F}} := \mathrm{i}\sin(\xi)\frac{d}{d\xi} + \mathrm{i}\frac{d}{d\xi}\sin(\xi), \quad \mathcal{D}(A_{\mathcal{F}}) := \{f \in L^2([-\pi, \pi], d\xi) : A_{\mathcal{F}}f \in L^2([-\pi, \pi], d\xi)\}.$$

3.1. $\mathcal{C}^1(A)$ Regularity.

We now show that H and H' are of class $\mathcal{C}^1(A)$.

Proposition 3.1. *The form $[\Delta, \mathrm{i}A]$ extends to a bounded form denoted $[\Delta, \mathrm{i}A]_\circ$ and*

$$[\Delta, \mathrm{i}A]_\circ = \Delta(4 - \Delta). \tag{3.2}$$

Furthermore Δ is of class $\mathcal{C}^\infty(A)$.

Proof. A straightforward and well-known computation shows that $\langle u, [\Delta, \mathrm{i}A]v\rangle = \langle u, \Delta(4 - \Delta)v\rangle$ for all $u, v \in \ell_0(\mathbb{Z})$. Thus $[\Delta, \mathrm{i}A]$ extends to a bounded form and we have (3.2). Using induction and applying Lemma 2.2 shows that $\mathrm{ad}_A^k(\Delta)$ is a polynomial of degree $k + 1$ in Δ. □

Define the bounded operators

(3.3) $K_W := 2^{-1}W(S^*+S)+2^{-1}(S^*+S)W, \quad \text{and} \quad B_W := U\tilde{W}(S^*-S)-(S^*-S)\tilde{W}U,$

where $\tilde{W}$ and U are respectively the operators

$$(\tilde{W}u)(n) := q\sin(kn)u(n), \quad \text{and} \quad (Uu)(n) := \operatorname{sign}(n)u(n).$$

We use the convention $\operatorname{sign}(0)=0$. A simple calculation shows that for all $u,v \in \ell_0(\mathbb{Z})$,

$$\langle u, [W, \mathrm{i}A]v\rangle = \langle u, K_W v\rangle + \langle u, B_W v\rangle.$$

We also investigate the form $[W', \mathrm{i}A]$. Define the bounded operators

(3.4) $K_{W'} := 2^{-1}W'(S^*+S)+2^{-1}(S^*+S)W', \quad \text{and} \quad B_{W'} := \tilde{W}(S^*-S)-(S^*-S)\tilde{W}.$

A straightforward computation shows that for all $u,v \in \ell_0(\mathbb{Z})$,

$$\langle u, [W', \mathrm{i}A]v\rangle = \langle u, K_{W'} v\rangle + \langle u, B_{W'} v\rangle.$$

Hence both $[W, \mathrm{i}A]$ and $[W', \mathrm{i}A]$ extend to bounded forms and we have

(3.5) $$[W, \mathrm{i}A]_\circ = K_W + B_W, \quad \text{and} \quad [W', \mathrm{i}A]_\circ = K_{W'} + B_{W'}.$$

Note that K_W and $K_{W'}$ are compact, while B_W and $B_{W'}$ are bounded (but not compact by Proposition 3.3). Finally, we turn to the form $[V, \mathrm{i}A]$. For $u \in \ell_0(\mathbb{Z})$ we have

$$((VA-AV)u)(n) = \mathrm{i}(n-2^{-1})(V(n)-V(n-1))u(n-1)+\mathrm{i}(n-2^{-1})(V(n)-V(n+1))u(n+1).$$

Therefore in the form sense, we have for $u,v \in \ell_0(\mathbb{Z})$,

(3.6) $$\langle u, [V, \mathrm{i}A]v\rangle = -\langle u, \big[(N-2^{-1})(V-\tau V)S+(N-2^{-1})(V-\tau^* V)S^*\big]v\rangle.$$

By hypothesis (1.8), we see that $[V, \mathrm{i}A]$ can be extended to a bounded form, and that $[V, \mathrm{i}A]_\circ$ is a compact operator. The above discussion leads to:

Proposition 3.2. *$H = \Delta + W + V$ and $H' = \Delta + W' + V$ are of class $\mathcal{C}^1(A)$.*

We now explain why the usual Mourre theory with conjugate operator A cannot be applied. We have proved that $H \in \mathcal{C}^1(A)$, however in order to apply the standard Mourre theory, one typically has to prove that H is in a better class of regularity w.r.t. A. As mentionned previously, the existing standard theory in [ABG] is optimal for the class $\mathcal{C}^{1,1}(A)$. However, we are not dealing with potentials in this class as shown in the following Proposition. The same phenomenon occurs in the case of the continuous Schrödinger operator (cf. [GJ2]).

Proposition 3.3. *H and H' are not of class $\mathcal{C}^{1,u}(A)$.*

Proof. We stick with H as the same proof works for H'. Since $\Delta \in \mathcal{C}^\infty(A)$, we have $\Delta \in \mathcal{C}^{1,\mathrm{u}}(A)$. Let us assume by contradiction that $H \in \mathcal{C}^{1,\mathrm{u}}(A)$. Then $H-\Delta \in \mathcal{C}^{1,\mathrm{u}}(A)$. In particular

$$\lim_{t\to 0}\big[e^{-\mathrm{i}tA}(H-\Delta)e^{\mathrm{i}tA}-(H-\Delta)\big]t^{-1} = [(H-\Delta), \mathrm{i}A]_\circ = [(W+V), \mathrm{i}A]_\circ$$

is a compact operator as the norm limit of compact operators. As explained before, $[V, \mathrm{i}A]_\circ$ is compact, and $[W, \mathrm{i}A]_\circ$ is the sum of the compact operator K_W and the bounded operator B_W. We show that B_W is not compact, and this will be our contradiction. Consider the sequence $(\delta_j)_{j\geqslant 2}$ of unit vectors in $\ell^2(\mathbb{Z})$ satisfying $(\delta_j)(n) = \delta_{j;n}$. Then

$$B_W\delta_j = q\left(\sin(k(j-1))-\sin(kj)\right)\delta_{j-1} - q\left(\sin(k(j+1))-\sin(kj)\right)\delta_{j+1}.$$

For this operator to be compact, we require

$$\begin{aligned}0 &= \lim_{j\to\infty} |q||\sin(k(j-1)) - \sin(kj)| + |q||\sin(k(j+1)) - \sin(kj)| \\ &= \lim_{j\to\infty} 2|q||\cos(kj - k/2)||\sin(k/2)| + 2|q||\cos(kj + k/2)||\sin(k/2)|.\end{aligned}$$

As $j \to \infty$, we would need $kj - k/2 \to \pi/2 \pmod \pi$ and $kj + k/2 \to \pi/2 \pmod \pi$, but this is not possible precisely because $k \neq \pi$. □

3.2. **Classical Mourre Theory.** In this section we derive the classical Mourre estimate (2.4) for the one-dimensional Schrödinger operator H. From the previous section, we know that $[V, \mathrm{i}A]_\circ$ is compact and that $[W, \mathrm{i}A]_\circ = K_W + B_W$, with K_W compact but B_W just bounded. Therefore, in order to derive the Mourre estimate, what really remains to show is that $E_{\mathcal{I}}(\Delta) B_W E_{\mathcal{I}}(\Delta)$ is compact for some well-chosen $\mathcal{I} \subset [0,4]$. We show precisely:

Lemma 3.4. *Recall that $E_\pm(k) := 2 \pm 2\cos(k/2)$. Let $E \in [0,4] \backslash \{E_\pm(k)\}$. Then there exists $\varepsilon = \varepsilon(E) > 0$ such that for all $\theta \in C_c^\infty(\mathbb{R})$ supported on $\mathcal{I} := (E-\varepsilon, E+\varepsilon)$, $\theta(\Delta)\tilde{W}\theta(\Delta) = 0$. Thus $\theta(\Delta) B_{W'} \theta(\Delta) = 0$ and $\theta(\Delta) B_W \theta(\Delta)$ is compact.*

The proof of this Lemma is deferred to the end of this section, but note that the last part of the Lemma is easy, since if $\theta(\Delta)\tilde{W}\theta(\Delta) = 0$, then

$$\theta(\Delta) B_{W'} \theta(\Delta) = \theta(\Delta)\tilde{W}\theta(\Delta)(S^* - S) - (S^* - S)\theta(\Delta)\tilde{W}\theta(\Delta) = 0.$$

Commuting U with Δ produces a finite rank, hence compact operator by (3.7), so $\theta(\Delta) B_W \theta(\Delta)$ is compact. The classical Mourre estimate for H and H' is easily deduced:

Proposition 3.5. *For every $E \in (0,4) \backslash \{E_\pm(k)\}$, there is an open interval $\mathcal{I}$ containing E such that the Mourre estimate (2.4) holds for H and H'. In particular, the number of eigenvalues of H and H' in $\mathcal{I}$ are finite and they are of finite multiplicity.*

Proof. For $E \in (0,4) \backslash \{E_\pm(k)\}$, let $\theta \in C_c^\infty(\mathbb{R})$ be as in Lemma 3.4, with $\mathrm{supp}(\theta) = \mathcal{I}$. By the resolvent identity, $\Omega := \theta(H) - \theta(\Delta)$ is compact. Indeed, by the Helffer-Sjöstrand formula,

$$\Omega = \frac{\mathrm{i}}{2\pi} \int_{\mathbb{C}} \frac{\partial \tilde{\theta}}{\partial \overline{z}} (z - H)^{-1} (W + V)(z - \Delta)^{-1} dz \wedge d\overline{z}$$

is a norm converging integral of compact operators. We have for some compact operator K:

$$\begin{aligned}\theta(H)[H, \mathrm{i}A]_\circ \theta(H) &= \theta(\Delta)[H, \mathrm{i}A]_\circ \theta(\Delta) + \Omega[H, \mathrm{i}A]_\circ \theta(H) + \theta(\Delta)[H, \mathrm{i}A]_\circ \Omega \\ &= \theta(\Delta)\Delta(4 - \Delta)\theta(\Delta) + K.\end{aligned}$$

By functional calculus, $\theta(\Delta)\Delta(4-\Delta)\theta(\Delta) \geqslant c\theta^2(\Delta)$, $c := \min_{x \in \mathcal{I}} x(4-x)$. Thus

$$\theta(H)[H, \mathrm{i}A]_\circ \theta(H) \geqslant c\theta^2(H) + K + c(\theta^2(\Delta) - \theta^2(H)).$$

For all open intervals $\mathcal{I}'$ with $\overline{\mathcal{I}'} \subset \mathcal{I}$, we obtain the Mourre estimate when applying $E_{\mathcal{I}'}(H)$ to either sides of the last inequality. □

We now show that compactness of $E_{\mathcal{I}}(H) B_W E_{\mathcal{I}}(H)$ is not possible for any interval $\mathcal{I}$ centered about $E_\pm(k)$. Let $B \subset \mathbb{Z}$ and let $\delta_B(n) = 1$ if $n \in B$ and $\delta_B(n) = 0$ if $n \notin B$. Thanks to

$$S^* U = U S^* + \delta_{\{0\}} S^* + \delta_{\{-1\}} S^*, \quad \text{and} \quad SU = US - \delta_{\{0\}} S - \delta_{\{1\}} S, \tag{3.7}$$

one shows that

$$\theta(\Delta) B_W \theta(\Delta) = U\theta(\Delta)\left(\tilde{W}(S^* - S) - (S^* - S)\tilde{W}\right)\theta(\Delta) + \text{ compact.} \tag{3.8}$$

Proposition 3.6. *Fix $E \in \{E_\pm(k)\}$, and suppose that $q \neq 0$, $k \in (0, 2\pi)\backslash\{\pi\}$. Then for all $\theta \in C_c^\infty(R)$ with $supp(\theta) \ni E$, $\theta(\Delta)B_W\theta(\Delta)$ and $\theta(\Delta)B_{W'}\theta(\Delta)$ are not compact.*

Proof. We show that $Q := \theta(\Delta)[\tilde{W}(S^* - S) - (S^* - S)\tilde{W}]\theta(\Delta) = \theta(\Delta)B_{W'}\theta(\Delta)$ is not compact for any θ supported about $E_\pm(k)$. Applying U to this operator does not make the product any more compact, and so the result will follow by (3.8). In Fourier space, Q becomes

$$q\theta\left(2 - 2\cos(\cdot)\right) \circ \left[\sin(\cdot) \circ (T_k - T_{-k}) - (T_k - T_{-k}) \circ \sin(\cdot)\right] \circ \theta\left(2 - 2\cos(\cdot)\right).$$

Here $T_{\pm k}$ is the operator of translation by $\pm k$. It is not hard to see that if ϕ solves

$$2 - 2\cos(\phi) = 2 - 2\cos(\phi + k), \quad \text{or} \quad 2 - 2\cos(\phi) = 2 - 2\cos(\phi - k)$$

then it is possible to construct a sequence of «delta» functions f_n supported in a neighborhood of ϕ converging weakly to zero, but $\|f_n\|_2 = 1$. The solutions to the previous equations are $\phi = k/2, \pi - k/2$ for the first, and $\phi = -k/2, \pi + k/2$ for the second. Either way, we retrieve the threshold energies $E_\pm(k) = 2 \pm 2\cos(k/2)$. □

The rest of the section is devoted to proving Lemma 3.4. Recall that $\mathcal{F}$ is the discrete Fourier transform defined in (1.4). Let T_k denote the multiplication operator on $\ell^2(\mathbb{Z})$ given by $(T_k u)(n) := e^{\mathrm{i}kn}u(n)$. Then T_k corresponds to a translation by k in the Fourier space of 2π-periodic functions, that is, $(\mathcal{F}T_k\mathcal{F}^{-1}f)(\xi) = f(\xi + k)$. Also denote $\check{\mathbb{1}}_{[0,\pi]}$ the operator on $\ell^2(\mathbb{Z})$ satisfying $(\mathcal{F}\check{\mathbb{1}}_{[0,\pi]}\mathcal{F}^{-1}f)(\xi) = \mathbb{1}_{[0,\pi]}(\xi)f(\xi)$. This operator is bounded, self-adjoint, commutes with Δ, and its spectrum is $\sigma(\check{\mathbb{1}}_{[0,\pi]}) = \text{ess ran}(\mathbb{1}_{[0,\pi]}(\xi)) = \{0, 1\}$. We need a formula describing how T_k and Δ commute.

Lemma 3.7. *Let $k \in [0, 2\pi]\backslash\{\pi\}$. Then for all $\theta \in C_c^\infty(\mathbb{R})$,*

$$T_k\theta(\Delta) = \theta(g_k(\Delta, \check{\mathbb{1}}_{[0,\pi]}))T_k, \tag{3.9}$$

where $g_k(x, y) : [0, 4] \times \{0, 1\} \mapsto \mathbb{R}$ is the function

$$g_k(x, y) := 2 + (x - 2)\cos(k) - \sin(k)\sqrt{x(4 - x)}(2y - 1). \tag{3.10}$$

Proof. First

$$\begin{aligned}(\mathcal{F}T_k\Delta\mathcal{F}^{-1}f)(\xi) &= (2 - 2\cos(\xi + k))f(\xi + k) \\ &= \left[2 - 2\cos(k)\cos(\xi) - 2\sin(k)\sqrt{1 - \cos^2(\xi)}(2\mathbb{1}_{[0,\pi]}(\xi) - 1)\right]f(\xi + k). \end{aligned}\tag{3.11}$$

Now,

$$g_k(\Delta, \check{\mathbb{1}}_{[0,\pi]}) := 2 + (\Delta - 2)\cos(k) - \sin(k)\sqrt{\Delta(4 - \Delta)}(2\check{\mathbb{1}}_{[0,\pi]} - 1).$$

Then (3.11) provides us with the following key relation:

$$T_k\Delta = g_k(\Delta, \check{\mathbb{1}}_{[0,\pi]})T_k.$$

In particular, for all $z \in \mathbb{C}\backslash\mathbb{R}$,

$$T_k(z - \Delta)^{-1} = \left(z - g_k(\Delta, \check{\mathbb{1}}_{[0,\pi]})\right)^{-1}T_k.$$

The result follows by applying the Helffer-Sjöstrand formula. □

We are now ready to prove Lemma 3.4.

Proof of Lemma 3.4. We apply (3.9) and get

$$\theta(\Delta)\tilde{W}\theta(\Delta) = \theta(\Delta)\theta(g_k(\Delta, \check{\mathbb{1}}_{[0,\pi]}))qT_k/(2\mathrm{i}) - \theta(\Delta)\theta(g_{2\pi-k}(\Delta, \check{\mathbb{1}}_{[0,\pi]}))qT_{2\pi-k}/(2\mathrm{i}).$$

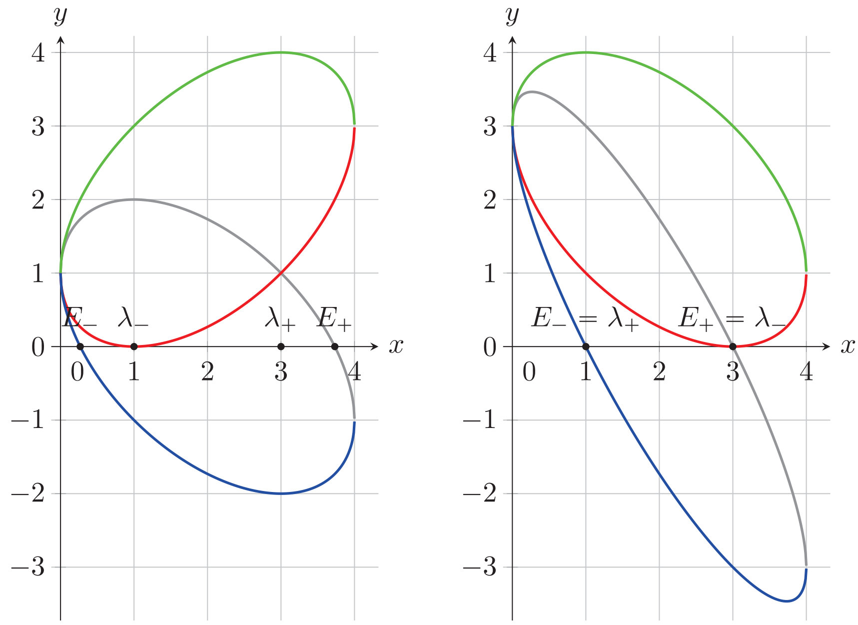

FIGURE 1. $g_{k;-}$, $g_{k;+}$, $h_{k;-}$ and $h_{k;+}$ for $k = \pi/3$ (left) and $k = 2\pi/3$ (right)

We show that for all $k \in [0, 2\pi]\backslash\{\pi\}$, one may choose θ appropriately so that

$$\theta(\Delta)\theta(g_k(\Delta, \check{\mathbb{1}}_{[0,\pi]})) = 0.$$

Also, as will be seen shortly, $\theta(\Delta)\theta(g_k(\Delta, \check{\mathbb{1}}_{[0,\pi]})) = 0$ iff $\theta(\Delta)\theta(g_{2\pi-k}(\Delta, \check{\mathbb{1}}_{[0,\pi]})) = 0$. We appeal to the functional calculus for two self-adjoint commuting operators. Consider the function $g_k(x, y)$ of (3.10) defined for $(x, y) \in \sigma(\Delta) \times \sigma(\check{\mathbb{1}}_{[0,\pi]}) = [0, 4] \times \{0, 1\}$. We show that for all $E \in [0, 4]\backslash\{E_\pm(k)\}$, there exists $\varepsilon = \varepsilon(E) > 0$ such that for the interval $\mathcal{I} := (E - \varepsilon, E + \varepsilon)$,

$$\mathcal{I} \cap \{g_k(x, y) : x \in \mathcal{I}, y \in \{0, 1\}\} = \varnothing. \tag{3.12}$$

In this way if $\mathrm{supp}(\theta) = \mathcal{I}$, then we will have $\theta(x)\theta(g_k(x, y)) = 0$ as required. Set

$$\mathcal{E}(k) := \{E \in [0, 4] : \text{ there exists } y \in \{0, 1\} \text{ such that } E = g_k(E, y)\}. \tag{3.13}$$

Clearly if $E \in \mathcal{E}(k)$, then (3.12) does not hold at E. To simplify the analysis, we let

$$g_{k;\pm}(x) := 2 + (x - 2)\cos(k) \pm \sin(k)\sqrt{x(4 - x)} \quad \text{and} \quad h_{k;\pm}(x) := g_{k;\pm}(x) - x. \tag{3.14}$$

Notice that $h_{k;\pm}(E_\pm(k)) = 0$, and so $E_\pm(k) \in \mathcal{E}(k)$. To show that $\mathcal{E}(k) = \{E_-(k), E_+(k)\}$, it is equivalent to show that these are the only roots of $h_{k;\pm}$. Because of the symmetry relations

$$g_{k;+}(x) = 4 - g_{k;-}(4 - x) \quad \text{and} \quad h_{k;+}(x) = -h_{k;-}(4 - x), \tag{3.15}$$

we may focus our analysis on $g_{k;-}$ and $h_{k;-}$. Define $\alpha(k) := (\cos(k) - 1)(\sin(k))^{-1}$. The equation

$$h'_{k;-}(x) = (\cos(k) - 1) - \sin(k)(-x + 2)(x(4 - x))^{-1/2} = 0$$

can be solved via the quadratic formula and yields a single solution given by

$$\begin{cases} 2 + 2\sqrt{1 - (1 + \alpha^2(k))^{-1}} & \text{if } k \in (0, \pi) \\ 2 - 2\sqrt{1 - (1 + \alpha^2(k))^{-1}} & \text{if } k \in (\pi, 2\pi). \end{cases}$$

Consequently $h_{k;-}$ has exactly one local extremum. Combining this with the fact that $h_{k;-}$ is continuous, $h_{k;-}(0) = 2 - 2\cos(k) > 0$ and $h_{k;-}(4) = -2 + 2\cos(k) < 0$, we conclude that $E_-(k)$ is the only root of $h_{k;-}$. By (3.15) we immediately get that $E_+(k)$ is the only root of $h_{k;+}$. We move on to the analysis of $g_{k;-}$. The equation

$$g'_{k;-}(x) = \cos(k) - \sin(k)(-x+2)(x(4-x))^{-1/2} = 0$$

has a single solution given by

$$\lambda_-(k) := \begin{cases} 2 - 2\sqrt{1-(1+\beta^2(k))^{-1}} = 2 - 2|\cos(k)| & \text{if } k \in (0, \pi/2] \cup (\pi, 3\pi/2] \\ 2 + 2\sqrt{1-(1+\beta^2(k))^{-1}} = 2 + 2|\cos(k)| & \text{if } k \in [\pi/2, \pi) \cup [3\pi/2, 2\pi). \end{cases}$$

Here $\beta(k) := \cot(k)$. We conclude that $g_{k;-}$ has exactly one local extremum. We note that $g_{k;-}(\lambda_-(k)) = 0$ when $k \in (0,\pi)$ and $g_{k;-}(\lambda_-(k)) = 4$ when $k \in (\pi, 2\pi)$. Finally, we have

$$h''_{k;-}(x) = g''_{k;-}(x) = 4\sin(k)(x(4-x))^{-3/2}.$$

The relevant details are summarized in Tables 1, 2, 3 and 4. We are ready to complete the proof.

k	$\lambda_-(k)$	$E_-(k)$		$g''_{k;-}(x) = h''_{k;-}(x)$
$\in (0,\pi)$	$= 2 - 2\cos(k)$	$= 2 - 2\cos(k/2)$	$E_-(k) < \lambda_-(k)$	$> 0\ \forall x \in [0,4]$
$\in (\pi, 2\pi)$	$= 2 + 2\cos(k)$	$= 2 - 2\cos(k/2)$	$\lambda_-(k) < E_-(k)$	$< 0\ \forall x \in [0,4]$

TABLE 1. Analysis of $g_{k;-}$ and $h_{k;-}$ for different values of k

x	0	$E_-(k)$	$\lambda_-(k)$	4	x	0	$\lambda_-(k)$	$E_-(k)$	4
$g_{k;-}(x)$	$\searrow$		$\searrow$ 0	$\nearrow$	$g_{k;-}(x)$	$\nearrow$ 4	$\searrow$		$\searrow$
$h_{k;-}(x)$	$+$	0	$-$	$-$	$h_{k;-}(x)$	$+$	$+$	0	$-$

TABLE 2. Variations of $g_{k;-}$ and sign of $h_{k;-}$ for $k \in (0,\pi)$ (left) and $k \in (\pi, 2\pi)$ (right)

k	$\lambda_+(k)$	$E_+(k)$		$g''_{k;+}(x) = h''_{k;+}(x)$
$\in (0,\pi)$	$= 2 + 2\cos(k)$	$= 2 + 2\cos(k/2)$	$\lambda_+(k) < E_+(k)$	$< 0\ \forall x \in [0,4]$
$\in (\pi, 2\pi)$	$= 2 - 2\cos(k)$	$= 2 + 2\cos(k/2)$	$E_+(k) < \lambda_+(k)$	$> 0\ \forall x \in [0,4]$

TABLE 3. Analysis of $g_{k;+}$ and $h_{k;+}$ for different values of k

x	0	$\lambda_+(k)$	$E_+(k)$	4	x	0	$E_+(k)$	$\lambda_+(k)$	4
$g_{k;+}(x)$	$\nearrow$ 4	$\searrow$		$\searrow$	$g_{k;+}(x)$	$\searrow$		$\searrow$ 0	$\nearrow$
$h_{k;+}(x)$	$+$	$+$	0	$-$	$h_{k;+}(x)$	$+$	0	$-$	$-$

TABLE 4. Variations of $g_{k;+}$ and sign of $h_{k;+}$ for $k \in (0,\pi)$ (left) and $k \in (\pi, 2\pi)$ (right)

Case $k \in (0,\pi)$, $y=0$: Depending on $E \in [0,4]\backslash\{E_-(k)\}$, we show that there exists an interval $\mathcal{I} \ni E$ such that one of the two following hold:

$$\mathcal{I} < g_{k;-}(\mathcal{I}), \tag{3.16}$$

$$\mathcal{I} > g_{k;-}(\mathcal{I}). \tag{3.17}$$

(A) For $E \in [0, E_-(k))$, there is $\varepsilon > 0$ such that $E+\varepsilon < g_{k;-}(E+\varepsilon)$. Thus (3.16) holds for $\mathcal{I} = (E-\varepsilon, E+\varepsilon)$. **(B)** For $E \in (E_-(k), \lambda_-(k))$, there is $\varepsilon > 0$ such that $g_{k;-}(E-\varepsilon) < E-\varepsilon$. Thus (3.17) holds for $\mathcal{I} = (E-\varepsilon, E+\varepsilon)$. **(C)** For $E = \lambda_-(k)$, there is $\varepsilon_1 > 0$ such that $g_{k;-}(\lambda_-(k)-\varepsilon_1) < \lambda_-(k)-\varepsilon_1$. Thus $[0, g_{k;-}(\lambda_-(k)-\varepsilon_1)] = g_{k;-}([\lambda_-(k)-\varepsilon_1, \lambda_-(k)]) < [\lambda_-(k)-\varepsilon_1, \lambda_-(k)]$. By continuity of $g_{k;-}$ there is $\varepsilon_2 > 0$ such that $g_{k;-}([\lambda_-(k), \lambda_-(k)+\varepsilon_2]) = [0, g_{k;-}(\lambda_-(k)+\varepsilon_2)] \subset [0, g_{k;-}(\lambda_-(k)-\varepsilon_1)]$. Thus (3.17) holds for $\mathcal{I} = (\lambda_-(k)-\varepsilon_1, \lambda_-(k)+\varepsilon_2)$. **(D)** Finally for $E \in (\lambda_-(k), 4]$, there is $\varepsilon > 0$ such that $h_{k;-}(t) < -2\varepsilon$ for all $t \in [E-\varepsilon, E+\varepsilon]$, and so $g_{k;-}(E+\varepsilon) < E-\varepsilon$. Thus (3.17) holds for $\mathcal{I} = (E-\varepsilon, E+\varepsilon)$.

Case $k \in (0,\pi)$, $y=1$: We denote $\lambda_+(k) = 4-\lambda_-(k)$ the location of the extremum of $g_{k;+}$. Depending on $E \in [0,4]\backslash\{E_+(k)\}$, one procedes in the same fashion as before to show that there exists an interval $\mathcal{I} \ni E$ such that one of the two following hold:

$$\mathcal{I} < g_{k;+}(\mathcal{I}), \tag{3.18}$$

$$\mathcal{I} > g_{k;+}(\mathcal{I}). \tag{3.19}$$

The case of $k \in (\pi, 2\pi)$ is also covered because $g_{(2\pi-k);+}(x) = g_{k;-}(x)$ for all $k \in (0,\pi)\backslash\{\pi\}$. ☐

4. The Multi-dimensional Case

We introduce the tensor product notation. The position space is the Hilbert space $\mathcal{H} = \ell^2(\mathbb{Z}^d) \approx \otimes_{i=1}^d \ell^2(\mathbb{Z})$. The d-dimensional Laplacian is equivalent to

$$\Delta \approx \Delta_1 \otimes \mathbb{1} \otimes \ldots \otimes \mathbb{1} \;+\; \mathbb{1} \otimes \Delta_2 \otimes \ldots \otimes \mathbb{1} \;+\; \ldots \;+\; \mathbb{1} \otimes \ldots \otimes \mathbb{1} \otimes \Delta_d$$

where the Δ_i are copies of the one-dimensional Laplacian. The potentials W and V cannot be written explicitely in tensor product notation, whereas W' can. The generator of dilations is

$$A \approx A_1 \otimes \mathbb{1} \otimes \ldots \otimes \mathbb{1} \;+\; \mathbb{1} \otimes A_2 \otimes \ldots \otimes \mathbb{1} \;+\; \ldots \;+\; \mathbb{1} \otimes \ldots \otimes \mathbb{1} \otimes A_d, \quad \mathcal{D}(A) := \otimes_{i=1}^d \mathcal{D}(A_i)$$

where the A_i are copies of the $1d$ generator of dilations defined as the closure of (3.1). Since the copies A_i are all self-adjoint, A is self-adjoint.

4.1. $\mathcal{C}^1(A)$ Regularity.

It is immediate that $[\Delta, \mathrm{i}A]$ extends to a bounded form and

$$[\Delta, \mathrm{i}A]_\circ \approx \Delta_1(4-\Delta_1) \otimes \mathbb{1} \ldots \otimes \mathbb{1} \;+\; \mathbb{1} \otimes \Delta_2(4-\Delta_2) \otimes \ldots \otimes \mathbb{1} \;+\; \ldots \;+\; \mathbb{1} \otimes \ldots \otimes \mathbb{1} \otimes \Delta_d(4-\Delta_d).$$

By induction, we have that $\Delta \in \mathcal{C}^\infty(A)$. We turn to the potential W. Define

$$K_W := 2^{-1} W \sum_{i=1}^d (S_i^* + S_i) + 2^{-1} \sum_{i=1}^d (S_i^* + S_i) W, \tag{4.1}$$

$$B_W := \sum_{i=1}^d U_i \tilde{W} (S_i^* - S_i) - \sum_{i=1}^d (S_i^* - S_i) \tilde{W} U_i, \tag{4.2}$$

where the U_i are the operators $(U_i u)(n) := n_i |n|^{-1} u(n)$ and $\tilde{W}$ is the operator $(\tilde{W} u)(n) := q \sin(k(n_1 + \ldots + n_d)) u(n)$. We have that for all $u, v \in \ell_0(\mathbb{Z}^d)$,

$$\langle u, [W, \mathrm{i}A] v \rangle = \langle u, K_W v \rangle + \langle u, B_W v \rangle.$$

Thus $[W, \mathrm{i}A]$ extends to a bounded operator and $[W, \mathrm{i}A]_\circ = K_W + B_W$. For the potential W',

$$\begin{aligned}[W', \mathrm{i}A]_\circ \approx & [W'_1, \mathrm{i}A_1]_\circ \otimes W'_2 \otimes ... \otimes W'_d \ + \ W'_1 \otimes [W'_2, \mathrm{i}A_2]_\circ \otimes ... \otimes W'_d \\ & + \ ... \ + \ W'_1 \otimes ... \otimes W'_{d-1} \otimes [W'_d, \mathrm{i}A_d]_\circ \\ := & K_{W'} + B_{W'}\end{aligned}$$

where

$$K_{W'} := K_{W'_1} \otimes W'_2 \otimes ... \otimes W'_d \ + \ W'_1 \otimes K_{W'_2} \otimes ... \otimes W'_d \ + \ ... \ + \ W'_1 \otimes ... \otimes W'_{d-1} \otimes K_{W'_d}, \tag{4.3}$$

$$B_{W'} := B_{W'_1} \otimes W'_2 \otimes ... \otimes W'_d \ + \ W'_1 \otimes B_{W'_2} \otimes ... \otimes W'_d \ + \ ... \ + \ W'_1 \otimes ... \otimes W'_{d-1} \otimes B_{W'_d}, \tag{4.4}$$

$$K_{W'_i} = 2^{-1} W'_i (S_i^* + S_i) + 2^{-1} (S_i^* + S_i) W'_i, \quad \text{and} \quad B_{W'_i} = \tilde{W}'_i (S_i^* - S_i) - (S_i^* - S_i) \tilde{W}'_i. \tag{4.5}$$

Here W'_i and $\tilde{W}'_i$ are one-dimensional operators defined by $(W'_i u)(n) = q_i \sin(k_i n) n^{-1} u(n)$, and $(\tilde{W}'_i u)(n) := q_i \sin(k_i n) u(n)$. Note that K_W and $K_{W'}$ are compact, while B_W and $B_{W'}$ are bounded but not compact by Proposition 4.2. As for the form $[V, \mathrm{i}A]$, we have as in (3.6) that for all $u, v \in \ell_0(\mathbb{Z}^d)$,

$$\langle u, [V, \mathrm{i}A] v \rangle = - \sum_{i=1}^{d} \langle u, \big[(N_i - 2^{-1})(V - \tau_i V) S_i + (N_i - 2^{-1})(V - \tau_i^* V) S_i^* \big] v \rangle. \tag{4.6}$$

Hypothesis (1.8) allows us to extend $[V, \mathrm{i}A]$ into a compact operator. This leads to the following

Proposition 4.1. *H and H' are of class $\mathcal{C}^1(A)$.*

As in the one-dimensional case, we have

Proposition 4.2. *H and H' are not of class $\mathcal{C}^{1,u}(A)$.*

Proof. As in the proof of Proposition 3.3, one shows that B_W and $B_{W'}$ are not compact. This can be done by considering the sequence $(\delta_j)_{j \geq 2}$ of unit vectors in $\ell^2(\mathbb{Z}^d)$ satisfying $(\delta_j)(n) = \delta_{j;n_1} \delta_{0;n_2} \cdots \delta_{0;n_d}$. This sequence is converging weakly to zero. If $B_{W'}$ was compact, we would require $B_{W'} \delta_j$ to converge strongly to zero, but this would lead to the same contradiction as in Proposition 3.3. As for B_W, we commute U_i with $(S_i^* - S_i)$ to produce a compact and get

$$B_W = \sum_{i=1}^{d} U_i [\tilde{W}(S_i^* - S_i) - (S_i^* - S_i) \tilde{W}] + \text{ compact}.$$

Again, applying this operator to δ_j and requiring the limit to converge strongly to zero would generate the same contradiction. □

4.2. **Classical Mourre Theory.** Recall that $\sigma(\Delta) = \overline{\sigma(\Delta_1) + ... + \sigma(\Delta_d)} = [0, 4d]$. We would like to identify the sub-intervals of $\sigma(\Delta)$ for which a strict Mourre estimate for Δ holds. Recall the function $\rho_T^A(E)$ introduced in paragraph 2.3. In the setting of the tensor product of two operators we have the standard result [ABG, Theorem 8.3.6]:

$$\varrho_T^A(E) = \inf_{E = x_1 + x_2} [\varrho_{T_1}^{A_1}(x_1) + \varrho_{T_2}^{A_2}(x_2)], \tag{4.7}$$

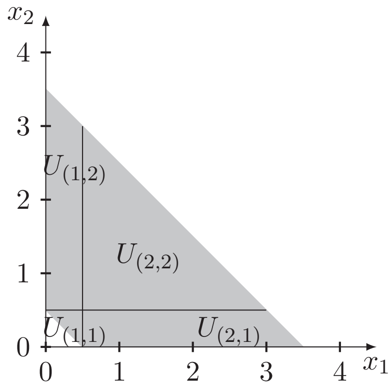

FIGURE 2. Support of $\chi_{\mathcal{I}}(x_1 + x_2)$ for $\mathcal{I} = (0.5, 3.5)$.

where $T := T_1 \otimes \mathbb{1} + \mathbb{1} \otimes T_2$ and $A := A_1 \otimes \mathbb{1} + \mathbb{1} \otimes A_2$ are an arbitrary pair of conjugate self-adjoint operators. Now, an easy consequence of the one-dimensional result (3.2) is that for all $x_i \in [0, 4]$

$$\varrho^A_{\Delta_i}(x_i) = x_i(4 - x_i).$$

Therefore we infer that in the case of $d = 2$, $0 < \varrho^A_{\Delta}(E) < \infty$ if and only if $E \in (0, 8)\backslash\{4\}$, so that the strict Mourre estimate for Δ holds at every point of the spectrum of Δ, except at the critical points $\{0, 4, 8\}$. If $d > 2$, then a similar formula to (4.7) holds with nested terms. One easily sees that $0 < \varrho^A_{\Delta}(E) < \infty$ if and only if $E \in (0, 4d)\backslash\{4j\}^{d-1}_{j=1}$, so that the strict Mourre estimate holds at every point of the spectrum of Δ, except at the critical points $\{4j\}^d_{j=0}$. For the special case of the discrete Laplacian, the classic strict Mourre estimate can be derived without resorting to formula (4.7) whose proof is somewhat elaborate. We show how this can be done.

We work in two dimensions, but remark that the same setup can be generalized for $d > 2$. Let $\varepsilon \in (0, 2)$ be given and let $\mathcal{I} = (\varepsilon, 4 - \varepsilon)$. By (3.2), we have

$$E_{\mathcal{I}}(\Delta_i)[\Delta_i, \mathrm{i}A_i]_\circ E_{\mathcal{I}}(\Delta_i) \geqslant \varepsilon(4 - \varepsilon) E_{\mathcal{I}}(\Delta_i), \quad \text{for all} \quad i = 1, 2. \tag{4.8}$$

The following Proposition converts the one-dimensional (optimal) strict Mourre estimate for Δ into a two-dimensional strict Mourre estimate.

Proposition 4.3. *For every $\varepsilon \in (0, 2)$, let $\mathcal{I} := (\varepsilon, 4 - \varepsilon)$, or $\mathcal{I} := (4 + \varepsilon, 8 - \varepsilon)$. Then the strict Mourre estimate holds for the two-dimensional Laplacian Δ on $\mathcal{I}$, namely:*

$$E_{\mathcal{I}}(\Delta)[\Delta, \mathrm{i}A]_\circ E_{\mathcal{I}}(\Delta) \geqslant \varepsilon(4 - \varepsilon) E_{\mathcal{I}}(\Delta). \tag{4.9}$$

Proof. We consider the case $\mathcal{I} = (\varepsilon, 4 - \varepsilon)$, as the other case is similar. Note that $\chi_{\mathcal{I}}(x_1 + x_2)$ is supported on the open set $U := \{(x_1, x_2) \in [0, 4] \times [0, 4] : x_1 + x_2 \in \mathcal{I}\}$ which has the form of a trapezoid. We decompose U in four regions, namely $U_{(1,1)} := U \cap [0, \varepsilon) \times [0, \varepsilon)$, $U_{(1,2)} := U \cap [0, \varepsilon) \times [\varepsilon, 4 - \varepsilon)$, $U_{(2,1)} := U \cap [\varepsilon, 4 - \varepsilon) \times [0, \varepsilon)$, and $U_{(2,2)} := U \cap [\varepsilon, 4 - \varepsilon) \times [\varepsilon, 4 - \varepsilon)$.

For $n \in \mathbb{N}$ and $(i, j) \in \{1, ..., 2^n\} \times \{1, ..., 2^n\}$, consider the disjoint intervals of the form

$$\mathcal{I}_{1;i;n} := \big[(i - 1)2^{-n}\varepsilon, i2^{-n}\varepsilon\big) \quad \text{and} \quad \mathcal{I}_{2;j;n} := \big[\varepsilon + (j - 1)2^{-n}(4 - 2\varepsilon), \varepsilon + j2^{-n}(4 - 2\varepsilon)\big)$$

which satisfy $\cup^{2^n}_{i=1} \mathcal{I}_{1;i;n} = [0, \varepsilon)$ and $\cup^{2^n}_{j=1} \mathcal{I}_{2;j;n} = [\varepsilon, 4 - \varepsilon)$. For $\alpha, \beta \in \{1, 2\}$, let

$$F_{\alpha,\beta,n} := \{(i, j) \in \{1, ..., 2^n\} \times \{1, ..., 2^n\} : \mathcal{I}_{\alpha;i;n} \times \mathcal{I}_{\beta;j;n} \subset U_{(\alpha,\beta)}\}.$$

Then

$$\lim_{n\to\infty} \bigcup_{(i,j)\in F_{\alpha,\beta,n}} \mathcal{I}_{\alpha;i;n} \times \mathcal{I}_{\beta;j;n} = U_{(\alpha,\beta)}.$$

In terms of operators, we have

$$\operatorname*{s-lim}_{n\to\infty} \sum_{\alpha,\beta=1,2} \sum_{(i,j)\in F_{\alpha,\beta,n}} E_{\mathcal{I}_{\alpha;i;n}}(\Delta_1) \otimes E_{\mathcal{I}_{\beta;j;n}}(\Delta_2) = E_{\mathcal{I}}(\Delta).$$

Now, $[\Delta, \mathrm{i}A]_\circ = [\Delta_1, \mathrm{i}A_1]_\circ \otimes \mathbb{1} + \mathbb{1} \otimes [\Delta_2, \mathrm{i}A_2]_\circ$, so for fixed n we calculate:

$$\begin{aligned}
&\left(\sum_{\alpha,\beta}\sum_{(i,j)} E_{\mathcal{I}_{\alpha;i;n}}(\Delta_1) \otimes E_{\mathcal{I}_{\beta;j;n}}(\Delta_2)\right)[\Delta, \mathrm{i}A]_\circ \left(\sum_{\alpha',\beta'}\sum_{(i',j')} E_{\mathcal{I}_{\alpha';i';n}}(\Delta_1) \otimes E_{\mathcal{I}_{\beta';j';n}}(\Delta_2)\right) \\
&= \sum_{\alpha,\beta}\sum_{(i,j)}\sum_{\alpha'}\sum_{(i',j)} E_{\mathcal{I}_{\alpha;i;n}}(\Delta_1)[\Delta_1, \mathrm{i}A_1]_\circ E_{\mathcal{I}_{\alpha';i';n}}(\Delta_1) \otimes E_{\mathcal{I}_{\beta;j;n}}(\Delta_2) \\
&\qquad + \sum_{\alpha,\beta}\sum_{(i,j)}\sum_{\beta'}\sum_{(i,j')} E_{\mathcal{I}_{\alpha;i;n}}(\Delta_1) \otimes E_{\mathcal{I}_{\beta;j;n}}(\Delta_2)[\Delta_2, \mathrm{i}A_2]_\circ E_{\mathcal{I}_{\beta';j';n}}(\Delta_2) \\
&\qquad \geqslant \sum_{\alpha,\beta}\sum_{(i,j)} E_{\mathcal{I}_{\alpha;i;n}}(\Delta_1)[\Delta_1, \mathrm{i}A_1]_\circ E_{\mathcal{I}_{\alpha;i;n}}(\Delta_1) \otimes E_{\mathcal{I}_{\beta;j;n}}(\Delta_2) \\
&\qquad\qquad + \sum_{\alpha,\beta}\sum_{(i,j)} E_{\mathcal{I}_{\alpha;i;n}}(\Delta_1) \otimes E_{\mathcal{I}_{\beta;j;n}}(\Delta_2)[\Delta_2, \mathrm{i}A_2]_\circ E_{\mathcal{I}_{\beta;j;n}}(\Delta_2) \\
&\qquad \geqslant \sum_{\alpha,\beta}\sum_{(i,j)} (c_{\alpha;i;n} + c_{\beta;j;n}) E_{\mathcal{I}_{\alpha;i;n}}(\Delta_1) \otimes E_{\mathcal{I}_{\beta;j;n}}(\Delta_2)
\end{aligned}$$

for some positive constants $c_{\alpha;i;n}$ and $c_{\beta;j;n}$ which can possibly be 0 if $\alpha = 1$ and $i = 1$ or if $\beta = 1$ and $j = 1$. However $c_{\alpha;i;n}$ and $c_{\beta;j;n}$ are not independent since $(i,j) \in F_{\alpha,\beta,n}$; in fact $c_{\alpha;i;n} + c_{\beta;j;n} \geqslant \varepsilon(4-\varepsilon) > 0$ for all $\alpha, \beta \in \{1,2\}$ and $(i,j) \in F_{\alpha,\beta,n}$. The case $\alpha = \beta = 1$ is the least obvious. Consider $\Gamma(x_1, x_2) = x_1(4-x_1) + x_2(4-x_2)$ defined for $(x_1, x_2) \in [0,\varepsilon) \times [0,\varepsilon)$ which represents how $c_{\alpha;i;n} + c_{\beta;j;n}$ varies. Then $c_{1;i;n} + c_{1;j;n} \geqslant \Gamma(x_1, \varepsilon - x_1) = -2x_1^2 + 2x_1\varepsilon - \varepsilon^2 + 4\varepsilon \geqslant -\varepsilon^2 + 4\varepsilon$. The proof is now complete by taking the limit $n \to \infty$. □

We are now working our way towards a classic Mourre estimate (2.4) for the full Schrödinger operator H. As in the one-dimensional case, $[V, \mathrm{i}A]_\circ$ is compact, and $[W, \mathrm{i}A]_\circ$ is the sum of a compact operator K_W and a bounded operator B_W defined by (4.2), so we really only have to show that $E_{\mathcal{I}}(H) B_W E_{\mathcal{I}}(H)$ is compact.

Let $k \in [0, 2\pi]\backslash\{\pi\}$, and let T_k be the multiplication operator on $\ell^2(\mathbb{Z}^d)$ given by $(T_k u)(n) := e^{\mathrm{i}k(n_1+\ldots+n_d)}u(n)$. Then T_k corresponds to a translation in the Fourier space of 2π-periodic functions by k in each direction, that is, $(\mathcal{F}T_k\mathcal{F}^{-1}f)(\xi) = f(\xi + k)$ (see (1.4) for the definition of the discrete Fourier transform). Denote by $\check{\mathbb{1}}_{[0,\pi],i}$ the operator on $\ell^2(\mathbb{Z}^d)$ satisfying $(\mathcal{F}\check{\mathbb{1}}_{[0,\pi],i}\mathcal{F}^{-1}f)(\xi) = \mathbb{1}_{[0,\pi]}(\xi_i)f(\xi)$. Note that $\check{\mathbb{1}}_{[0,\pi],i}$ is a bounded self-adjoint operator with spectrum $\sigma(\check{\mathbb{1}}_{[0,\pi],i}) = \text{ess ran}\,(\mathbb{1}_{[0,\pi]}(\xi_i)) = \{0,1\}$. Moreover $\check{\mathbb{1}}_{[0,\pi],i}$ commutes with $\check{\mathbb{1}}_{[0,\pi],j}$ and Δ_j for all $1 \leqslant i,j \leqslant d$. Here Δ_j is the Laplacian restricted to the j^{th} dimension : $(\mathcal{F}\Delta_j\mathcal{F}^{-1}f)(\xi) = f(\xi)(2 - 2\cos(\xi_j))$ and $\sigma(\Delta_j) = [0,4]$. We need a formula describing how Δ and T_k commute.

Lemma 4.4. *Let $k \in [0, 2\pi]\backslash\{\pi\}$. Then for all $\theta \in C_c^\infty(\mathbb{R})$,*

$$T_k \theta(\Delta) = \theta \left(\sum_{i=1}^{d} g_k(\Delta_i, \check{\mathbb{1}}_{[0,\pi],i}) \right) T_k, \tag{4.10}$$

where $g_k(x, y) : [0, 4] \times \{0, 1\} \mapsto \mathbb{R}$ is the function defined in (3.10).

Proof. First

$$\begin{aligned}(\mathcal{F} T_k \Delta \mathcal{F}^{-1} f)(\xi) &= f(\xi + k) \sum_{i=1}^{d} (2 - 2\cos(\xi_i + k)) \\ &= f(\xi + k) \sum_{i=1}^{d} \left[2 - 2\cos(k)\cos(\xi_i) - 2\sin(k)\sqrt{1 - \cos^2(\xi_i)}(2\mathbb{1}_{[0,\pi]}(\xi_i) - 1) \right]. \qquad (4.11)\end{aligned}$$

Letting $g_k(\Delta_i, \check{\mathbb{1}}_{[0,\pi],i}) := 2 + (\Delta_i - 2)\cos(k) - \sin(k)\sqrt{\Delta_i(4 - \Delta_i)}(2\check{\mathbb{1}}_{[0,\pi],i} - 1)$ and continuing as in Lemma 3.7 leads to the required formula. □

Since $\{\Delta_i, \check{\mathbb{1}}_{[0,\pi],i}\}_{i=1}^d$ forms a family of $2d$ self-adjoint commuting operators, we may apply the functional calculus for such operators. We are now ready to prove that θ can be chosen so that $\theta(H) B_W \theta(H)$ is compact.

Proposition 4.5. *Let*

$$E(k) := \begin{cases} 4 - 4\cos(k/2) & \text{for } k \in (0, \pi) \\ 4 + 4\cos(k/2) & \text{for } k \in (\pi, 2\pi) \end{cases} \quad \text{and} \quad \mu(H) := (0, E(k)) \cup (4d - E(k), 4d). \tag{4.12}$$

For each $E \in \mu(H)$ there exists $\varepsilon = \varepsilon(E) > 0$ such that for all $\theta \in C_c^\infty(\mathbb{R})$ supported on $\mathcal{I} := (E - \varepsilon, E + \varepsilon)$, $\theta(\Delta) \tilde{W} \theta(\Delta) = 0$. In particular, $\theta(\Delta) B_W \theta(\Delta)$ is compact. Consequently, for every $E \in \mu(H)$, the classical Mourre estimate (2.4) holds for H on $\mathcal{I}'$, where $\overline{\mathcal{I}'} \subset \mathcal{I}$.

Remark 4.1. *The unitary transformation $u(n) \mapsto (-1)^{n_1 + \ldots + n_d} u(n)$ for all $u \in \mathcal{H} := \ell^2(\mathbb{Z}^d)$ shows that Δ and $4d - \Delta$ are unitarily equivalent, (and likewise for $H := \Delta + W + V$ and $4d - \Delta + W + V$). Because of this symmetry, showing that $\theta(\Delta) B_W \theta(\Delta)$ is compact for θ supported on $\mathcal{I} = (E - \varepsilon, E + \varepsilon)$ and $E \in (0, E(k))$ implies it for $E \in (4d - E(k), 4d)$ (and vice versa). This symmetry is due to the bipartite structure of $\mathbb{Z}^d$.*

Remark 4.2. *That $\theta(\Delta) B_W \theta(\Delta)$ is compact and not zero is because commuting U_i with Δ produces a compact operator. Then using the strict Mourre estimate for Δ from Proposition 4.3 or (4.7), one derives the Mourre estimate for H in the same way as in Proposition 3.5.*

Proof. The strategy is the same as in 1d (cf. Lemma 3.4 for the notation). Thanks to (4.10),

$$\begin{aligned}&\theta(\Delta)\tilde{W}\theta(\Delta) \\ &\quad = \theta(\Delta)\theta\left(\sum_{i=1}^{d} g_k(\Delta_i, \check{\mathbb{1}}_{[0,\pi],i})\right) qT_k/(2\mathrm{i}) - \theta(\Delta)\theta\left(\sum_{i=1}^{d} g_{2\pi-k}(\Delta_i, \check{\mathbb{1}}_{[0,\pi],i})\right) qT_{2\pi-k}/(2\mathrm{i}),\end{aligned}$$

and so it is enough to show that $\theta(\Delta)\theta\left(\sum_i g_k(\Delta_i, \check{\mathbb{1}}_{[0,\pi],i})\right) = 0$ for $k \in (0, 2\pi)\backslash\{\pi\}$ and θ appropriately chosen. Consider the function $g_k(x, y)$ of (3.10) defined for $(x, y) \in \sigma(\Delta_i) \times$

$\sigma(\check{\mathbb{1}}_{[0,\pi],i}) = [0,4] \times \{0,1\}$. We want to find $\varepsilon = \varepsilon(E) > 0$ such that for the interval $\mathcal{I} := (E-\varepsilon, E+\varepsilon)$.

$$\mathcal{I} \cap \Big\{ \sum_{1 \leqslant i \leqslant d} g_k(x_i, y_i) : (x_1, ..., x_d) \in R \ \text{ and } \ (y_1, ..., y_d) \in \{0,1\}^d \Big\} = \varnothing. \tag{4.13}$$

Here R is the region defined by $R := \{(x_1, ..., x_d) \in [0,4]^d : x_1 + ... + x_d \in \mathcal{I}\}$. In this way if $\text{supp}(\theta) = \mathcal{I}$, then we will have $\theta(x_1 + ... + x_d)\theta(\sum_i g_k(x_i, y_i)) = 0$ as required. Set

$$\begin{aligned}\mathcal{E}_d(k) := \{E \in [0,4d] :\ & \text{there exist } (x_1, ..., x_d) \in [0,4]^d \text{ and } (y_1, ..., y_d) \in \{0,1\}^d \\ & \text{such that } E = x_1 + ... + x_d = g_k(x_1, y_1) + ... + g_k(x_d, y_d)\}.\end{aligned} \tag{4.14}$$

If $E \in \mathcal{E}_d(k)$, then (4.13) does not hold at E. Note also that $\mathcal{E}_d(k) = \mathcal{E}_d(2\pi - k)$. First we work in $d = 2$, and extend the result for $d \geqslant 3$ at the very end. To identify the set $\mathcal{E}_2(k)$, we solve

$$\mathscr{E}_{k;*;\diamond} : \quad h_{k;*}(x_1) + h_{k;\diamond}(x_2) = 0, \quad \text{for } *, \diamond \in \{-,+\}. \tag{4.15}$$

We denote by $S_{k;*;\diamond}$ the solutions to $\mathscr{E}_{k;*;\diamond}$ and let $E_{k;*;\diamond} := \{x_1 + x_2 : (x_1, x_2) \in S_{k;*;\diamond}\}$. By (3.15), $(x_1, x_2) \in S_{k;-;-}$ iff $(4 - x_1, 4 - x_2) \in S_{k;+;+}$. By symmetry, $(x_1, x_2) \in S_{k;-;+}$ iff $(x_2, x_1) \in S_{k;+;-}$. We focus first on $\mathscr{E}_{k;-;-}$. In this case, note that (x_1, x_2) is a solution iff (x_2, x_1) is a solution. With the change of variables $(x_1, x_2) = (2 - 2\cos(\phi), 2 - 2\cos(\varphi))$, $(\phi, \varphi) \in [0,\pi]^2$, $\mathscr{E}_{k;-;-}$ becomes

$$-2\cos(\phi)(\cos(k) - 1) - 2\sin(k)\sin(\phi) - 2\cos(\varphi)(\cos(k) - 1) - 2\sin(k)\sin(\varphi) = 0$$

which reduces to

$$-8\sin(k/2)\sin((\phi + \varphi - k)/2)\cos((\phi - \varphi)/2) = 0. \tag{4.16}$$

Thus $(\phi + \varphi - k)/2 = 0$ [mod π] or $(\phi - \varphi)/2 = \pi/2$ [mod π]. Considering $(\phi, \varphi) \in [0,\pi]^2$ and the cases $k \in (0,\pi)$ and $k \in (\pi, 2\pi)$ separately, one can rule out several possibilities. Let $J_k := [0,k]$ if $k \in (0,\pi)$, and $J_k := [k - \pi, \pi]$ if $k \in (\pi, 2\pi)$. The valid solutions of the previous equation are $(\phi, \varphi) \in \{(0,\pi), (\pi, 0), (\phi, k - \phi), \text{with } \phi \in J_k\}$. The solutions to $\mathscr{E}_{k;-;-}$ are

$$S_{k;-;-} = \{(0,4), (4,0), (2 - 2\cos(\phi), 2 - 2\cos(k - \phi)), \phi \in J_k\},$$

Let $f_{k;-;-}(\phi) := 2 - 2\cos(\phi) + 2 - 2\cos(k - \phi) = 4 - 4\cos(k/2)\cos(\phi - k/2)$. Thus

$$\mathcal{E}_2(k) \supset E_{k;-;-} = \{4\} \cup f_{k;-;-}(J_k) = \begin{cases} \{4\} \cup [4 - 4\cos(k/2), 2 - 2\cos(k)] & \text{for } k \in (0,\pi) \\ \{4\} \cup [6 + 2\cos(k), 4 - 4\cos(k/2)] & \text{for } k \in (\pi, 2\pi). \end{cases}$$

The solutions of $\mathscr{E}_{k;+;+}$ are

$$S_{k;+;+} = \{(0,4), (4,0), (2 + 2\cos(\phi), 2 + 2\cos(k - \phi)), \phi \in J_k\}.$$

Let $f_{k;+;+}(\phi) := 2 + 2\cos(\phi) + 2 + 2\cos(k - \phi) = 4 + 4\cos(k/2)\cos(\phi - k/2)$. Then

$$\mathcal{E}_2(k) \supset E_{k;+;+} = \{4\} \cup f_{k;+;+}(J_k) = \begin{cases} \{4\} \cup [6 + 2\cos(k), 4 + 4\cos(k/2)] & \text{for } k \in (0,\pi) \\ \{4\} \cup [4 + 4\cos(k/2), 2 - 2\cos(k)] & \text{for } k \in (\pi, 2\pi). \end{cases}$$

We now solve $\mathscr{E}_{k;-;+}$. With the same change of variables as before, this equation becomes

$$8\sin(k/2)\sin((\varphi - \phi + k)/2)\cos((\phi + \varphi)/2) = 0. \tag{4.17}$$

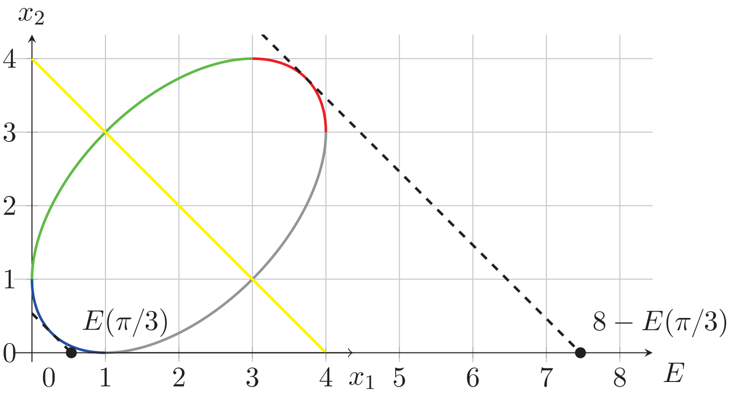

FIGURE 3. Solutions $S_{-;-}$, $S_{+;+}$, $S_{-;+}$ and $S_{+;-}$ to $\mathscr{E}_{k;*;\diamond}$ for $k=\pi/3$ and $*,\diamond\in\{-,+\}$, $d=2$

Let $J'_k := [k,\pi]$ for $k\in(0,\pi)$ and $J'_k := [0,k-\pi]$ for $k\in(\pi,2\pi)$. The solutions to this equation are $(\phi,\varphi)\in\{(\phi,\pi-\phi),\ \text{with}\ \phi\in[0,\pi],(\phi,\phi-k),\ \text{with}\ \phi\in J'_k\}$. Thus

$$S_{k;-;+}=\{(t,4-t),t\in[0,4],(2-2\cos(\phi),2-2\cos(k-\phi)),\phi\in J'_k\}.$$

Note that $f_{k;-;-}$ is strictly increasing on J'_k. Thus

$$\mathcal{E}_2(k)\supset E_{k;-;+}=\{4\}\cup f_{k;-;-}(J'_k)=\begin{cases}\{4\}\cup[2-2\cos(k),6+2\cos(k)] & \text{for } k\in(0,\pi)\\ \{4\}\cup[2-2\cos(k),6+2\cos(k)] & \text{for } k\in(\pi,2\pi).\end{cases}$$

Finally, by symmetry, $E_{k;+;-}=E_{k;-;+}$. Putting together our previous results, we have

$$\mathcal{E}_2(k)=[\lambda_\ell(k),\lambda_r(k)]=E_{k;-;-}\cup E_{k;+;+}\cup E_{k;-;+}\cup E_{k;+;-}. \tag{4.18}$$

We now aim to derive (4.13) on $\mathcal{L}_k:=[0,E(k))$. Fix $k\in\mathcal{T}:=(0,2\pi)\backslash\{\pi\}$. For $\lambda\in\mathcal{L}_k$ define the function $F_{\lambda;k}$ on $[0,\lambda]$ by

$$F_{\lambda;k}(x):=\begin{cases}h_{k;-}(x)+h_{k;-}(\lambda-x) & \text{for } (\lambda,k)\in\mathcal{M}_k:=\mathcal{L}_k\times(0,\pi)\\ h_{k;+}(x)+h_{k;+}(\lambda-x) & \text{for } (\lambda,k)\in\mathcal{N}_k:=\mathcal{L}_k\times(\pi,2\pi)\end{cases}$$

$$=\begin{cases}(\lambda-4)(\cos(k)-1)-\sin(k)\sqrt{x(4-x)}-\sin(k)\sqrt{(-x+\lambda)(4+x-\lambda)} & \text{for } (\lambda,k)\in\mathcal{M}_k\\ (\lambda-4)(\cos(k)-1)+\sin(k)\sqrt{x(4-x)}+\sin(k)\sqrt{(-x+\lambda)(4+x-\lambda)} & \text{for } (\lambda,k)\in\mathcal{N}_k.\end{cases}$$

A surprising calculation yields the single solution $x=\lambda/2$ to the equation $F'_{\lambda;k}(x)=0$ for all $k\in\mathcal{T}$ and $\lambda\in\mathcal{L}_k$. Also, when $(\lambda,k)\in\mathcal{L}_k\times\mathcal{T}$, $F_{\lambda;k}(0)=F_{\lambda;k}(\lambda)>F_{\lambda;k}(\lambda/2)$. Hence

$$\forall\lambda\in\mathcal{L}_k,\ \forall k\in\mathcal{T},\ \min_{x\in[0,\lambda]}F_{\lambda;k}(x)=F_{\lambda;k}(\lambda/2).$$

Define for $\lambda\in\overline{\mathcal{L}_k}\times\mathcal{T}$ the function

$$f_k(\lambda):=F_{\lambda;k}(\lambda/2)=\begin{cases}(\lambda-4)(\cos(k)-1)-\sin(k)\sqrt{\lambda(8-\lambda)} & \text{for } (\lambda,k)\in\mathcal{M}_k\\ (\lambda-4)(\cos(k)-1)+\sin(k)\sqrt{\lambda(8-\lambda)} & \text{for } (\lambda,k)\in\mathcal{N}_k.\end{cases}$$

Then for all $k\in\mathcal{T}$, $f_k(0)=4(1-\cos(k))>0$ and $f_k(E(k))=0$. We claim that for all $k\in\mathcal{T}$, f_k is strictly decreasing and positive on $\mathcal{L}_k$. To prove this, consider the functions

$$m_{k;\mp}(\lambda):=(\lambda-4)(\cos(k)-1)\mp\sin(k)\sqrt{\lambda(8-\lambda)}$$

defined on $[0,8]\times\mathcal{T}$. The equation $m'_{k;*}(\lambda)=0$ has a single solution

$$\lambda = 4+4\sqrt{1-(1+\alpha(k)^2)^{-1}} > E(k) \quad \text{when } (k,*)\in(0,\pi)\times\{-\}\cup(\pi,2\pi)\times\{+\}.$$

Recall $\alpha(k) := (\cos(k)-1)(\sin(k))^{-1}$. The claim is therefore verified. Now let $E\in\mathcal{L}_k$, and choose $\varepsilon'>0$ such that $\mathcal{I} := (E-\varepsilon', E+\varepsilon')\subset\mathcal{L}_k$. Recall that R is the region defined after (4.13). Let $(k,*)\in(0,\pi)\times\{-\}\cup(\pi,2\pi)\times\{+\}$. We have:

$$\begin{aligned}\inf\{g_{k;*}(x_1)+g_{k;*}(x_2) : (x_1,x_2)\in R\} &= \inf\{g_{k;*}(x)+g_{k;*}(\lambda-x) : \lambda\in\mathcal{I}, x\in[0,\lambda]\}\\ &\geqslant \inf\{f_k(\lambda)+\lambda : \lambda\in\mathcal{I}\}\\ &\geqslant \varepsilon+E-\varepsilon'.\end{aligned}$$

Here ε is any real in $(0, f_k(E+\varepsilon'))$. Taking ε' even smaller, the above inequalities remain valid with the same ε since f_k is decreasing. Thus we may take $\varepsilon'=\varepsilon/2$ for example. Moreover, since $g_{k;+}\geqslant g_{k;-}(x)$ for all $(x,k)\in[0,4]\times(0,\pi)$ and $g_{k;-}\geqslant g_{k;+}(x)$ for all $(x,k)\in[0,4]\times(\pi,2\pi)$, we have proven that for all $(k,*,\diamond)\in\mathcal{T}\times\{-,+\}\times\{-,+\}$,

$$\inf\{g_{k;*}(x_1)+g_{k;\diamond}(x_2) : (x_1,x_2)\in R\}\geqslant E+\varepsilon/2. \tag{4.19}$$

This proves (4.13) for $E\in\mathcal{L}_k$, with $\mathcal{I}=(E-\varepsilon/2,E+\varepsilon/2)$ and $k\in\mathcal{T}$.

Now we proceed to extend the results for $d\geqslant 3$. Recall the properties of the function $g_{k;\pm}$ listed in Tables 2 and 4. In particular, $g_{k;-}(x)\geqslant 0$ for all $(x,k)\in[0,\lambda_-(k)]\times(0,\pi)$ where $\lambda_-(k) = 2-2\cos(k)$, and $g_{k;+}(x)\geqslant 0$ for all $(x,k)\in[0,\lambda_+(k)]\times(\pi,2\pi)$ where $\lambda_+(k)=2-2\cos(k)$. We take advantage of the fact that $E(k)<\lambda_-(k)$ for all $k\in(0,\pi)$ and $E(k)<\lambda_+(k)$ for all $k\in(\pi,2\pi)$. Again, let $E\in\mathcal{L}_k$, and choose $\varepsilon>0$ such that $\mathcal{I} := (E-\varepsilon/2,E+\varepsilon/2)\subset\mathcal{L}_k$. Let $(k,*)\in(0,\pi)\times\{-\}\cup(\pi,2\pi)\times\{+\}$. Applying the two-dimensional result we obtain

$$\begin{aligned}&\inf\left\{\sum_{i=1}^d g_k(x_i,y_i) : (x_i)_{i=1}^d\in R, (y_i)_{i=1}^d\in\{0,1\}^d\right\}\\ &\qquad\geqslant \inf\left\{\sum_{i=1}^d g_{k;*}(x_i) : (x_i)_{i=1}^d\in R\right\}\\ &\qquad\geqslant \inf\{g_{k;*}(x)+g_{k;*}(\lambda-x) : \lambda\in\mathcal{I}, x\in[0,\lambda]\}\\ &\qquad\geqslant E+\varepsilon/2.\end{aligned}$$

As this implies (4.13) for $E\in\mathcal{L}_k$, the proof is now complete. □

The method employed is optimal in the following sense: let $d=2$, $q\neq 0$ and $k\in(0,2\pi)\backslash\{\pi\}$. Then for all $E\in(0,8)\backslash\mu(H)=[E(k),8-E(k)]$ and for all $\theta\in C_c^\infty(\mathbb{R})$ with $\mathrm{supp}(\theta)\ni E$, $\theta(\Delta)B_W\theta(\Delta)$ is not compact. Indeed, it is not hard to see that if $\xi=(\xi_1,...,\xi_d)\in[-\pi,\pi]^d$ solves

$$\sum_{i=1}^d(2-2\cos(\xi_i)) = \sum_{i=1}^d(2-2\cos(\xi_i+k)) \quad\text{or}\quad \sum_{i=1}^d(2-2\cos(\xi_i)) = \sum_{i=1}^d(2-2\cos(\xi_i-k)), \tag{4.20}$$

then $\theta(\Delta)B_W\theta(\Delta)$ is not compact for all θ with $\mathrm{supp}(\theta)\ni E=\sum_i(2-2\cos(\xi_i))$. We note that (4.20) is precisely the same as (4.16) and (4.17) when $d=2$. By using the method of Lagrange multipliers for example, a slightly better value for $E(k)$ can be found when $d\geqslant 3$ (a value increasing with d). The method consists in extremizing $E=\sum_i(2-2\cos(\xi_i))$ with the constraints given in (4.20). We move on to derive the classic Mourre estimate (2.4) for the full Schrödinger operator H'. We really only have to show that $E_{\mathcal{I}}(H')B_{W'}E_{\mathcal{I}}(H')$ is compact.

Proposition 4.6. *Let $k = (k_1, ..., k_d) \in ([0, 2\pi]\backslash\{\pi\})^d$ be given parameters, and let*

(4.21)

$$E'(k) := \min\{\ell(k_i) : 1 \leqslant i \leqslant d\}, \quad \text{where} \quad \ell(k_i) := \begin{cases} 2 - 2\cos(k_i/2), & k_i \in (0, 2\pi/3] \\ 2 + 2\cos(k_i), & k_i \in (2\pi/3, \pi) \cup (\pi, 4\pi/3] \\ 2 + 2\cos(k_i/2), & k_i \in (4\pi/3, 2\pi). \end{cases}$$

Denote $\mu(H') := (0, E'(k)) \cup (4d - E'(k), 4d)$. Then for every $E \in \mu(H')$ there exists $\varepsilon = \varepsilon(E) > 0$ such that for all $\theta \in C_c^\infty(\mathbb{R})$ supported on $\mathcal{I} := (E - \varepsilon, E + \varepsilon)$, $\theta(\Delta)B_{W'}\theta(\Delta) = 0$. In particular, for every $E \in \mu(H')$, the classical Mourre estimate (2.4) holds for H' on $\mathcal{I}'$, where $\overline{\mathcal{I}'} \subset \mathcal{I}$.

Proof. As mentioned in Remark 4.1, we show the result for $E \in (0, E'(k))$ and apply symmetry to get the result at the other end of the spectrum. We use the results from the one-dimensional case and follow the notation of Lemma 3.4. For now we denote by Δ the $1d$ Laplacian. The idea is the following : given $\lambda \in \sigma(\Delta) = [0, 4]$, we want to find an interval $\mathcal{I}$ satisfying:

$$(4.22) \qquad \begin{cases} \mathcal{I} \text{ is of the form } \mathcal{I} = [0, \lambda) \ \text{ or } \ \mathcal{I} = (\lambda, 4], \text{ and} \\ \mathcal{I} \cap g_k(\mathcal{I}, y) = \varnothing \ \text{ for } \ y \in \{0, 1\}. \end{cases}$$

Here $g_k(x, y)$ is the function defined in (3.10). The motivation for wanting $\mathcal{I}$ of this form will be clear later in the proof. We examine the inequalities (3.16), (3.17), (3.18) and (3.19). Fix $k \in (0, \pi)$. (3.16) gives us (4.22) for $\lambda \in [0, E_-(k))$ and $y = 0$, whereas (3.18) gives us (4.22) for $\lambda \in [0, \lambda_+(k))$ and $y = 1$, however with the condition that $\lambda < g_{k;+}(0)$. We therefore let $\ell'(k) := \min(E_-(k), \lambda_+(k), g_{k;+}(0)) = \min(2 - 2\cos(k/2), 2 + 2\cos(k), 2 - 2\cos(k))$, and it is readily checked that $\ell(k) = \ell'(k)$. Similarly, for $k \in (\pi, 2\pi)$, we find $\ell(k) = \min(\lambda_-(k), E_+(k), g_{k;-}(0)) = \min(2+2\cos(k), 2+2\cos(k/2), 2-2\cos(k))$. All intervals of the form $\mathcal{I} = [0, \lambda)$ with $\lambda < \ell(k)$ will satisfy (4.22).

Now we show how this can be of use for the two-dimensional case, although one can generalize for $d > 2$. Let $k = (k_1, k_2)$ be the Wigner-von Neumann paramters and let $E'(k) := \min(\ell(k_1), \ell(k_2))$. Let $E \in \mathcal{L}_k := [0, E'(k))$ be given. Choose $\varepsilon > 0$ such that $\mathcal{I} := (E - \varepsilon, E + \varepsilon) \subset \mathcal{L}_k$. If $E = 0$ was chosen, take $\mathcal{I} := [0, \varepsilon) \subset \mathcal{L}_k$. Now let $\mathcal{I}_1 = \mathcal{I}_2 := [0, E + \varepsilon)$. Notice that

$$(4.23) \qquad \{(x_1, x_2) : x_1 + x_2 \in \mathcal{I}\} \cap (\sigma(\Delta_1) \times \sigma(\Delta_2)) \subset \mathcal{I}_1 \times \mathcal{I}_2,$$

so that as functions on $(x_1, x_2) \in \sigma(\Delta_1) \times \sigma(\Delta_2)$, $\chi_{\mathcal{I}}(x_1 + x_2) = \chi_{\mathcal{I}}(x_1 + x_2)\chi_{\mathcal{I}_1}(x_1)\chi_{\mathcal{I}_2}(x_2)$. Thus as operators on $\ell^2(\mathbb{Z}) \otimes \ell^2(\mathbb{Z})$, $E_{\mathcal{I}}(\Delta) = E_{\mathcal{I}}(\Delta) \cdot E_{\mathcal{I}_1}(\Delta_1) \otimes E_{\mathcal{I}_2}(\Delta_2)$. By (4.22),

$$E_{\mathcal{I}_i}(\Delta_i)\tilde{W'}_i E_{\mathcal{I}_i}(\Delta_i) = 0 \text{ for } i = 1, 2.$$

Recall that $B_{W_i'}$ is given by (4.5). For $i = 1, 2$,

$$E_{\mathcal{I}_i}(\Delta_i)B_{W_i'}E_{\mathcal{I}_i}(\Delta_i) = E_{\mathcal{I}_i}(\Delta_i)\tilde{W'}_i E_{\mathcal{I}_i}(\Delta_i)(S_i^* - S_i) - (S_i^* - S_i)E_{\mathcal{I}_i}(\Delta_i)\tilde{W'}_i E_{\mathcal{I}_i}(\Delta_i) = 0.$$

Therefore

$$\begin{aligned} &E_{\mathcal{I}}(\Delta) \cdot B_{W_1'} \otimes W_2' \cdot E_{\mathcal{I}}(\Delta) \\ &= E_{\mathcal{I}}(\Delta) \cdot E_{\mathcal{I}_1}(\Delta_1) \otimes E_{\mathcal{I}_2}(\Delta_2) \cdot B_{W_1'} \otimes W_2' \cdot E_{\mathcal{I}_1}(\Delta_1) \otimes E_{\mathcal{I}_2}(\Delta_2) \cdot E_{\mathcal{I}}(\Delta) \\ &= E_{\mathcal{I}}(\Delta) \cdot E_{\mathcal{I}_1}(\Delta_1)B_{W_1'}E_{\mathcal{I}_1}(\Delta_1) \otimes E_{\mathcal{I}_2}(\Delta_2)W_2'E_{\mathcal{I}_2}(\Delta_2) \cdot E_{\mathcal{I}}(\Delta) \\ &= 0. \end{aligned}$$

Similarly, $E_{\mathcal{I}}(\Delta) \cdot W_1' \otimes B_{W_2'} \cdot E_{\mathcal{I}}(\Delta) = 0$. Thus $E_{\mathcal{I}}(\Delta) B_{W'} E_{\mathcal{I}}(\Delta) = 0$, and the proof is complete. □

5. Weighted Mourre Theory : Proof of Theorem 1.1

In this section we prove the main result Theorem 1.1. For $s \in \mathbb{R}$, let $\langle N \rangle^s$ be the operator on $\ell_0(\mathbb{Z}^d)$ defined by $(\langle N \rangle^s u)(n) = \langle n \rangle^s u(n)$. The following Lemma says that the conjugate operator A is comparable to the position operator N:

Lemma 5.1. *For all $\varepsilon \in [0,1]$, both $\langle A \rangle^{\varepsilon} \langle N \rangle^{-\varepsilon}$ and $\langle N \rangle^{-\varepsilon} \langle A \rangle^{\varepsilon}$ are bounded operators.*

Proof. We use the notation $\|f\| \lesssim \|g\|$ if there is $c > 0$ such that $\|f\| \leqslant c\|g\|$. Let $u \in \otimes_{i=1}^d \ell_0(\mathbb{Z})$, which is dense in $\otimes_{i=1}^d \ell^2(\mathbb{Z})$. We have:

$\|\langle A \rangle u\|^2 = \|u\|^2 + \|Au\|^2 \lesssim \|u\|^2 + (\sum_i \|u\| + \|N_i u\|)^2 \lesssim \|u\|^2 + \sum_i \left(\|u\|^2 + \|N_i u\|^2\right) \lesssim \|\langle N \rangle u\|^2.$

The first inequality follows from (1.9), and the second inequality holds by equivalence of the norms on $\ell^1(G)$ and $\ell^2(G)$ for finite dimensional Hilbert spaces G. By complex interpolation, $\|\langle A \rangle^{\varepsilon} u\| \lesssim \|\langle N \rangle^{\varepsilon} u\|$. Hence, for a dense set of $u' \in \otimes_{i=1}^d \ell^2(\mathbb{Z})$, we have $\|\langle A \rangle^{\varepsilon} \langle N \rangle^{-\varepsilon} u'\| \lesssim \|u'\|$. This shows that $\langle A \rangle^{\varepsilon} \langle N \rangle^{-\varepsilon}$ extends to a bounded operator, and taking adjoints yields the result. □

In our proof of the projected weighted Mourre estimate (2.6), the following Lemma is crucial. At this point we will be using the full strength of hypothesis (1.7) on V, namely $\langle N \rangle^{\rho} |V| \leqslant C$.

Lemma 5.2. *Let $\theta \in C_c^{\infty}(\mathbb{R})$, and ρ be as in (1.7). Then for all $\varepsilon \in [0, \min(\rho, 1))$, the following operators are compact :*

$$(\theta(H) - \theta(\Delta)) \langle A \rangle^{\varepsilon} \quad \text{and} \quad (\theta(H') - \theta(\Delta)) \langle A \rangle^{\varepsilon}. \tag{5.1}$$

Proof. First, by Proposition 6.6, $\Delta \in \mathcal{C}^1(\langle A \rangle^{\varepsilon})$ since $f(x) = \langle x \rangle^{\varepsilon} \in \mathcal{S}^{\varepsilon}$, thus $[\Delta, \langle A \rangle^{\varepsilon}]_{\circ}$ exists as a bounded operator. By the Helffer-Sjöstrand formula and the resolvent identity,

$$\begin{aligned}
(\theta(H) - \theta(\Delta)) \langle A \rangle^{\varepsilon} &= \frac{\mathrm{i}}{2\pi} \int_{\mathbb{C}} \frac{\partial \tilde{\theta}}{\partial \bar{z}} (z - H)^{-1} (W + V)(z - \Delta)^{-1} \langle A \rangle^{\varepsilon} dz \wedge d\bar{z} \\
&= \frac{\mathrm{i}}{2\pi} \int_{\mathbb{C}} \frac{\partial \tilde{\theta}}{\partial \bar{z}} (z - H)^{-1} (W + V) \langle A \rangle^{\varepsilon} (z - \Delta)^{-1} dz \wedge d\bar{z} \\
&\quad + \frac{\mathrm{i}}{2\pi} \int_{\mathbb{C}} \frac{\partial \tilde{\theta}}{\partial \bar{z}} (z - H)^{-1} (W + V)[(z - \Delta)^{-1}, \langle A \rangle^{\varepsilon}]_{\circ} dz \wedge d\bar{z} \\
&= \frac{\mathrm{i}}{2\pi} \int_{\mathbb{C}} \frac{\partial \tilde{\theta}}{\partial \bar{z}} (z - H)^{-1} (W + V) \langle N \rangle^{\varepsilon} \langle N \rangle^{-\varepsilon} \langle A \rangle^{\varepsilon} (z - \Delta)^{-1} dz \wedge d\bar{z} \\
&\quad + \frac{\mathrm{i}}{2\pi} \int_{\mathbb{C}} \frac{\partial \tilde{\theta}}{\partial \bar{z}} (z - H)^{-1} (W + V)(z - \Delta)^{-1} [\Delta, \langle A \rangle^{\varepsilon}]_{\circ} (z - \Delta)^{-1} dz \wedge d\bar{z}.
\end{aligned}$$

By (1.2), W and $W \langle N \rangle^{\varepsilon}$ are compact, and so are V and $V \langle N \rangle^{\varepsilon}$ by assumption (1.7). By Lemma 5.1, $\langle N \rangle^{-\varepsilon} \langle A \rangle^{\varepsilon}$ is bounded, and so the integrands of the last two integrals are compact operators. With the support of θ compact, the integrals are converging in norm, and so the compactness of $(\theta(H) - \theta(\Delta)) \langle A \rangle^{\varepsilon}$ is preserved in the limit. As for the Schrödinger operator H' the same proof works, but the additional point that has to be verified is that $W' \langle N \rangle^{\varepsilon}$ is compact. Indeed, since

$$\left(\prod_{i=1}^d q_i \sin(k_i n_i) n_i^{-1} \right)^2 \langle n \rangle^{2\varepsilon} \leqslant \left(\prod_{i=1}^d q_i^2 \sin^2(k_i n_i) n_i^{-2} \right) \left(1 + \sum_{i=1}^d n_i^2 \right) \langle n \rangle^{2(\varepsilon - 1)} \leqslant c \langle n \rangle^{2(\varepsilon - 1)},$$

it follows that $W'(n)\langle n\rangle^{\varepsilon} \to 0$ as $|n| \to \infty$. $\square$

Because we are aiming at a projected Mourre estimate, we need some information on possible eigenvalues embedded in the interval on which the LAP takes place. Recall that P denotes the orthogonal projection onto the pure point spectral subspace of H (resp. H'), and $\mu(H)$ and $\mu(H')$ are points where the classical Mourre estimate hold for H and H' respectively.

Lemma 5.3. *Let $E \in \mu(H)$ and suppose that $\ker(H-E) \in \mathcal{D}(A)$. Then there is an interval $\mathcal{I} \subset \mu(H)$ containing E such that $PE_{\mathcal{I}}(H)$ and $P^{\perp}\eta(H)$ are of class $\mathcal{C}^1(A)$ for all $\eta \in C_c^{\infty}(\mathbb{R})$ with supp$(\eta) = \mathcal{I}$. The corresponding statement also holds for H'.*

Proof. Since the Mourre estimate holds at E, the point spectrum is finite in a neighborhood $\mathcal{I}$ of E. Therefore $PE_{\mathcal{I}}(H)$ is a finite rank operator. Further shrinking $\mathcal{I}$ around E if necessary, we have that $\ker(H-\lambda) \in \mathcal{D}(A)$ for all $\lambda \in \mathcal{I}$. We may therefore apply Lemma 2.3 to get $PE_{\mathcal{I}}(H) \in \mathcal{C}^1(A)$. In addition, $P^{\perp}\eta(H) = \eta(H) - PE_{\mathcal{I}}(H)\eta(H) \in \mathcal{C}^1(A)$. $\square$

We are now ready to prove the *projected weighted Mourre estimate* (2.6). The proof makes use of almost analytic extensions of $C^{\infty}(\mathbb{R})$ bounded functions. The reader is invited to consult the appendix for some notation and useful results about these functions. We also mention that the proof is essentially the same as that of [GJ2][Theorem 4.15], but we display it in detail for the reader's convenience.

Theorem 5.4. *Let $E \in \mu(H)$ be such that $\ker(H-E) \subset \mathcal{D}(A)$. Then there exists an open interval $\mathcal{I} \ni E$ such that the projected weighted Mourre estimate (2.6) holds on $\mathcal{I}$ for all $s > 1/2$. Thus, for all compact $\mathcal{I}'$ with $\overline{\mathcal{I}'} \subset \mathcal{I}$, the LAP for H holds with respect to $(\mathcal{I}', s, A)$. The corresponding result holds for H'.*

Proof. First choose $\mathcal{I} \ni E$ so that for all $\lambda \in \mathcal{I}$, $\ker(H-\lambda) \in \mathcal{D}(A)$. This is of course possible as explained in Lemma 5.3. Let $\theta, \eta, \chi \in C_c^{\infty}(\mu(H))$ be bump functions such that $\eta\theta = \theta$, $\chi\eta = \eta$ and supp$(\chi) \subset \mathcal{I}$. Later we will shrink $\mathcal{I}$ appropriately. Let $s \in (1/2, 2/3)$ be given. Define

$$\varphi : \mathbb{R} \to \mathbb{R}, \qquad \varphi(t) := \int_{-\infty}^{t} \langle x\rangle^{-2s} dx. \tag{5.2}$$

Note that $\varphi \in \mathcal{S}^0$ (see (6.1) for the definition of $\mathcal{S}^0$). For $R \geqslant 1$, consider the bounded operator

$$\begin{aligned} F &:= P^{\perp}\theta(H)[H, \mathrm{i}\varphi(A/R)]_{\circ}\theta(H)P^{\perp} \\ &= \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial\tilde{\varphi}}{\partial\overline{z}}(z)P^{\perp}\theta(H)(z-A/R)^{-1}[H, \mathrm{i}A/R]_{\circ}(z-A/R)^{-1}\theta(H)P^{\perp}dz \wedge d\overline{z}. \end{aligned}$$

By Lemma 5.3, $P^{\perp}\eta(H) \in C^1(A)$, so

$$[P^{\perp}\eta(H), (z-A/R)^{-1}]_{\circ} = (z-A/R)^{-1}[P^{\perp}\eta(H), A/R]_{\circ}(z-A/R)^{-1}. \tag{5.3}$$

Next to $P^{\perp}\theta(H)$ we introduce $P^{\perp}\eta(H)$ and commute it with $(z-A/R)^{-1}$:

$$\begin{aligned} F = &\frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial\tilde{\varphi}}{\partial\overline{z}}(z)P^{\perp}\theta(H)\left((z-A/R)^{-1}P^{\perp}\eta(H) + [P^{\perp}\eta(H), (z-A/R)^{-1}]_{\circ}\right)[H, \mathrm{i}A/R]_{\circ} \\ &\qquad \left(\eta(H)P^{\perp}(z-A/R)^{-1} + [(z-A/R)^{-1}, P^{\perp}\eta(H)]_{\circ}\right)\theta(H)P^{\perp}dz \wedge d\overline{z} \\ = &\frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial\tilde{\varphi}}{\partial\overline{z}}(z)P^{\perp}\theta(H)(z-A/R)^{-1}P^{\perp}\eta(H)[H, \mathrm{i}A/R]_{\circ} \\ &\qquad \eta(H)P^{\perp}(z-A/R)^{-1}\theta(H)P^{\perp}dz \wedge d\overline{z} + I_1 + I_2 + I_3 \end{aligned}$$

where I_1, I_2, I_3 are the 3 other integrals one obtains when expanding. For example

$$I_1 = \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial\tilde{\varphi}}{\partial\overline{z}}(z)P^{\perp}\theta(H)(z-A/R)^{-1}[P^{\perp}\eta(H),A/R]_{\circ}(z-A/R)^{-1}[H,\mathrm{i}A/R]_{\circ} \eta(H)P^{\perp}(z-A/R)^{-1}\theta(H)P^{\perp}dz\wedge d\overline{z}$$
$$= P^{\perp}\theta(H)\Big\langle\frac{A}{R}\Big\rangle^{-s}\frac{B_1}{R^2}\Big\langle\frac{A}{R}\Big\rangle^{-s}\theta(H)P^{\perp}$$

for some bounded operator B_1 whose norm is uniformly bounded with respect to R, as shown in Lemma 6.5 with $\rho = 0$ and $n = 3$. The same holds for I_2 and I_3, so for $i = 1, 2, 3$,

$$I_i = P^{\perp}\theta(H)\Big\langle\frac{A}{R}\Big\rangle^{-s}\frac{B_i}{R^2}\Big\langle\frac{A}{R}\Big\rangle^{-s}\theta(H)P^{\perp}.$$

Next to either $\eta(H)$ we insert $\chi(H)$, and we let $G := \eta(H)[H,\mathrm{i}A/R]_{\circ}\eta(H)$. We have:

$$F = \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial\tilde{\varphi}}{\partial\overline{z}}(z)P^{\perp}\theta(H)(z-A/R)^{-1}P^{\perp}\chi(H)G\chi(H)P^{\perp}(z-A/R)^{-1}\theta(H)P^{\perp}dz\wedge d\overline{z}$$
$$+ P^{\perp}\theta(H)\Big\langle\frac{A}{R}\Big\rangle^{-s}\left(\frac{B_1+B_2+B_3}{R^2}\right)\Big\langle\frac{A}{R}\Big\rangle^{-s}\theta(H)P^{\perp}.$$

We decompose G as follows

$$G = R^{-1}\Big(\eta(\Delta)[\Delta,\mathrm{i}A]_{\circ}\eta(\Delta) + \eta(\Delta)[W,\mathrm{i}A]_{\circ}\eta(\Delta) + \eta(\Delta)[V,\mathrm{i}A]_{\circ}\eta(\Delta)$$
$$+ (\eta(H)-\eta(\Delta))[H,\mathrm{i}A]_{\circ}\eta(\Delta) + \eta(H)[H,\mathrm{i}A]_{\circ}(\eta(H)-\eta(\Delta))\Big).$$

We put into action our previous results. Shrink the support of η if necessary to ensure that $\eta(\Delta)B_W\eta(\Delta)$ is compact (or zero) according to Lemma 3.4 and Propositions 4.5 and 4.6. Thus $G = R^{-1}(\eta(\Delta)[\Delta,\mathrm{i}A]_{\circ}\eta(\Delta) + K_0)$ where $K_0 := \eta(\Delta)K_W\eta(\Delta) + \eta(\Delta)B_W\eta(\Delta) +$

$$+\ \eta(\Delta)[V,\mathrm{i}A]_{\circ}\eta(\Delta) + (\eta(H)-\eta(\Delta))[H,\mathrm{i}A]_{\circ}\eta(\Delta) + \eta(H)[H,\mathrm{i}A]_{\circ}(\eta(H)-\eta(\Delta)).$$

We claim that

$$K_1 := \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial\tilde{\varphi}}{\partial\overline{z}}(z)\Big\langle\frac{A}{R}\Big\rangle^{s}(z-A/R)^{-1}P^{\perp}\chi(H)K_0\chi(H)P^{\perp}\Big\langle\frac{A}{R}\Big\rangle^{s}(z-A/R)^{-1}dz\wedge d\overline{z}, \tag{5.4}$$

converges in norm to a compact operator for s sufficiently close to $1/2$. Although K_0 is clearly compact, convergence in norm requires careful justification. Define

$$K_{11} := \langle A\rangle^{\varepsilon}P^{\perp}\chi(H)\eta(\Delta)K_W\eta(\Delta),$$
$$K_{12} := \langle A\rangle^{\varepsilon}P^{\perp}\chi(H)\eta(\Delta)B_W\eta(\Delta),$$
$$K_{13} := \langle A\rangle^{\varepsilon}P^{\perp}\chi(H)\eta(\Delta)[V,\mathrm{i}A]_{\circ}\eta(\Delta),$$
$$K_{14} := \langle A\rangle^{\varepsilon}P^{\perp}\chi(H)(\eta(H)-\eta(\Delta))[H,\mathrm{i}A]_{\circ}\eta(\Delta),$$
$$K_{15} := \eta(H)[H,\mathrm{i}A]_{\circ}(\eta(H)-\eta(\Delta))\chi(H)P^{\perp}\langle A\rangle^{\varepsilon}.$$

Let $\varepsilon \in [0,\min(\rho,1))$. Since $P^{\perp}\chi(H)\eta(\Delta) \in \mathcal{C}^1(A)$ and $f(x) = \langle x\rangle^{\varepsilon} \in \mathcal{S}^{\varepsilon}$, $[\langle A\rangle^{\varepsilon}, P^{\perp}\chi(H)\eta(\Delta)]_{\circ}$ exists by Proposition 6.6. Moreover, $\langle N\rangle^{\varepsilon}K_W$ is compact and $\langle A\rangle^{\varepsilon}\langle N\rangle^{-\varepsilon}$ is bounded. Thus

$$K_{11} = P^{\perp}\chi(H)\eta(\Delta)\langle A\rangle^{\varepsilon}\langle N\rangle^{-\varepsilon}\langle N\rangle^{\varepsilon}K_W\eta(\Delta) + [\langle A\rangle^{\varepsilon}, P^{\perp}\chi(H)\eta(\Delta)]_{\circ}K_W\eta(\Delta)$$

is compact. We turn to K_{12}. Commuting $\langle A\rangle^{\varepsilon}$ with $P^{\perp}\chi(H)$ gives

$$K_{12} = P^{\perp}\chi(H)\langle A\rangle^{\varepsilon}\langle N\rangle^{-\varepsilon}\langle N\rangle^{\varepsilon}\eta(\Delta)B_W\eta(\Delta) + [\langle A\rangle^{\varepsilon}, P^{\perp}\chi(H)]_{\circ}\eta(\Delta)B_W\eta(\Delta).$$

Applying the mean value theorem shows that $\langle N\rangle^{\varepsilon}[S_j, U_i]_{\circ}$ and $\langle N\rangle^{\varepsilon}[S_j^*, U_i]_{\circ}$ are compact $\forall\ i, j = 1, ..., d$. Since

$$\eta(\Delta)B_W\eta(\Delta) = \sum_i [\eta(\Delta), U_i]_{\circ}\tilde{W}(S_i^* - S_i)\eta(\Delta) - \eta(\Delta)(S_i^* - S_i)\tilde{W}[U_i, \eta(\Delta)]_{\circ},$$

we see that $\langle N\rangle^{\varepsilon}\eta(\Delta)B_W\eta(\Delta)$, and hence K_{12} is compact. As for K_{13}, we use the full strength of hypothesis (1.8) on V to guarantee compactness of $\langle N\rangle^{\varepsilon}[V, \mathrm{i}A]_{\circ}$. Commuting $\langle A\rangle^{\varepsilon}$ with $P^{\perp}\chi(H)\eta(\Delta)$ as before shows that K_{13} is compact. By Lemma 5.2, $(\eta(H)-\eta(\Delta))\langle A\rangle^{\varepsilon}$ and its adjoint $\langle A\rangle^{\varepsilon}(\eta(H) - \eta(\Delta))$ are compact. Recall that this Lemma uses the full strength of hypothesis (1.7) on V. Commuting $\langle A\rangle^{\varepsilon}$ with $P^{\perp}\chi(H)$ and using the fact that $[P^{\perp}\chi(H), \langle A\rangle^{\varepsilon}]_{\circ}$ exists shows that K_{14} and K_{15} are compact. Finally, $\langle A/R\rangle^{\varepsilon}\langle A\rangle^{-\varepsilon}$ and $\langle A\rangle^{-\varepsilon}\langle A/R\rangle^{\varepsilon}$ are uniformly bounded operators w.r.t. R. Thus invoking (6.5) for $\ell = 2$ and (6.11) we see that K_1 is a norm converging integral of compact operators provided s additionally satisfies $s < 1/2 + \varepsilon/2$. This proves the claim. Another important point to take into consideration is that $\|K_1\|$ is bounded above by

(5.5)

$$C_1\left(\|K_{11}\chi(H)P^{\perp}\| + \|K_{12}\chi(H)P^{\perp}\| + \|K_{13}\chi(H)P^{\perp}\| + \|K_{14}\chi(H)P^{\perp}\| + \|P^{\perp}\chi(H)K_{15}\|\right)$$

for some finite $C_1 > 0$ independent of R. Hence $\|K_1\|$ vanishes as the support of χ gets tighter around E. Let

$$M := P^{\perp}\chi(H)\eta(\Delta)[\Delta, \mathrm{i}A]_{\circ}\eta(\Delta)\chi(H)P^{\perp}.$$

So far we have

$$\begin{aligned} F = &\frac{\mathrm{i}}{2\pi}\frac{1}{R}\int_{\mathbb{C}}\frac{\partial\tilde{\varphi}}{\partial\overline{z}}(z)P^{\perp}\theta(H)(z - A/R)^{-1}M(z - A/R)^{-1}\theta(H)P^{\perp}dz \wedge d\overline{z} \\ &+ P^{\perp}\theta(H)\left\langle\frac{A}{R}\right\rangle^{-s}\left(\frac{B_1 + B_2 + B_3}{R^2} + \frac{K_1}{R}\right)\left\langle\frac{A}{R}\right\rangle^{-s}\theta(H)P^{\perp}. \end{aligned}$$

Next we commute $(z - A/R)^{-1}$ with M:

$$\begin{aligned} F = &\frac{\mathrm{i}}{2\pi}\frac{1}{R}\int_{\mathbb{C}}\frac{\partial\tilde{\varphi}}{\partial\overline{z}}(z)P^{\perp}\theta(H)(z - A/R)^{-2}M\theta(H)P^{\perp}dz \wedge d\overline{z} \\ &+ \frac{\mathrm{i}}{2\pi}\frac{1}{R}\int_{\mathbb{C}}\frac{\partial\tilde{\varphi}}{\partial\overline{z}}(z)P^{\perp}\theta(H)(z - A/R)^{-1}[M, (z - A/R)^{-1}]_{\circ}\theta(H)P^{\perp}dz \wedge d\overline{z} \\ &+ P^{\perp}\theta(H)\left\langle\frac{A}{R}\right\rangle^{-s}\left(\frac{B_1 + B_2 + B_3}{R^2} + \frac{K_1}{R}\right)\left\langle\frac{A}{R}\right\rangle^{-s}\theta(H)P^{\perp}. \end{aligned}$$

We apply (6.9) to the first integral (which converges in norm), while for the second integral we use the fact that $M \in \mathcal{C}^1(A)$ to conclude that there exists a uniformly bounded operator B_4 such that

$$\begin{aligned} F = &R^{-1}P^{\perp}\theta(H)\varphi'(A/R)M\theta(H)P^{\perp} \\ &+ P^{\perp}\theta(H)\left\langle\frac{A}{R}\right\rangle^{-s}\left(\frac{B_1 + B_2 + B_3 + B_4}{R^2} + \frac{K_1}{R}\right)\left\langle\frac{A}{R}\right\rangle^{-s}\theta(H)P^{\perp}. \end{aligned}$$

Now $\varphi'(A/R) = \langle A/R\rangle^{-2s}$. As a result of the Helffer-Sjöstrand formula, (6.5) and (6.11),

$$[\langle A/R\rangle^{-s}, M]_{\circ}\langle A/R\rangle^{s} = R^{-1}B_5$$

for some uniformly bounded operator B_5. Thus commuting $\langle A/R\rangle^{-s}$ and M gives

$$\begin{aligned}
F &= R^{-1}P^\perp\theta(H)\Big\langle\frac{A}{R}\Big\rangle^{-s}M\Big\langle\frac{A}{R}\Big\rangle^{-s}\theta(H)P^\perp \\
&+ P^\perp\theta(H)\Big\langle\frac{A}{R}\Big\rangle^{-s}\left(\frac{B_1+B_2+B_3+B_4+B_5}{R^2}+\frac{K_1}{R}\right)\Big\langle\frac{A}{R}\Big\rangle^{-s}\theta(H)P^\perp \\
&\geqslant CR^{-1}P^\perp\theta(H)\Big\langle\frac{A}{R}\Big\rangle^{-s}P^\perp\chi(H)\eta^2(\Delta)\chi(H)P^\perp\Big\langle\frac{A}{R}\Big\rangle^{-s}\theta(H)P^\perp \\
&+ P^\perp\theta(H)\Big\langle\frac{A}{R}\Big\rangle^{-s}\left(\frac{B_1+B_2+B_3+B_4+B_5}{R^2}+\frac{K_1}{R}\right)\Big\langle\frac{A}{R}\Big\rangle^{-s}\theta(H)P^\perp
\end{aligned}$$

where $C>0$ comes from applying the Mourre estimate. Let

$$K_2 := P^\perp\chi(H)(\eta^2(\Delta)-\eta^2(H))\chi(H)P^\perp. \tag{5.6}$$

Note that K_2 is compact with $\|K_2\|$ vanishing as the support of χ gets tighter around E. Thus

$$\begin{aligned}
F &\geqslant CR^{-1}P^\perp\theta(H)\Big\langle\frac{A}{R}\Big\rangle^{-s}P^\perp\chi(H)\eta^2(H)\chi(H)P^\perp\Big\langle\frac{A}{R}\Big\rangle^{-s}\theta(H)P^\perp \\
&+ P^\perp\theta(H)\Big\langle\frac{A}{R}\Big\rangle^{-s}\left(\frac{B_1+B_2+B_3+B_4+B_5}{R^2}+\frac{K_1+K_2}{R}\right)\Big\langle\frac{A}{R}\Big\rangle^{-s}\theta(H)P^\perp.
\end{aligned}$$

Finally, we commute $P^\perp\chi(H)\eta^2(H)\chi(H)P^\perp = P^\perp\eta^2(H)P^\perp$ with $\langle A/R\rangle^{-s}$, and see that

$$[P^\perp\eta^2(H)P^\perp,\langle A/R\rangle^{-s}]_\circ\langle A/R\rangle^{s} = R^{-1}B_6$$

for some uniformly bounded operator B_6. Thus we have

$$\begin{aligned}
F &\geqslant CR^{-1}P^\perp\theta(H)\Big\langle\frac{A}{R}\Big\rangle^{-2s}\theta(H)P^\perp \\
&+ P^\perp\theta(H)\Big\langle\frac{A}{R}\Big\rangle^{-s}\left(\frac{B_1+B_2+B_3+B_4+B_5+B_6}{R^2}+\frac{K_1+K_2}{R}\right)\Big\langle\frac{A}{R}\Big\rangle^{-s}\theta(H)P^\perp.
\end{aligned}$$

To conclude, we shrink the support of χ to ensure that $\|K_1+K_2\|<C/3$ and choose $R\geqslant 1$ so that $\|\sum_{i=1}^6 B_i\|/R<C/3$. Then $K_1+K_2\geqslant -C/3$ and $\sum_{i=1}^6 B_i/R\geqslant -C/3$, so

$$F\geqslant \frac{C}{3R}P^\perp\theta(H)\Big\langle\frac{A}{R}\Big\rangle^{-2s}\theta(H)P^\perp. \tag{5.7}$$

Let $\mathcal{I}'$ be any open interval with $\overline{\mathcal{I}'}\subset\mathcal{I}$. Applying $E_{\mathcal{I}'}(H)$ on both sides of this inequality yields the projected weighted Mourre estimate (2.6), with $c=C/(3R)$, $K=0$, and $s\in(1/2,\min(2/3,1/2+\rho/2))$. As a result of Theorem 2.4, the proof is complete. □

6. Appendix : Review of Almost Analytic Extenstions

We refer to [D], [DG], [GJ1], [GJ2], [HS] and [Mo] for more details. We collect basic and essential results that are spread out in the mentioned literature. Let $\rho\in\mathbb{R}$ and denote by $\mathcal{S}^\rho(\mathbb{R})$ the class of functions φ in $C^\infty(\mathbb{R})$ such that

$$|\varphi^{(k)}(x)|\leqslant C_k\langle x\rangle^{\rho-k},\quad \text{for all } k\geqslant 0. \tag{6.1}$$

For $\rho<0$, $\mathcal{S}^\rho$ consists of the slowly decreasing functions at infinity, and contains every rational function whose denominator doesn't vanish on $\mathbb{R}$ and is of degree higher than its numerator. On the other hand, for $\rho>0$, $\mathcal{S}^\rho$ also allows for slowly increasing functions at infinity.

Lemma 6.1. [D] *and* [DG] *Let* $\varphi \in \mathcal{S}^\rho$*,* $\rho \in \mathbb{R}$*. Then for every* $N \in \mathbb{Z}^+$ *there exists a smooth function* $\tilde{\varphi}_N : \mathbb{C} \to \mathbb{C}$*, called an almost analytic extension of* φ*, satisfying:*

$$\tilde{\varphi}_N(x + \mathrm{i}0) = \varphi(x) \ \forall x \in \mathbb{R}; \tag{6.2}$$

$$\mathrm{supp}\ (\tilde{\varphi}_N) \subset \{x + \mathrm{i}y : |y| \leqslant \langle x\rangle\}; \tag{6.3}$$

$$\tilde{\varphi}_N(x + \mathrm{i}y) = 0 \ \forall y \in \mathbb{R} \text{ whenever } \varphi(x) = 0; \tag{6.4}$$

$$\forall \ell \in \mathbb{N} \cap [0, N], \left|\frac{\partial \tilde{\varphi}_N}{\partial \bar{z}}(x + \mathrm{i}y)\right| \leqslant c_\ell \langle x\rangle^{\rho-1-\ell}|y|^\ell \text{ for some constants } c_\ell > 0. \tag{6.5}$$

Proof. Let $\theta \in C_c^\infty(\mathbb{R})$ be a bump function such that $\theta(x) = 1$ for $x \in [-1/2, 1/2]$ and $\theta(x) = 0$ for $x \in \mathbb{R}\backslash[-1, 1]$, and consider

$$\tilde{\varphi}_N(x + \mathrm{i}y) := \sum_{n=0}^{N} \varphi^{(n)}(x)\frac{(\mathrm{i}y)^n}{n!}\theta\left(\frac{y}{\langle x\rangle}\right). \tag{6.6}$$

The Wirtinger derivative is easily calculated:

$$\frac{\partial \tilde{\varphi}_N}{\partial \bar{z}}(z) = \frac{1}{2}\sum_{n=0}^{N} \frac{\varphi^{(n)}(x)}{\langle x\rangle}\frac{(\mathrm{i}y)^n}{n!}\theta'\left(\frac{y}{\langle x\rangle}\right)\left(\mathrm{i} - \frac{yx}{\langle x\rangle^2}\right) \ + \ \frac{1}{2}\varphi^{(N+1)}(x)\frac{(\mathrm{i}y)^N}{N!}\theta\left(\frac{y}{\langle x\rangle}\right).$$

Therefore,

$$\left|\frac{\partial \tilde{\varphi}_N}{\partial \bar{z}}(z)\right| \leqslant \sum_{n=0}^{N} \frac{|\varphi^{(n)}(x)|}{\langle x\rangle}\frac{|y|^n}{n!}\chi_{\left\{\frac{\langle x\rangle}{2} \leqslant y \leqslant \langle x\rangle\right\}}(x, y) \ + \ \frac{1}{2}|\varphi^{(N+1)}(x)|\frac{|y|^N}{N!}\chi_{\left\{|y| \leqslant \langle x\rangle\right\}}(x, y).$$

It follows that:

$$\begin{aligned}\left|\langle x\rangle^{\ell+1-\rho}|y|^{-\ell}\frac{\partial \tilde{\varphi}_N}{\partial \bar{z}}(x + \mathrm{i}y)\right| &\leqslant \sum_{n=0}^{\ell} C_n\frac{\langle x\rangle^{\ell-n}}{n!}\left(\frac{\langle x\rangle}{2}\right)^{n-\ell} + \sum_{n=\ell+1}^{N} C_n\frac{\langle x\rangle^{\ell-n}}{n!}\langle x\rangle^{n-\ell} + \frac{1}{2}\frac{C_{N+1}}{N!}\\ &= \sum_{n=0}^{\ell}\frac{C_n}{n!}\frac{1}{2^{n-\ell}} + \sum_{n=\ell+1}^{N}\frac{C_n}{n!} + \frac{1}{2}\frac{C_{N+1}}{N!} := c_\ell.\end{aligned}$$

□

Moreover, for $\varphi \in C_c^\infty(\mathbb{R})$, we have the following key formula (cf. [DG]):

$$\varphi(t) = \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}}\frac{\partial \tilde{\varphi}_N}{\partial \bar{z}}(z)(z - t)^{-1}dz \wedge d\bar{z}, \quad \forall N \in \mathbb{Z}^+.$$

By a limiting argument, this formula holds pointwise when $\varphi \in \mathcal{S}^\rho, \rho < 0$. Now let A be a self-adjoint operator acting on a Hilbert space $\mathcal{H}$. In terms of operators, we have

$$\varphi(A) = \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}}\frac{\partial \tilde{\varphi}_N}{\partial \bar{z}}(z)(z - A)^{-1}dz \wedge d\bar{z}. \tag{6.7}$$

Thus, in the case where $\varphi \in \mathcal{S}^\rho, \rho < 0$, the point of the analytic extension is that it allows for an explicit expression of the operator $\varphi(A)$ whose existence is known from the spectral theorem. This formula can be extended for $\rho \geqslant 0$ as follows:

Lemma 6.2. [GJ1] *Let $\rho \geqslant 0$ and $\varphi \in \mathcal{S}^\rho$. Let $\varphi(A)$ with domain $\mathcal{D}(\varphi(A)) \supset \mathcal{D}(\langle A\rangle^\rho)$ be the operator whose existence is assured by the spectral theorem. Then for $f \in \mathcal{D}(\langle A\rangle^\rho)$,*

$$\varphi(A)f = \lim_{R\to\infty} \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial(\widetilde{\varphi\theta_R})_N}{\partial\bar z}(z)(z-A)^{-1} f dz\wedge d\bar z, \tag{6.8}$$

where $\theta_R(x) := \theta(x/R)$ and θ is like in Lemma 6.1.

Proof.

$$\frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial(\widetilde{\varphi\theta_R})_N}{\partial\bar z}(z)(z-A)^{-1} f dz\wedge d\bar z = (\varphi\theta_R)(A)f = (\varphi_\rho\theta_R)(A)\langle A\rangle^\rho f,$$

where $\varphi_\rho(t) := \varphi(t)\langle t\rangle^{-\rho}$ is a bounded function. Thus $(\varphi_\rho\theta_R)(A)$ is converging strongly to $\varphi(A)\langle A\rangle^{-\rho}$, and this shows (6.8). □

Notice that when $\rho < 0$, the r.h.s. of (6.8) is equal to the r.h.s of (6.7) applied to f by the dominated convergence theorem.

Lemma 6.3. *Let $\rho < 0$ and $\varphi \in \mathcal{S}^\rho$. Then for all $k \in \mathbb{N}$ and $N \in \mathbb{N}$:*

$$\varphi^{(k)}(A) = \frac{\mathrm{i}(k!)}{2\pi}\int_{\mathbb{C}} \frac{\partial\tilde\varphi_N}{\partial\bar z}(z)(z-A)^{-1-k} dz\wedge d\bar z \tag{6.9}$$

where the integral exists in the norm topology. For $\rho \geqslant 0$, the following limit exists:

$$\varphi^{(k)}(A)f = \lim_{R\to\infty} \frac{\mathrm{i}(k!)}{2\pi}\int_{\mathbb{C}} \frac{\partial(\widetilde{\varphi\theta_R})_N}{\partial\bar z}(z)(z-A)^{-1-k} f dz\wedge d\bar z, \quad \textit{for all } f \in \mathcal{D}(\langle A\rangle^\rho). \tag{6.10}$$

In particular, if $\varphi \in \mathcal{S}^\rho$ with $0 \leqslant \rho < k$ and $\varphi^{(k)}$ is a bounded function, then $\varphi^{(k)}(A)$ is a bounded operator and (6.9) holds (with the integral converging in norm).

Proof. First we show (6.9). Assume for now that $\varphi \in C_c^\infty(\mathbb{R})$. By definition,

$$\varphi^{(k)}(A) = \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial\widetilde{\varphi^{(k)}}_N}{\partial\bar z}(z)(z-A)^{-1} dz\wedge d\bar z.$$

Now consider $\widetilde{\varphi^{(k)}}_N$ and the k^{th} partial derivative of $\tilde\varphi_N$ in x respectively given by

$$\widetilde{\varphi^{(k)}}_N(x+\mathrm{i}y) = \sum_{n=0}^N \varphi^{(k+n)}(x)\frac{(\mathrm{i}y)^n}{n!}\theta\left(\frac{y}{\langle x\rangle}\right), \text{ and}$$

$$\partial_x^k\tilde\varphi_N(x+\mathrm{i}y) = \sum_{n=0}^N \varphi^{(k+n)}(x)\frac{(\mathrm{i}y)^n}{n!}\theta\left(\frac{y}{\langle x\rangle}\right) + \sum_{n=0}^N \frac{(\mathrm{i}y)^n}{n!}\sum_{j=1}^k \frac{k!}{j!(k-j)!}\varphi^{(n+k-j)}(x)\partial_x^j\theta\left(\frac{y}{\langle x\rangle}\right).$$

Notice that $|\widetilde{\varphi^{(k)}}_N(x+\mathrm{i}y) - \partial_x^k\tilde\varphi_N(x+\mathrm{i}y)|$ is identically zero in a small strip around the x-axis, and so by [D, Lemma 2.2.3], we have that

$$\varphi^{(k)}(A) = \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial\widetilde{\varphi^{(k)}}_N}{\partial\bar z}(z)(z-A)^{-1} dz\wedge d\bar z = \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial\partial_x^k\tilde\varphi_N}{\partial\bar z}(z)(z-A)^{-1} dz\wedge d\bar z.$$

The result follows by performing k partial integrations w.r.t. x. The formula extends to $\varphi \in \mathcal{S}^\rho$ by density of $C_c^\infty(\mathbb{R})$ in $\mathcal{S}^\rho$ for $\rho < 0$. As for (6.10), let $\phi_\rho(t) := \langle t\rangle^{-\rho}$. We have, using (6.9),

$$\frac{\mathrm{i}(k!)}{2\pi}\int_{\mathbb{C}} \frac{\partial(\widetilde{\varphi\theta_R})_N}{\partial\bar z}(z)(z-A)^{-1-k} f dz\wedge d\bar z = (\varphi\theta_R)^{(k)}(A)f = \left(\sum_{j=0}^k c_j\varphi^{(k-j)}\phi_\rho(\theta_R)^{(j)}\right)(A)\langle A\rangle^\rho f.$$

Here $c_j := k!(j!(k-j)!)^{-1}$. First note that $(\theta_R)^{(j)}(x) = R^{-j}\theta^{(j)}(x/R)$. Moreover, $\varphi^{(k-j)}\phi_\rho$ are bounded functions for $0 \leqslant j \leqslant k$, so $(\varphi^{(k-j)}\phi_\rho)(A)$ are bounded operators and

$$(\varphi^{(k-j)}\phi_\rho)(A) = \underset{R\to\infty}{\text{s-lim}}(\varphi^{(k-j)}\phi_\rho)(A)\theta^{(j)}(A/R).$$

Thus

$$\underset{R\to\infty}{\text{s-lim}}\left(\sum_{j=1}^{k} c_j\varphi^{(k-j)}\phi_\rho(\theta_R)^{(j)}\right)(A) = 0$$

and this implies (6.10). Finally, if $0 \leqslant \rho < k$ and $\varphi^{(k)}$ is a bounded function, then we use (6.5) with $\ell = k+1$ and apply the dominated convergence theorem to pass the limit inside the integral. □

Lemma 6.4. [GJ2] *Let $s \in [0,1]$ and $D := \{(x,y) \in \mathbb{R}^2 : 0 < |y| \leqslant \langle x\rangle\}$. Then there exists $c > 0$ independent of A such that for all $z = x + \mathrm{i}y \in D$:*

$$\|\langle A\rangle^s (A-z)^{-1}\| \leqslant c \cdot \langle x\rangle^s \cdot |y|^{-1}. \tag{6.11}$$

Lemma 6.5. *Let $\varphi \in \mathcal{S}^\rho$, and let $B_1, ..., B_n$ be bounded operators. Then for $s \in [0,1]$ satisfying $s < 1 - (1+\rho)/n$, and any $N \geqslant n$, the following integral*

$$\frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial\tilde{\varphi}_N}{\partial\bar{z}} \prod_{i=1}^{n} \langle A\rangle^s (z-A)^{-1} B_i \, dz \wedge d\bar{z} \tag{6.12}$$

converges in norm to a bounded operator. In particular, for $\rho = 0$ and $n \geqslant 3$, (6.12) converges to a bounded operator for $s \in [0, 2/3)$.

Proof. Combine (6.11) and (6.5) for $\ell = n$. □

We end this section with two very useful formulas.

Proposition 6.6. [GJ1] *Let T be a bounded self-adjoint operator satisfying $T \in C^1(A)$. Then:*

$$[T, (z-A)^{-1}]_\circ = (z-A)^{-1}[T, A]_\circ (z-A)^{-1}, \tag{6.13}$$

and for any $\varphi \in \mathcal{S}^\rho$ with $\rho < 1$, $T \in \mathcal{C}^1(\varphi(A))$ and

$$[T, \varphi(A)]_\circ = \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial\tilde{\varphi}_N}{\partial\bar{z}} (z-A)^{-1}[T, A]_\circ (z-A)^{-1} dz \wedge d\bar{z}. \tag{6.14}$$

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SUB-EXPONENTIAL DECAY OF EIGENFUNCTIONS FOR SOME DISCRETE SCHRÖDINGER OPERATORS

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Abstract. Following the method of Froese and Herbst, we show for a class of potentials V that an eigenfunction ψ with eigenvalue E of the multi-dimensional discrete Schrödinger operator $H = \Delta + V$ on $\mathbb{Z}^d$ decays sub-exponentially whenever the Mourre estimate holds at E. In the one-dimensional case we further show that this eigenfunction decays exponentially with a rate at least of $\cosh^{-1}((E-2)/(\theta_E-2))$, where θ_E is the nearest threshold of H located between E and 2. A consequence of the latter result is the absence of eigenvalues between 2 and the nearest thresholds above and below this value. The method of Combes-Thomas is also reviewed for the discrete Schrödinger operators.

1. Introduction

The analysis of the decay rate of eigenfunctions of Schrödinger operators goes back to the famous works of Slaggie and Wichmann [SW], Agmon [A1], and Combes and Thomas [CT]. Their results showed that eigenfunctions corresponding to eigenvalues located outside the essential spectrum decay exponentially. Subsequently, Froese and Herbst [FH], but also [FHHO1] and [FHHO2], investigated the decay of eigenfunctions corresponding to eigenvalues located in the essential spectrum of Schrödinger operators. They showed that eigenfunctions of the continuous Schrödinger operator on $\mathbb{R}^n$ decay exponentially at non-threshold energies for a large class of potentials. Since their pioneering work a solid literature has grown using these ideas. For example, these ideas have been applied to Schrödinger operators on manifolds [V], Schrödinger operators in PDE's [HS], and self-adjoint operators in Mourre theory [FMS]. This short list is by no means complete. The question however does not seem to have been investigated for the discrete Schrödinger operator on the lattice and constitutes the subject of this paper. For completeness and convenience, this paper will also review the Combes-Thomas method for the discrete Schrödinger operators. A nice historical review on the exponential decay of eigenfunctions is done by Hislop in [Hi].

We now describe the mathematical setup of the article. The configuration space is the multi-dimensional lattice $\mathbb{Z}^d$ for some integer $d \geqslant 1$. For a multi-index $n = (n_1, ..., n_d) \in \mathbb{Z}^d$, we set $|n|^2 := n_1^2 + ... + n_d^2$. Consider the complex Hilbert space $\mathcal{H} := \ell^2(\mathbb{Z}^d)$ of square summable sequences $(u(n))_{n\in\mathbb{Z}^d}$. The discrete Schrödinger operator acting on $\mathcal{H}$ is

$$H := \Delta + V, \tag{1.1}$$

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where Δ is the non-negative discrete Laplacian defined by

$$(\Delta u)(n) := \sum_{\substack{m\in\mathbb{Z}^d,\\ |n-m|=1}} (u(n) - u(m)), \quad \text{for all } n \in \mathbb{Z}^d, u \in \mathcal{H},$$

and V is a multiplication operator by a bounded real-valued sequence $(V(n))_{n\in\mathbb{Z}^d}$. It is common knowledge that the spectrum of Δ, denoted $\sigma(\Delta)$, is purely absolutely continuous and equals $[0, 4d]$. Define for $(\alpha, \gamma) \in [0, \infty) \times [0, 1]$ the operator of multiplication on $\mathcal{H}$ by

$$\vartheta_{\alpha,\gamma} := \exp\left(\alpha\left(1 + |n|^2\right)^{\gamma/2}\right), \quad \text{with domain} \tag{1.2}$$

$$\mathcal{D}(\vartheta_{\alpha,\gamma}) := \left\{ u \in \mathcal{H} : \sum_{n\in\mathbb{Z}^d} \exp\left(2\alpha\left(1 + |n|^2\right)^{\gamma/2}\right) |u(n)|^2 < +\infty \right\}.$$

In this manuscript, we will say that $\psi \in \mathcal{H}$ decays sub-exponentially (resp. exponentially) if $\psi \in \mathcal{D}(\vartheta_{\alpha,\gamma})$ for some $\gamma < 1$ (resp. for $\gamma = 1$) and some $\alpha > 0$. Write $\vartheta_\alpha := \vartheta_{\alpha,1}$. We begin with a well-known fact and formulate a version of the main result of Combes and Thomas in the context of multi-dimensional discrete Schrödinger operators:

Theorem 1.1. *Let $(V(n))_{n\in\mathbb{Z}^d}$ be a bounded sequence. Suppose that $H\psi = E\psi$, with $\psi \in \mathcal{H}$ and $E \in \mathbb{R} \setminus \sigma(\Delta) = (-\infty, 0) \cup (4d, +\infty)$. If $\limsup_{|n|\to+\infty} |V(n)| < \operatorname{dist}(\sigma(\Delta), E)$, then there exists $\nu > 0$ depending on $\operatorname{dist}(\sigma(\Delta), E)$ such that for all $\alpha \in [0, \nu)$, $\psi \in \mathcal{D}(\vartheta_\alpha)$.*

Remark 1.1. *We recall that in the discrete setting, a multiplication operator V is compact if and only if $\lim_{|n|\to+\infty} V(n) = 0$. If V is compact, then $0 = \limsup_{|n|\to+\infty} |V(n)| < \operatorname{dist}(\sigma(\Delta), E)$ is automatically verified and also $\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(\Delta) = \sigma(\Delta)$ by Weyl's Theorem. So in this case, Theorem 1.1 is indeed proving the exponential decay of the eigenfunction ψ when the eigenvalue E is located outside the essential spectrum of H.*

The advantage of the perturbative method of Combes-Thomas is that it yields exponential decay of eigenfunctions with a convenient and explicit geometric bound under rather general assumptions for the potential. Another big plus is that it is easy to implement in many different scenarios. The drawback however is that it does not work if the eigenvalue E belongs to the spectrum of the free operator Δ. In addition to the aforementioned references, we refer to [BCH] for an improved Combes-Thomas method with optimal exponential bounds.

The method of Froese and Herbst does not exploit a condition like $\operatorname{dist}(\sigma(\Delta), E) > 0$, but rather a Mourre estimate, which is a local positivity condition on the commutator between H and some appropriate conjugate operator. The article is largely devoted to the study of this method. Before presenting the results, we elaborate on the Mourre estimate, the key relation in the theory developed by Mourre [Mo]. We refer to [ABG] and references therein for a thorough overview of the improved theory. The position operator $N = (N_1, ..., N_d)$ is defined by

$$(N_i u)(n) := n_i u(n), \quad \mathcal{D}(N_i) := \left\{ u \in \ell^2(\mathbb{Z}^d) : \sum_{n\in\mathbb{Z}^d} |n_i u(n)|^2 < +\infty \right\}, \tag{1.3}$$

and the shift operators S_i and S_i^* to the right and to left respectively act on $\mathcal{H}$ by

$$(S_i u)(n) := u(n_1, ..., n_i - 1, ..., n_d), \quad \text{for all } n \in \mathbb{Z}^d \text{ and } u \in \mathcal{H}, \tag{1.4}$$

and correspondingly for S_i^*. We note that the Laplacian may alternatively be written as $\Delta = \sum_{i=1}^d (2 - S_i^* - S_i)$. The conjugate operator to H that is used in this manuscript is the discrete version of the so-called generator of dilations. We denote it by A and it is the closure of the operator A_0 given by

$$A_0 := \mathrm{i} \sum_{i=1}^{d} 2^{-1}(S_i^* + S_i) - (S_i^* - S_i)N_i = -\mathrm{i} \sum_{i=1}^{d} 2^{-1}(S_i^* + S_i) + N_i(S_i^* - S_i) \tag{1.5}$$

with domain $\mathcal{D}(A_0) = \ell_0(\mathbb{Z}^d)$, the collection of sequences with compact support. It is well-known that A is a self-adjoint operator, see e.g. [GGo]. Let T be an arbitrary bounded self-adjoint operator on $\mathcal{H}$. If the form

$$(u, v) \mapsto \langle u, [T, A]v\rangle := \langle Tu, Av\rangle - \langle Au, Tv\rangle$$

defined on $\mathcal{D}(A) \times \mathcal{D}(A)$ extends to a bounded form on $\mathcal{H} \times \mathcal{H}$, we denote by $[T, A]_\circ$ the bounded operator extending the form, and say that T is of class $C^1(A)$, cf. [ABG][Lemma 6.2.9]. We refer the reader to [ABG][Theorem 6.2.10] for equivalent definitions of this class. We have that

$$[\Delta, \mathrm{i}A]_\circ = \sum_{i=1}^{d} \Delta_i(4 - \Delta_i) = \sum_{i=1}^{d} (2 - (S_i^*)^2 - (S_i)^2) \tag{1.6}$$

and this is a non-negative operator. We must also discuss the commutator between the potential V and A. To this end, denote by $\tau_i V$ and $\tau_i^* V$ the operators of multiplication by the shifted sequence $(V(n))_{n\in\mathbb{Z}^d}$ to the right and left respectively on the i^{th} coordinate, namely

$$[(\tau_i V)u](n) := V(n_1, ..., n_i - 1, ..., n_d)u(n), \quad \forall n \in \mathbb{Z}^d, u \in \mathcal{H}, \text{and } i = 1, ..., d,$$

and correspondingly for $\tau_i^* V$. The commutator between V and A is given by

$$\langle u, [V, \mathrm{i}A]v\rangle = \sum_{i=1}^{d} \langle u, [(2^{-1} - N_i)(V - \tau_i V)S_i + (2^{-1} + N_i)(V - \tau_i^* V)S_i^*]v\rangle, \quad \forall u, v \in \ell_0(\mathbb{Z}^d). \tag{1.7}$$

Assuming V to be bounded, note that $[V, \mathrm{i}A]_\circ$ exists if and only if Hypothesis 1 stated below holds. Assuming $[H, \mathrm{i}A]_\circ$ to exist, we say that the Mourre estimate holds at $\lambda \in \mathbb{R}$ if there exists an open interval Σ containing λ, a constant $c > 0$ and a compact operator K such that

$$E_\Sigma(H)[H, \mathrm{i}A]_\circ E_\Sigma(H) \geqslant cE_\Sigma(H) + K, \tag{1.8}$$

in the form sense on $\mathcal{H} \times \mathcal{H}$. Here $E_\Sigma(H)$ is the spectral projector of H onto the interval Σ. Denote $\Theta(H)$ the set of points where a Mourre estimate (1.8) holds for H with respect to A. In other words, $\mathbb{R} \setminus \Theta(H)$ is the set of *thresholds* of H. In addition to V bounded, two hypotheses on the potential appear in this manuscript:
Hypothesis 1: The potential V satisfies

$$\max_{1\leqslant i\leqslant d} \sup_{n\in\mathbb{Z}^d} |n_i(V - \tau_i V)(n)| < +\infty. \tag{1.9}$$

Hypothesis 2: V is compact, i.e.

$$V(n) \to 0, \quad \text{as } |n| \to +\infty. \tag{1.10}$$

The main result of the paper concerning the one-dimensional operator H is:

Theorem 1.2. *Assume Hypotheses 1 and 2, and $d = 1$. If $H\psi = E\psi$ with $\psi \in \ell^2(\mathbb{Z})$, then if*

$$\theta_E := \begin{cases} \sup\{2 + (E-2)/\cosh\alpha : \alpha \geqslant 0 \text{ and } \psi \in \mathcal{D}(\vartheta_\alpha)\}, & \text{for } E < 2 \\ \inf\{2 + (E-2)/\cosh\alpha : \alpha \geqslant 0 \text{ and } \psi \in \mathcal{D}(\vartheta_\alpha)\}, & \text{for } E > 2, \end{cases} \tag{1.11}$$

one has that either $\theta_E \in \mathbb{R} \setminus \Theta(H)$ or $\theta_E = 2$. If $E = 2$, the statement is that either $\psi \in \mathcal{D}(\vartheta_\alpha)$ for all $\alpha \geqslant 0$ or $2 \in \mathbb{R} \setminus \Theta(H)$. Moreover, if $\psi \in \mathcal{D}(\vartheta_\alpha)$ for all $\alpha \geqslant 0$, then $\psi = 0$.

Remark 1.2. *The function $\mathbb{R}^+ \ni \alpha \mapsto \theta_E(\alpha) := 2 + (E-2)/\cosh(\alpha) \in [E, 2)$ is increasing to two when $E < 2$ so that $E \leqslant \theta_E \leqslant 2$, whereas the function is decreasing to two when $E > 2$ in which case $E \geqslant \theta_E \geqslant 2$. This function is graphed in Figure 1 for four different values of E.*

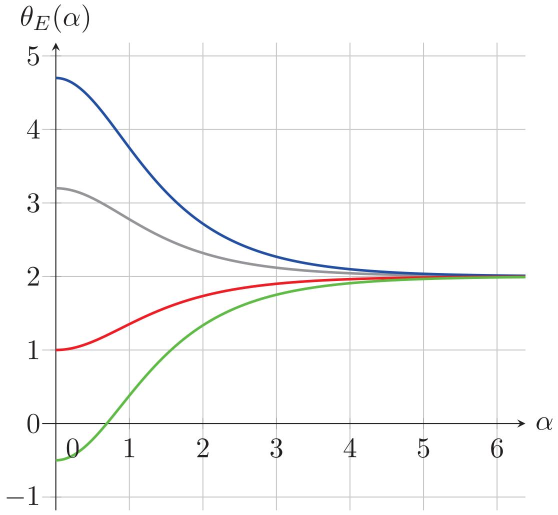

Figure 1. Graph of $\theta_E(\alpha) = 2 + (E-2)/\cosh(\alpha)$ for four different values of E.

If E is both an eigenvalue and a threshold, Theorem 1.2 does not give any information about the rate of decay of the corresponding eigenfunction, whereas if E is not a threshold, the corresponding eigenfunction decays at a rate at least of $\cosh^{-1}((E-2)/(\theta_E - 2))$. As in the continuous operator setting, the possibility of $\psi \in \mathcal{D}(\vartheta_\alpha)$ for all $\alpha \geqslant 0$ can be eliminated. The last part of Theorem 1.2 implies the absence of eigenvalues in the middle of the band $[0, 4]$, more precisely between 2 and the nearest thresholds above and below this value.

The study of the absence of positive eigenvalues for Schrödinger operators has a long history. For continuous Schrödinger operators, it was shown in the sixties in articles by Kato [K2], Simon [Si1] and Agmon [A2] that the multi-dimensional operator $-\Delta + V_1 + V_2$ has no eigenvalues in $[0, +\infty)$ whenever $\lim_{|x|\to+\infty} |x||V_1(x)| = 0$ and $\lim_{|x|\to+\infty} |(x \cdot \nabla)V_2(x)| = 0$. In fact, the method of Froese and Herbst allows to extend this result to N-body Hamiltonians, see [CFKS, Theorem 4.19]. So, if the discrete case were to resemble the continuous case, it is not unreasonable to expect the multi-dimensional operator $\Delta + V$ to have no eigenvalues in $(0, 4d)$ whenever $|n_i(V - \tau_i V)(n)| \to 0$ as $|n| \to +\infty$. A one-dimensional result pointing in this direction is the following. It actually comes as a corollary of Theorem 1.2.

Theorem 1.3. *Let $d = 1$. Suppose that V satisfies $\lim_{|n|\to+\infty} |n||V(n) - V(n-1)| = 0$ and $\lim_{|n|\to+\infty} |V(n)| = 0$. Then $H := \Delta + V$ has no eigenvalues in $(0, 4)$.*

Proof. First, if $|n(V(n)-V(n-1))| \to 0$, we see from (1.7) that $[V, \mathrm{i}A]_\circ$ is not only a bounded operator but also compact. It follows by [GMa, Proposition 2.1] that $V \in C^1_{\mathrm{u}}(A)$. Let $\mathcal{B}(\mathcal{H})$ denote the bounded operators on $\mathcal{H}$. We recall that a bounded operator T belongs to the $C^1_{\mathrm{u}}(A)$ class if the map $\mathbb{R} \mapsto e^{-\mathrm{i}tA}Te^{\mathrm{i}tA}$ is of class $C^1(\mathbb{R}; \mathcal{B}(\mathcal{H}))$, with $\mathcal{B}(\mathcal{H})$ endowed with the norm operator topology. It is well-known that Δ is of class $C^1_{\mathrm{u}}(A)$, see e.g. [Man]. We then apply [ABG, Theorem 7.2.9] to conclude that $\Theta(H) = \Theta(\Delta) = (0, 4)$. Here $\Theta(\Delta)$ denotes the set of points where a Mourre estimate holds for Δ with respect to A, and $\Theta(\Delta) = (0, 4)$ is a direct consequence of(1.6). Since H does not have any thresholds in $(0, 4)$, it must be that H has no eigenvalues in this interval, by Theorem 1.2. □

This is very much related to Remling's optimal result [R], that if $\lim_{|n|\to+\infty} |n||V(n)| = 0$, then the spectrum of the one-dimensional discrete operator $\Delta + V$ is purely absolutely continuous on $(0, 4)$. Of course, Remling's result is stronger than that of Theorem 1.3, but the assumptions are also stronger. Also related is a one-dimensional discrete version of Weidmann's Theorem proven in [Si2], namely if V is compact and of bounded variation, then the spectrum of $\Delta + V$ is purely absolutely continuous on $(0, 4)$. Finally, another interesting result is that of [JS] where it is shown that the spectrum of the half-line discrete Schrödinger operator $\Delta + W + V$ is purely absolutely continuous on $(0, 4) \setminus \{2 \pm 2\cos(k/2)\}$, where $W(n) = q \sin(kn)/n^\beta$ with $q, k \in \mathbb{R}, \beta \in (1/2, 1]$ and $(V(n)) \in \ell^1(\mathbb{Z}_+)$. Note that Theorem 1.2 is in conformity with their example when $\beta = 1$ and $V \equiv 0$. In the same spirit, we provide a simple application of Theorem 1.3:

Proposition 1.4. *Let $d = 1$ and $W(n) := q \sin(k|n|^\alpha)/|n|^\beta$ be a Wigner-von Neumann potential, with $q, k \in \mathbb{R}$. Then for $\beta > \alpha > 0$, $\sigma_{\mathrm{ess}}(\Delta + W) = [0, 4]$ and $(0, 4)$ is void of eigenvalues.*

An analogous result for continuous Schrödinger operators is obtained and thoroughly discussed in [JM], and is also inspired from [FH]. We now turn to the multi-dimensional discrete Schrödinger operators. The main result concerning these is:

Theorem 1.5. *Let $d \geqslant 1$. Suppose that Hypothesis 1 holds for the potential V. If $H\psi = E\psi$ with $\psi \in \ell^2(\mathbb{Z}^d)$ and $E \in \Theta(H)$, then $\psi \in \mathcal{D}(\vartheta_{\alpha,\gamma})$ for all $(\alpha, \gamma) \in [0, \infty) \times [0, 2/3)$.*

Although Theorem 1.5 does not yield exponential decay of eigenfunctions at non-threshold energies as in the continuous operator case, the result is still useful for applications in Mourre theory. It appears that the method of Froese and Herbst adapts quite well for the one-dimensional discrete operator; however, there seems to be a non-trivial difference between the dimensions $d \geqslant 2$ and $d = 1$ in the discrete setting as far as the method is concerned. The exponential decay of eigenfunctions at non-threshold energies in higher dimensions therefore remains an open question because our proof does not attain it. Yet an indication it may occur comes from the Combes-Thomas method presented above.

On the one hand, if E belongs to the discrete spectrum of H, then for any interval Σ containing E and located outside the essential spectrum of H, $E_\Sigma(H)$ is simply a finite rank eigenprojection and so the Mourre estimate holds by default, both sides of (1.8) being compact operators. So under Hypothesis 1 only, the corresponding eigenfunction decays sub-exponentially according to Theorem 1.5. In this case, the Combes-Thomas method is clearly superior. On the other hand, the Mourre estimate typically holds above the essential spectrum of H. So Theorem 1.5 is able to characterize the decay of eigenfunctions for non-threshold eigenvalues embedded in the essential spectrum, if *any* exist. We emphasize the last point, because to our knowledge there is no example of a Schrödinger operator with a non-threshold embedded eigenvalue. What is certainly known however is the existence of operators with a threshold embedded eigenvalue, the Wigner-von Neumann operator being the classical illustration of it, see e.g. [RS4].

Let us provide an example of a discrete Wigner-von Neumann type operator H that has an eigenvalue embedded in its essential spectrum. An eigenvector for this eigenvalue will be given explicitly. Here's how Theorem 1.5 turns out to be useful: as the eigenvector will have slow decay at infinity, we infer that the eigenvalue is a threshold, in the sense that no Mourre estimate holds for the pair of self-adjoint operators (H, A) above any interval containing this value. Our example and approach is inspired from the one that appears in [RS4, Section XIII.13, Example 1].

Proposition 1.6. *For given $k_1, ..., k_d \in (0, \pi)$, let $(t_{k_i})_{i=1}^d$ be real numbers such that*

$$t_{k_i} + \sin(2k_i)n_i - \sin(2k_i n_i) \neq 0, \quad \textit{for all } n_i \in \mathbb{Z}.$$

Then there exists an oscillating potential V on $\mathbb{Z}^d$ that has the asymptotic behavior

$$V(n_1, ..., n_d) = \sum_{i=1}^{d} -\frac{4\sin(k_i)\sin(2k_i n_i)}{n_i} + O_{k_i,t_{k_i}}(n_i^{-2})$$

and such that $E := 2d - \sum_{i=1}^d 2\cos(k_i)$ is both a threshold and an eigenvalue for $H := \Delta + V$, with eigenvector $\psi(n_1, ..., n_d) = \prod_{i=1}^d \sin(k_i n_i)[t_{k_i} + \sin(2k_i)n_i - \sin(2k_i n_i)]^{-1}$ belonging to $\ell^2(\mathbb{Z}^d)$. Moreover, $E \in [0, 4d] \subset \sigma_{\text{ess}}(H)$.

The exact expression of the potential V is given in the proof. By the notation $O_{k_i,t_{k_i}}(n_i^{-2})$, we mean that this decaying term depends on the choice of k_i and t_{k_i}. It is interesting to further note that the eigenvector ψ does not belong to the domain of A, for $(N_i(S_i^* - S_i)\psi)(n_1, ..., n_d)$ does not go to zero as $|n_i| \to +\infty$. To further motivate Theorem 1.5, let us give another application to discrete Wigner-von Neumann operators.

Example 1.7 (from [Man]). *Let W be the discrete Wigner-von Neumann potential given by*

$$(Wu)(n) = W(n)u(n) := \frac{q\sin(k(n_1 + ... + n_d))}{|n|}u(n), \quad \forall n \in \mathbb{Z}^d, u \in \mathcal{H},$$

for some $(q, k) \in \mathbb{R} \times (-\pi, \pi)$, and let V be a multiplication operator satisfying for some $\rho > 0$,

$$\sup_{n\in\mathbb{Z}^d} \langle n\rangle^\rho |V(n)| < \infty, \quad \textit{and} \quad \max_{1\leqslant i\leqslant d} \sup_{n\in\mathbb{Z}^d} \langle n\rangle^\rho |n_i||(V - \tau_i V)(n)| < +\infty.$$

Here $\langle n\rangle := \sqrt{1 + |n|^2}$. Let $H := \Delta + W + V$ be the Schrödinger operator on $\mathcal{H}$, and let P and $P^\perp$ respectively denote the spectral projectors onto the pure point subspace of H and its complement. Let $E(k) := 4 - 4 \cdot \text{sign}(k)\cos(k/2)$, and consider the sets

$$\mu(H) := (0, 4) \setminus \{2 \pm 2\cos(k/2)\}, \quad \textit{for } d = 1,$$
$$\mu(H) := (0, E(k)) \cup (4d - E(k), 4d), \quad \textit{for } d \geqslant 2.$$

By combining Theorem 1.5 with [Man, Theorem 1.1], *one can remove the abstract assumption* $\ker(H - E) \subset \mathcal{D}(A)$ *that appears in the latter Theorem; and for the one-dimensional result, we can use the stronger result of Theorem 1.2. We get the following improved result:*

Theorem 1.8. *We have that $\mu(H) \subset \Theta(H)$. For all $E \in \mu(H)$ there is an open interval Σ containing E such that for all $s > 1/2$ and all compact intervals $\Sigma' \subset \Sigma$, the reduced limiting* *absorption principle for H holds for with respect to (Σ', s, A), that is,*

$$\sup_{x\in\Sigma', y\neq 0} \|\langle A\rangle^{-s}(H-x-\mathrm{i}y)^{-1}P^{\perp}\langle A\rangle^{-s}\| < \infty.$$

In particular, the spectrum of H is purely absolutely continuous on Σ' whenever $P=0$ on Σ', and for $d=1$, H does not have any eigenvalues in the interval $(2-2\cos(k/2), 2+2\cos(k/2))$.

From a perspective of Mourre theory and in an abstract setting, an area of research is to show that the eigenfunction $\psi \in \mathcal{D}(A^n)$ for some $n \geqslant 1$. The first results of this kind were obtained in [Ca] and [CGH], where it was shown that if $H\psi = E\psi$ with E embedded in the continuous spectrum of H, and the iterated commutators $\mathrm{ad}_A^k(H)$ are bounded for $k=1,...,\nu$ together with appropriate domain conditions being satisfied by H and A, then $\psi \in \mathcal{D}(A^n)$ for all $n \geqslant 0$ satisfying $n+2 \leqslant \nu$, whenever the Mourre estimate holds at E. Here A is the conjugate operator to the Hamiltonian H in the abstract framework, and the iterated commutators are defined by $\mathrm{ad}_A^1(H) := [H, \mathrm{i}A]_\circ$ and $\mathrm{ad}_A^k(H) := [\mathrm{ad}_A^{k-1}(H), \mathrm{i}A]_\circ$. So in the simplest case, one would obtain $\psi \in \mathcal{D}(A)$ provided $\mathrm{ad}_A^3(H)$ exists. Then in [FMS], the authors reduce by one, from $n+2$ to $n+1$ the number of commutators that need to be bounded in order to obtain $\psi \in \mathcal{D}(A^n)$, and show that the result is optimal. In counterpart of these abstract results, we should point out that in the framework of Schrödinger operators, minimal hypotheses yield much stronger results. Indeed, a direct consequence of Theorem 1.5 is that $\psi \in \mathcal{D}(A^n)$ for all $n \geqslant 0$ assuming only $[H, \mathrm{i}A]_\circ$ bounded.

Finally, we point out that the notion of the $C^1(A)$ class of operators also exists for unbounded operators. It appears to us that the results of this paper could also apply to Schrödinger operators with unbounded potentials satisfying the $C^1(A)$ condition. A simple criterion to check if the potential belongs to this class is given in [GMo][Lemma A.2]. This criterion is straightforward to verify in the setting of this paper. It is however doubtful to us if the generalization of the result to unbounded potentials is significant.

The plan of the paper is as follows: in Section 2, we provide a proof of Theorem 1.1 for the reader's convenience. Section 3 is devoted to the proof of the main result for the multi-dimensional Schrödinger operator, namely Theorem 1.5. In Section 4, we prove Proposition 1.6. In Section 5, we further develop the method of Section 3 in the case of the one-dimensional operator, and prove Theorem 1.2. Finally Section 6 is the Appendix and contains a long technical calculation proving a key relation required for both Sections 3 and 5.

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2. The method of Combes-Thomas: Proof of Theorem 1.1

We follow the approach given in [Hi] and to a lesser extent [BCH]. We point out that the Combes-Thomas method typically involves techniques of analytic continuation which require some care if the operators are unbounded, see e.g. [RS4, Section XII.2]. However, since all operators are bounded in this setting, things are simpler. Let $\mathcal{B}(\mathcal{H})$ be the bounded operators on $\mathcal{H}$, and let $\rho = \rho(n) := \sqrt{1+|n|^2}$, $n \in \mathbb{Z}^d$. First we need an estimate:

Proposition 2.1. *Let V be any bounded real-valued potential, and denote $T := \Delta + V$. Then $\mathbb{C} \ni \lambda \mapsto T(\lambda) := e^{\mathrm{i}\lambda\rho} T e^{-\mathrm{i}\lambda\rho} \in \mathcal{B}(\mathcal{H})$ is an analytic map. If $E \in \mathbb{R} \setminus \sigma(T)$, then for λ satisfying*

$$\frac{2d \cdot e^{|\lambda|}|\lambda|}{\operatorname{dist}(\sigma(T), E)} < \frac{1}{2}, \tag{2.1}$$

$$\|(T(\lambda) - E)^{-1}\| \leqslant 2/\operatorname{dist}(\sigma(T), E). \tag{2.2}$$

Proof. A first calculation gives that

$$T(\lambda) := e^{\mathrm{i}\lambda\rho} T e^{-\mathrm{i}\lambda\rho} = T + D(\lambda),$$

where

$$D(\lambda) := \sum_{i=1}^{d} \left(1 - e^{\mathrm{i}\lambda(\rho - \tau_i\rho)}\right) S_i + \left(1 - e^{-\mathrm{i}\lambda(\rho - \tau_i^*\rho)}\right) S_i^*.$$

By the Mean Value Theorem, $|\rho - \tau_i\rho|$ and $|\rho - \tau_i^*\rho|$ are bounded above by one. Also, $\|S_i\| = \|S_i^*\| = 1$. Thus $D(\lambda) : \mathbb{C} \mapsto \mathcal{B}(\mathcal{H})$ is a differentiable function, and so $\lambda \mapsto T(\lambda)$ is an analytic family of bounded operators on $\mathbb{C}$. Suppose that $E \in \mathbb{R} \setminus \sigma(T)$. Then

$$(T(\lambda) - E) = \left(1 + D(\lambda)(T - E)^{-1}\right)(T - E).$$

Thanks to the inequality $|1 - e^z| \leqslant |z| e^{|z|}$, for all $z \in \mathbb{C}$, we get

$$\|D(\lambda)\| \leqslant 2d \cdot e^{|\lambda|}|\lambda|.$$

Also note that $\|(T - E)^{-1}\| \leqslant 1/\operatorname{dist}(\sigma(T), E)$ since T is self-adjoint. Therefore if we require that $|\lambda|$ satisfies (2.1), it follows that $\|D(\lambda)(T - E)^{-1}\| < 1/2$ and we may invert $(T(\lambda) - E)$. Consequently, bounding above by a geometric series gives

$$\|(T(\lambda) - E)^{-1}\| \leqslant \|(T - E)^{-1}\| \|(1 + D(\lambda)(T - E)^{-1})^{-1}\| \leqslant 2/\operatorname{dist}(\sigma(T), E).$$

□

Proof of Theorem 1.1: Suppose first that V has compact support in $\mathbb{Z}^d$. Then the condition $\operatorname{dist}(\sigma(\Delta), E) > \limsup_{|n| \to +\infty} |V(n)|$ is automatically true since the right side equals zero. Since $H\psi = (\Delta + V)\psi = E\psi$, we write, for $\lambda \in \mathbb{R}$,

$$e^{\mathrm{i}\lambda\rho}\psi = -\left(e^{\mathrm{i}\lambda\rho}(\Delta - E)^{-1} e^{-\mathrm{i}\lambda\rho}\right)(e^{\mathrm{i}\lambda\rho} V\psi) = -(\Delta(\lambda) - E)^{-1}(e^{\mathrm{i}\lambda\rho} V\psi).$$

Because of the analyticity of $\Delta(\lambda)$ and the compactness of the support of V, both terms on the right of the previous equation admit an analytic continuation to all of $\mathbb{C}$. Let ν be the unique positive solution to the equation

$$\mathbb{R}^+ \ni \mu \mapsto \frac{2d \cdot e^{\mu}\mu}{\operatorname{dist}(\sigma(\Delta), E)} = \frac{1}{2}. \tag{2.3}$$

Set $\lambda = -\mathrm{i}\alpha$, with $\alpha \in (0, \nu)$. Taking norms and applying Proposition 2.1 with $T \equiv \Delta$, we see that there exists a constant $C_{E,V,\psi}$ depending on E, V and ψ, so that

$$\|e^{\alpha\rho}\psi\| \leqslant 2\|\psi\| \cdot \sup_{n \in \mathbb{Z}^d} |e^{\alpha\rho} V(n)| / \operatorname{dist}(\sigma(\Delta), E) := C_{E,V,\psi}.$$

We now assume that the support of V is not compact, but $\limsup_{|n| \to +\infty} |V(n)| < \operatorname{dist}(\sigma(\Delta), E)$ holds. We may write $V = V_c + V_l$, where V_c is compactly supported and $\|V_l\| = \sup_{n \in \mathbb{Z}^d} |V_l(n)| \leqslant l$ for some $l < \operatorname{dist}(\sigma(\Delta), E)$. Consider the operator $H_l := \Delta + V_l$. Since V_l is a bounded operator, $H_l(\lambda)$ is an analytic family. If $\epsilon > 0$ is any number verifying $\epsilon < \operatorname{dist}(\sigma(\Delta), E) - l$, then H_l has a spectral gap around E of size at least ϵ. This is due to the following spectral inclusion formula, see e.g. [K1, Theorem 3.1]:

$$\sigma(H_l) \subset \{\mu \in \mathbb{R} : \text{dist}\,(\sigma(\Delta), \mu) \leqslant \|V_l\|\}.$$

In particular, $(H_l - E)$ is invertible. Since

$$(H_l - E) = \left(1 + V_l(\Delta - E)^{-1}\right)(\Delta - E)$$

and $\|V_l(\Delta - E)^{-1}\| < l/\text{dist}(\sigma(\Delta), E) < 1$, we get

$$(H_l - E)^{-1} = (\Delta - E)^{-1}\left(1 + V_l(\Delta - E)^{-1}\right)^{-1}.$$

From the eigenvalue equation $H\psi = (H_l + V_c)\psi = E\psi$, we may write

$$e^{\mathrm{i}\lambda\rho}\psi = -(H_l(\lambda) - E)^{-1}(e^{\mathrm{i}\lambda\rho}V_c\psi).$$

Let ν be the unique positive solution to the equation

$$\mathbb{R}^+ \ni \mu \mapsto \frac{2d \cdot e^{\mu}\mu}{\text{dist}(\sigma(H_l), E)} = \frac{1}{2}. \tag{2.4}$$

Set $\lambda = -\mathrm{i}\alpha$, with $\alpha \in (0, \nu)$. Taking norms and applying Proposition 2.1 with $T \equiv H_l$, we see that there exists a constant $C_{E,V,\psi}$ so that

$$\|e^{\alpha\rho}\psi\| \leqslant 2\|\psi\| \cdot \sup_{n \in \mathbb{Z}^d} |e^{\alpha\rho}V_c(n)|/\text{dist}(\sigma(H_l), E) := C_{E,V,\psi}.$$

□

3. The multidimensional case : sub-exponential decay of eigenfunctions

We begin this section by fixing more notation, and build on the one introduced above. Let

$$\Delta_i := 2 - S_i^* - S_i \quad \text{and}$$

$$A_{0,i} := -\mathrm{i}\left(2^{-1}(S_i^* + S_i) + N_i(S_i^* - S_i)\right) = \mathrm{i}\left(2^{-1}(S_i^* + S_i) - (S_i^* - S_i)N_i\right).$$

Let

$$A_i' := \mathrm{i}A_{0,i}, \quad \text{and} \quad A' := \sum_{i=1}^{d} A_i' = iA_0, \quad \text{with} \quad \mathcal{D}(A') = \mathcal{D}(A_0). \tag{3.1}$$

Then the following is a non-negative operator on $\mathcal{H}$:

$$[\Delta_i, A_i']_\circ = \Delta_i(4 - \Delta_i) = 2 - (S_i^*)^2 - (S_i)^2.$$

A useful identity relating the shift operators and the potential is:

$$S_i V = (\tau_i V)S_i \quad \text{and} \quad S_i^* V = (\tau_i^* V)S_i^*. \tag{3.2}$$

Consider an increasing function $F \in C^3([0, \infty))$ with bounded derivative away from the origin. Ideally we would like to take $F(x) = \alpha x$ later on, with $\alpha \geqslant 0$ as in [FH], but it will turn out that slightly better decay conditions on the derivative are required. So examples to keep in mind for a later application are $F_{s,\alpha,\gamma} : [0, \infty) \mapsto [0, \infty)$, where $(s, \alpha, \gamma) \in [0, \infty) \times [0, \infty) \times [0, 2/3)$ and

$$F_{s,\alpha,\gamma}(x) := \Upsilon_s(\alpha x^\gamma). \tag{3.3}$$

Here Υ_s is an interpolating function defined for $s \geqslant 0$ by

$$\Upsilon_s(x) := \int_0^x \langle st \rangle^{-2} dt. \tag{3.4}$$

Then $\Upsilon_s(x) \uparrow x$ as $s \downarrow 0$, and

$$\Upsilon_s(x) \leqslant c_s \quad \text{for} \quad s > 0, \quad \text{and} \quad |\Upsilon_s^{(n)}(x)| \leqslant cx^{-n+1}, \tag{3.5}$$

where the first constant in (3.5) depends on s whereas the second one does not. It is readily seen that there are constants $C > 0$ not depending on s and γ such that

$$|F'_{s,\alpha,\gamma}(x)| \leqslant Cx^{\gamma-1} \quad \text{and} \quad |F''_{s,\alpha,\gamma}(x)| \leqslant Cx^{\gamma-2}. \tag{3.6}$$

We also have that for all $x \geqslant 0$,

$$F'_{s,\alpha,\gamma}(x) \geqslant 0 \quad \text{and} \quad F''_{s,\alpha,\gamma}(x) \leqslant 0. \tag{3.7}$$

So $F_{s,\alpha,\gamma}$ is increasing and concave.

For $n = (n_1, ..., n_d) \in \mathbb{Z}^d$, let $\langle n \rangle := \sqrt{1 + |n|^2}$. The function F induces a radial operator of multiplication on $\mathcal{H}$, also denoted by F and acting as follows: $(Fu)(n) := F(\langle n \rangle)u(n)$, $\forall u \in \mathcal{H}$. For $i = 1, ..., d$, we introduce the multiplication operators on $\mathcal{H}$:

$$\varphi_{\ell_i} := (\tau_i e^F - e^F)/e^F = e^{\tau_i F - F} - 1 \quad \text{and} \quad \varphi_{r_i} := (\tau_i^* e^F - e^F)/e^F = e^{\tau_i^* F - F} - 1, \tag{3.8}$$

$$g_{\ell_i} := \varphi_{\ell_i}/N_i \quad \text{and} \quad g_{r_i} := \varphi_{r_i}/N_i. \tag{3.9}$$

In other words, if $U_i : \mathbb{Z}^d \mapsto \mathbb{Z}^d$ denotes the flow $(n_1, ..., n_d) \mapsto (n_1, ..., n_i - 1, ..., n_d)$ and U_i^{-1} its inverse, then φ_{ℓ_i} and φ_{r_i} are multiplication at n respectively by $\varphi_{\ell_i}(n) = e^{F(\langle U_i n \rangle) - F(\langle n \rangle)} - 1$ and $\varphi_{r_i}(n) = e^{F(\langle U_i^{-1} n \rangle - F(\langle n \rangle)} - 1$, while g_{ℓ_i} and g_{r_i} are multiplication at n respectively by $g_{\ell_i}(n) = \varphi_{\ell_i}(n)/n_i$ and $g_{r_i}(n) = \varphi_{r_i}(n)/n_i$. Since $g_{\ell_i}(n)$ and $g_{r_i}(n)$ are not well-defined when $n_i = 0$, set $g_{\ell_i}(n) = g_{r_i}(n) := 0$ in that case. We will need the operator g on $\mathcal{H}$ given by

$$(gu)(n) = g(n)u(n) := \frac{F'(\langle n \rangle)}{\langle n \rangle} u(n). \tag{3.10}$$

Three remarks are in order. First, by the Mean Value Theorem, F' bounded away from the origin ensures that φ_{ℓ_i}, φ_{r_i}, g_{ℓ_i} and g_{r_i} are bounded operators on $\mathcal{H}$; secondly, F increasing implies $\text{sign}(n_i)\varphi_{r_i}(n) \geqslant 0$, $\text{sign}(n_i)\varphi_{\ell_i}(n) \leqslant 0$, $g_{r_i}(n) \geqslant 0$, $g_{\ell_i}(n) \leqslant 0$ and $g(n) \geqslant 0$; and thirdly, we remark that F, φ_{ℓ_i}, φ_{r_i} and g are radial potentials on $\mathcal{H}$.

Proposition 3.1. *Suppose that Hypothesis 1 holds for the potential V. Let F be a general function as described above and suppose that for all $i, j = 1, ..., d$,*

- $\dagger_1$ $|g_{r_i}| \in O(1)$ *and* $|g_{\ell_i}| \in O(1)$,
- $\dagger_2$ $|\tau_i g - g| N_j \in O(1)$,
- $\dagger_3$ $|\tau_i \varphi_{r_i} - \varphi_{r_i}| N_j$, $|\tau_i \varphi_{\ell_i} - \varphi_{\ell_i}| N_j$, $|\tau_i \varphi_{r_j} - \varphi_{r_j}| N_i$ *and* $|\tau_i \varphi_{\ell_j} - \varphi_{\ell_j}| N_i \in O(1)$,
- $\dagger_4$ $|(g_{r_i} - g) - (g_{\ell_i} + g)| N_i N_j \in O(1)$.

Suppose that $H\psi = E\psi$, with $\psi \in \mathcal{H}$. Let $\psi_F := e^F \psi$, and assume $\psi_F \in \mathcal{H}$. Then $\psi_F \in \mathcal{D}(\sqrt{g}A')$ and there exist bounded operators $(W_i)_{i=1}^d$, $\mathcal{L}$, $\mathcal{M}$ and $\mathcal{G}$ on $\mathcal{H}$ depending on F such that

$$\begin{aligned} \langle \psi_F, [H, A']_\circ \psi_F \rangle = -2\big\|\sqrt{g}A'\psi_F\big\|^2 - \sum_{i=1}^d \big\|\sqrt{\Delta_i(4-\Delta_i)}W_i\psi_F\big\|^2 \\ + 2^{-1}\langle \psi_F, (\mathcal{L} + \mathcal{M} + \mathcal{G})\psi_F \rangle. \end{aligned} \tag{3.11}$$

The W_i are multiplication operators given by $W_i = W_{F;i} := \sqrt{\cosh(\tau_i F - F) - 1}$. The expressions of $\mathcal{L}$, $\mathcal{M}$ and $\mathcal{G}$ are involved; they are given by (6.9), (6.10) *and* (6.11) *respectively. The relevant point is that these three operators are a finite sum of terms, each one of the form*

$$P_1(S_1, ..., S_d, S_1^*, ..., S_d^*) T P_2(S_1, ..., S_d, S_1^*, ..., S_d^*), \tag{3.12}$$

where P_1 and P_2 are multivariable polynomials in $S_1, ..., S_d, S_1^*, ..., S_d^*$ and T are multiplication operators of the kind listed in $\dagger_1 - \dagger_4$.

Remark 3.1. *Formula* (3.11) *has an additional negative term compared to the corresponding formula for the continuous Schrödinger operator, cf.* [FH, Lemma 2.2]*:*

$$\langle \psi_F, [H, A']_\circ \psi_F \rangle = -4\|\sqrt{g} A' \psi_F\|^2 + \langle \psi_F, \mathcal{Q}\psi_F \rangle, \quad \textit{with} \quad \mathcal{Q} = (x \cdot \nabla)^2 g - x \cdot \nabla (\nabla F)^2.$$

Remark 3.2. *As mentioned in* [FH]*, if we consider the Virial Theorem disregarding operator domains, it is reasonable to expect $\langle \psi, [H, e^F A' e^F]\psi \rangle = 0$. This idea underlies* (3.11)*.*

Proof. Let $\phi \in \ell_0(\mathbb{Z}^d)$, the sequences with compact support, and $\phi_F := e^F \phi$. The first step of the proof consists in establishing the following identity :

$$\begin{aligned} \big\langle \phi, [e^F A' e^F, \Delta]\phi \big\rangle &= \big\langle \phi_F, [A', \Delta]\phi_F \big\rangle - 2\big\|\sqrt{g} A' \phi_F\big\|^2 \\ &\quad - \sum_{1 \leqslant i \leqslant d} \big\|\sqrt{\Delta_i(4 - \Delta_i)} W_i \phi_F\big\|^2 + 2^{-1}\big\langle \phi_F, (\mathcal{L} + \mathcal{M} + \mathcal{G})\phi_F \big\rangle. \end{aligned} \tag{3.13}$$

The proof of (3.13) is technical and long, so it is done in the Appendix. The assumptions of this Proposition together with F' bounded away from the origin imply that the W_i, $\mathcal{L}$, $\mathcal{M}$ and $\mathcal{G}$ stemming from this calculation are bounded operators. Exactly where these assumptions are applied are indicated in the Appendix by (‡). The second step consists in using (3.13) to prove (3.11). For $m \geqslant 1$, define the cut-off potentials $\chi_m(n) := \chi(\langle n \rangle / m)$ on $\mathbb{Z}^d$, where $\chi \in C_c^\infty(\mathbb{R})$ and χ equals one in a neighborhood of the origin. Then (3.13) holds with $\phi = \chi_m \psi$ and $\phi_F = e^F \chi_m \psi$. Adding $\big\langle \chi_m \psi, [e^F A' e^F, V]\chi_m \psi \big\rangle = \big\langle e^F \chi_m \psi, [A', V] e^F \chi_m \psi \big\rangle$ to each side of (3.13), and introducing the constant E in the commutator on the left gives

$$\begin{aligned} \big\langle \chi_m \psi, [e^F A' e^F, H - E]\chi_m \psi \big\rangle &= \big\langle e^F \chi_m \psi, [A', H] e^F \chi_m \psi \big\rangle - 2\big\|\sqrt{g} A' e^F \chi_m \psi\big\|^2 \\ &\quad - \sum_{1 \leqslant i \leqslant d} \big\|\sqrt{\Delta_i(4 - \Delta_i)} W_i e^F \chi_m \psi\big\|^2 \\ &\quad + 2^{-1}\big\langle e^F \chi_m \psi, (\mathcal{L} + \mathcal{M} + \mathcal{G}) e^F \chi_m \psi \big\rangle. \end{aligned} \tag{3.14}$$

Since $e^F \chi_m \psi \to \psi_F$ in $\mathcal{H}$ as $m \to \infty$, the first, third and fourth terms on the right side of (3.14) converge. The left side of (3.14) is handled in the same way as in [CFKS, Proposition 4.16]:

$$\begin{aligned} \big\langle \chi_m \psi, [e^F A' e^F, H - E]\chi_m \psi \big\rangle &= -2\Re\big(\big\langle e^F A' e^F \chi_m \psi, (H - E)\chi_m \psi \big\rangle\big) \\ &= -2\Re\big(\big\langle \langle N \rangle^{-1} A' e^F \chi_m \psi, \langle N \rangle e^F (H - E)\chi_m \psi \big\rangle\big). \end{aligned}$$

Since $\text{supp}(\chi_m) \subset [-2m, 2m]^d$, $\text{supp}((H - E)\chi_m \psi) \subset K := [-2m - 1, 2m + 1]^d$ and so commuting χ_m with $(H - E)$ gives

$$\begin{aligned} \langle N \rangle e^F (H - E)\chi_m \psi &= \langle N \rangle e^F \mathbf{1}_K (H - E)\chi_m \psi \\ &= \sum_{1 \leqslant i \leqslant d} \langle N \rangle (\chi_m - \tau_i \chi_m) e^F S_i \psi + \langle N \rangle (\chi_m - \tau_i^* \chi_m) e^F S_i^* \psi. \end{aligned} \tag{3.15}$$

An application of the Mean Value Theorem shows that $|\langle N\rangle(\chi_m - \tau_i \chi_m)|$ and $|\langle N\rangle(\chi_m - \tau_i^* \chi_m)|$ are bounded by a constant independent of m. Moreover, $\psi_F \in \mathcal{H}$ and F' bounded imply that $e^F S_i \psi = S_i e^{\tau_i^* F - F} \psi_F$ and $e^F S_i^* \psi = S_i^* e^{\tau_i F - F} \psi_F \in \mathcal{H}$. Thus the sequence (3.15) is uniformly bounded in absolute value in $\mathcal{H}$. Furthermore, it converges pointwise to zero. By Lebesgue's Dominated Convergence Theorem,

$$\big\| \langle N\rangle e^F (H-E) \chi_m \psi \big\| \to 0 \quad \text{as} \quad m \to \infty. \tag{3.16}$$

Since $\langle N\rangle^{-1} A'$ is a bounded operator on $\mathcal{H}$, the left side of (3.14) converges to zero as $m \to \infty$. The only remaining term in (3.14) is $2\|\sqrt{g} A' e^F \chi_m \psi\|^2$, hence it must also converge as $m \to \infty$. To finish the proof, it remains to show that $\psi_F \in \mathcal{D}(\sqrt{g} A')$. Let $\phi \in \ell_0(\mathbb{Z})$. Then

$$\big|\langle \psi_F, A' \sqrt{g} \phi \rangle\big| = \lim_{m\to\infty} \big|\langle e^F \chi_m \psi, A' \sqrt{g} \phi\rangle\big| \leqslant \Big(\lim_{m \to \infty} \|\sqrt{g} A' e^F \chi_m \psi\| \Big) \|\phi\|.$$

This shows that $\psi_F \in \mathcal{D}\big((-A'\sqrt{g})^*\big) = \mathcal{D}(\sqrt{g} A')$. Then it must be that $\|\sqrt{g} A' e^F \chi_m \psi\|^2 \to \|\sqrt{g} A' \psi_F\|^2$ and the proof is complete after rearranging the terms accordingly in (3.14). □

As mentionned in the last Proposition, $\mathcal{L}, \mathcal{M}$ and $\mathcal{G}$ are a finite sum of terms of the form

$$P_1(S_1, ..., S_d, S_1^*, ..., S_d^*) T P_2(S_1, ..., S_d, S_1^*, ..., S_d^*)$$

for some polynomials P_1 and P_2. Going forward, it is essential that the multiplication operators $T = T(n)$ decay radially at infinity. In other words, for the minimal assumptions $\dagger_1 - \dagger_4$, we will need $o(1)$ instead of $O(1)$. The following Lemma shows that this is the case for $F = F_{s,\alpha,\gamma}$.

Lemma 3.2. *Let $F = F_{s,\alpha,\gamma}$ be the function defined in (3.3). Consider its corresponding functions $\varphi_{r_i}, \varphi_{\ell_i}, g_{r_i}, g_{\ell_i}$ and g. The following estimates hold uniformly with respect to s and γ:*

- $\ddagger_1$ $|g_{r_i}|$ *and* $|g_{\ell_i}| \in O_\alpha(\langle n\rangle^{\gamma-2})$,
- $\ddagger_2$ $|\tau_i g - g| \in O_\alpha(\langle n\rangle^{\gamma-3})$,
- $\ddagger_3$ $|\tau_i^* \varphi_{r_j} - \varphi_{r_j}|$ *and* $|\tau_i^* \varphi_{\ell_j} - \varphi_{\ell_j}| \in O_\alpha(\langle n\rangle^{\gamma-2})$,
- $\ddagger_4$ $|(g_{r_i} - g) - (g_{\ell_i} + g)| \in O_\alpha(\langle n\rangle^{3\gamma-4})$,
- $\ddagger_5$ $|(\tau_i F - F) - \tau_i(\tau_i F - F)| \in O_\alpha(\langle n\rangle^{\gamma-2})$.

Therefore $\ddagger_i$ improve $\dagger_i$ for $i = 1,2,3,4$ respectively.

Proof. These estimates are simple applications of the Mean Value Theorem (MVT). Let $n = (n_1, ..., n_d) \in \mathbb{Z}^d$ and fix $i \in \{1, ..., d\}$. There is $n' = (n_1', ..., n_d')$ with $n_i' \in (n_i, n_i+1)$ and $n_j' = n_j$ for $j \neq i$ such that

$$g_{r_i}(n) = \frac{n_i'}{\langle n'\rangle} \frac{F'(\langle n'\rangle) e^{F(\langle n'\rangle)}}{n_i e^{F(\langle n\rangle)}}.$$

This, together with (3.6), and an analogous calculation for $g_{\ell_i}(n)$ shows $\ddagger_1$. Define $g : \mathbb{R}^d \to \mathbb{R}$, $g(x) := F'(\langle x\rangle)\langle x\rangle^{-1}$. Then $\ddagger_2$ follows from

$$\frac{\partial g}{\partial x_i}(x) = \frac{x_i}{\langle x\rangle} \frac{F''(\langle x\rangle)\langle x\rangle - F'(\langle x\rangle)}{\langle x\rangle^2}.$$

Now fix $i, j \in \{1, ..., d\}$. First there is $n' = (n_1', ..., n_d')$ with $n_j' \in (n_j, n_j+1)$ and $n_k' = n_k$ for $k \neq j$ such that

$$(\tau_j^* F - F)(n) = \frac{\partial \tilde{F}}{\partial x_j}(n') = \frac{n_j'}{\langle n'\rangle} F'(\langle n'\rangle), \quad \text{with} \quad \tilde{F}(x) = F(\langle x\rangle).$$

Then there is $n'' = (n''_1, ..., n''_d)$ with $n''_i \in (n'_i, n'_i + 1)$ and $n''_k = n'_k$ for $k \neq i$ such that

$$(\tau_i^* \varphi_{r_j} - \varphi_{r_j})(n) = \frac{\partial^2 \tilde{F}}{\partial x_i \partial x_j}(n'') e^{\frac{\partial \tilde{F}}{\partial x_j}(n'')}.$$

This proves $\ddagger_3$ since

$$\left| \frac{\partial^2 \tilde{F}}{\partial x_i \partial x_j}(x) \right| \leqslant \frac{|F'(\langle x \rangle)|}{\langle x \rangle} + |F''(\langle x \rangle)|.$$

The latter estimate on $\partial^2 \tilde{F}/(\partial x_i \partial x_j)$ also implies $\ddagger_5$. Finally, for $\ddagger_4$, we start with

$$g_{r_i}(n) - g(n) = \frac{1}{n_i e^{F(\langle n \rangle)}} \left[\frac{n'_i}{\langle n' \rangle} F'(\langle n' \rangle) e^{F(\langle n' \rangle)} - \frac{n_i}{\langle n \rangle} F'(\langle n \rangle) e^{F(\langle n \rangle)} \right] = \frac{1}{n_i e^{F(\langle n \rangle)}} \frac{\partial k}{\partial x_i}(n'')$$

where

$$k : \mathbb{R}^d \to \mathbb{R}, \quad k(x) := \frac{x_i}{\langle x \rangle} F'(\langle x \rangle) e^{F(\langle x \rangle)},$$

and $n'' = (n''_1, ..., n''_d)$ with $n''_i \in (n_i, n'_i)$ and $n''_j = n_j$ for $j \neq i$. We compute

$$\frac{\partial k}{\partial x_i}(x) = \left(\frac{F'(\langle x \rangle)}{\langle x \rangle} - \frac{x_i^2 F'(\langle x \rangle)}{\langle x \rangle^3} + \frac{x_i^2 F''(\langle x \rangle)}{\langle x \rangle^2} + \frac{x_i^2 (F'(\langle x \rangle))^2}{\langle x \rangle^2} \right) e^{F(\langle x \rangle)}.$$

Thus for some $n''' = (n'''_1, ..., n'''_d)$ with $n'''_i \in (n_i - 1, n_i + 1)$ and $n'''_j = n_j$ for $j \neq i$, we have

$$(g_{r_i}(n) - g(n)) - (g_{\ell_i}(n) + g(n)) = \frac{1}{n_i e^{F(\langle n \rangle}} \frac{\partial^2 k}{\partial x_i^2}(n''').$$

A calculation of $\partial^2 k / \partial x_i^2$ yields the required estimate. □

We are now ready to prove the main result concerning the multi-dimensional operator H:

Proof of Theorem 1.5. Let $\psi_{F_{s,\alpha,\gamma}} := e^{F_{s,\alpha,\gamma}} \psi$, and let $\Psi_s := \psi_{F_{s,\alpha,\gamma}} / \|\psi_{F_{s,\alpha,\gamma}}\|$. We suppose that for some $(\alpha, \gamma) \in [0, \infty) \times [0, 2/3)$, $\psi \notin \mathcal{D}(\vartheta_{\alpha,\gamma})$ and derive a contradiction. Of course, $\psi_{F_{s,\alpha,\gamma}} \in \mathcal{H}$ for all $s > 0$, but by the Monotone Convergence Theorem, $\|\psi_{F_{s,\alpha,\gamma}}\| \to +\infty$ as $s \downarrow 0$. Thus, for any bounded set $B \subset \mathbb{Z}^d$,

$$\lim_{s \downarrow 0} \sum_{n \in B} |\Psi_s(n)|^2 = 0. \tag{3.17}$$

In particular, Ψ_s converges weakly to zero. As α and γ are fixed, we shall write F_s instead of $F_{s,\alpha,\gamma}$ for simplicity. Introduce the operator $H_{F_s} := e^{F_s} H e^{-F_s}$. Then H_{F_s} is a bounded operator and $H_{F_s} \Psi_s = E \Psi_s$. We claim that

$$\lim_{s \downarrow 0} \|(H - E) \Psi_s\| = 0. \tag{3.18}$$

To see this, write H_{F_s} as follows:

$$H_{F_s} = H + \sum_{1 \leqslant i \leqslant d} S_i (1 - e^{\tau_i^* F_s - F_s}) + S_i^* (1 - e^{\tau_i F_s - F_s}).$$

To show (3.18), it is therefore enough to show that

$$\lim_{s \downarrow 0} \|(1 - e^{\tau_i^* F_s - F_s}) \Psi_s\| = \lim_{s \downarrow 0} \|(1 - e^{\tau_i F_s - F_s}) \Psi_s\| = 0. \tag{3.19}$$

Let $B(N) = \{n \in \mathbb{Z}^d : \langle n \rangle \leqslant N\}$, and $B(N)^c$ the complement set. For all $\epsilon > 0$, there is $N > 0$ such that

$$\sup_{\substack{n \in B(N)^c \\ s>0}} \left| 1 - e^{(\tau_i^* F_s - F_s)(n)} \right| = \sup_{\substack{n \in B(N)^c \\ s>0}} \left| 1 - e^{\alpha\gamma \langle n' \rangle^{\gamma-1} \Upsilon_s'(\alpha \langle n' \rangle^\gamma)} \right| \leqslant \epsilon$$

(here $n' = (n_1', ..., n_d')$ with $n_i' \in (n_i, n_i + 1)$ and $n_j' = n_j$ for $j \neq i$). Combining this with (3.17) proves the first limit in (3.19), and the second one is shown in the same way. Thus the claim is proven. Because $E \in \Theta(H)$, there exists an interval $\Sigma := (E - \delta, E + \delta)$ with $\delta > 0$, $\eta > 0$ and a compact K such that

$$E_\Sigma(H)[H, A']_\circ E_\Sigma(H) \geqslant \eta E_\Sigma(H) + K. \tag{3.20}$$

By functional calculus,

$$\lim_{s \downarrow 0} \|E_{\mathbb{R}\setminus\Sigma}(H)\Psi_s\| \leqslant \lim_{s\downarrow 0} \delta^{-1} \|E_{\mathbb{R}\setminus\Sigma}(H)(H - E)\Psi_s\| = 0. \tag{3.21}$$

It follows by the Mourre estimate (3.20) and (3.21) that

$$\liminf_{s\downarrow 0} \langle \Psi_s, E_\Sigma(H)[H, A']_\circ E_\Sigma(H)\Psi_s \rangle \geqslant \eta \liminf_{s\downarrow 0} \|E_\Sigma(H)\Psi_s\|^2 = \eta > 0. \tag{3.22}$$

We now look to contradict this equation. We start with

$$\langle \Psi_s, E_\Sigma(H)[H, A']_\circ E_\Sigma(H)\Psi_s \rangle = \langle \Psi_s, [H, A']_\circ \Psi_s \rangle - f_1(s) - f_2(s), \quad \text{where} \tag{3.23}$$

$$f_1(s) = \langle \Psi_s, E_{\mathbb{R}\setminus\Sigma}(H)[H, A']_\circ E_\Sigma(H)\Psi_s \rangle \quad \text{and} \quad f_2(s) = \langle \Psi_s, [H, A']_\circ E_{\mathbb{R}\setminus\Sigma}(H)\Psi_s \rangle.$$

Applying (3.21) gives

$$\lim_{s\downarrow 0} |f_1(s)| = \lim_{s\downarrow 0} |f_2(s)| = 0.$$

Now apply (3.11) with $F = F_{s,\alpha,\gamma}$, and after dividing this equation by $\|\Psi_s\|^2$, we have

$$\limsup_{s\downarrow 0} \langle \Psi_s, [H, A']_\circ \Psi_s \rangle \leqslant 0.$$

Here we took advantage of the negativity of the first two terms on the right side of (3.11), and used the uniform decay of $\mathcal{L} + \mathcal{M} + \mathcal{G}$ together with the weak convergence of Ψ_s to get $\langle \Psi_s, (\mathcal{L} + \mathcal{M} + \mathcal{G})\Psi_s \rangle \to 0$ as $s \downarrow 0$. To check this thoroughly, one needs to apply the estimates of Lemma 3.2 to where indicated in the Appendix by a (‡). Note that $\mathcal{L}$ given by (6.9) is the most constraining term; it has the necessary decay provided $3\gamma - 4 < -2$, i.e. $\gamma < 2/3$. Note also that $\ddagger_5$ allows to conclude, by continuity of the map $x \mapsto \sqrt{\cosh(x) - 1}$, that $\langle \Psi_s, (W_{F_s;i} - \tau_i W_{F_s;i})\Psi_s \rangle$ and like terms converge to zero. Thus by (3.23),

$$\limsup_{s\downarrow 0} \langle \Psi_s, E_\Sigma(H)[H, A']_\circ E_\Sigma(H)\Psi_s \rangle \leqslant 0.$$

This is in contradiction with (3.22), so the proof is complete. □

4. Proof of Proposition 1.6

As an application of Theorem 1.5, we display a Wigner-von Neumann type operator that has an eigenvalue embedded in the essential spectrum. The eigenvalue is proven to be a threshold.

Proof of Proposition 1.6. First, we construct the potential in dimension one. Second, we generalize this potential to higher dimensions. Third, we show that the eigenvalue is also a threshold and belongs to the essential spectrum.

Part 1. We follow [RS4, Section XIII.13, Example 1]. Starting with the eigenvalue equation

$$2\psi(n) - \psi(n+1) - \psi(n-1) + V(n)\psi(n) = E\psi(n),$$

we shift terms to write

$$V(n) = (E-2) + \frac{\psi(n+1)}{\psi(n)} + \frac{\psi(n-1)}{\psi(n)}.$$

We try the Ansatz $\psi(n) := \sin(kn)w_k(n)$, $k \in (0,\pi)$. For simplicity, write $w(n)$ instead of $w_k(n)$. We get

$$\begin{aligned}
V(n) &= (E-2)\\
&\quad + \frac{\sin(kn)\cos(k)+\cos(kn)\sin(k)}{\sin(kn)}\frac{w(n+1)}{w(n)} + \frac{\sin(kn)\cos(k)-\cos(kn)\sin(k)}{\sin(kn)}\frac{w(n-1)}{w(n)}\\
&= (E-2) + \cos(k)\left(\frac{w(n+1)}{w(n)} + \frac{w(n-1)}{w(n)}\right) + \sin(k)\frac{\cos(kn)}{\sin(kn)}\left(\frac{w(n+1)}{w(n)} - \frac{w(n-1)}{w(n)}\right).
\end{aligned}$$

For the moment, let us assume that

$$\frac{w(n+1)}{w(n)} \to 1, \quad \text{as } |n| \to +\infty \tag{4.1}$$

and

$$\sin(k)\frac{\cos(kn)}{\sin(kn)}\left(\frac{w(n+1)}{w(n)} - \frac{w(n-1)}{w(n)}\right) \to 0, \quad \text{as } |n| \to +\infty. \tag{4.2}$$

Thus if we want $V(n) \to 0$, we must have $(E-2)+2\cos(k) = 0$, i.e. $E = 2-2\cos(k)$. We now seek a suitable w_k. Let

$$g_k(n) = g(n) := \sin(2k)n - \sin(2kn).$$

For simplicity, we would like to define $w_k(n) := 1/g_k(n)$. But then $w_k(-1)$, $w_k(0)$ and $w_k(1)$ are not well-defined, nor is w_k for that matter if $k = \pi/2$. To circumvent this problem, we could define $w_k(n) := (1+(g_k(n))^2)^{-1}$ instead, as it is done in [RS4, Section XIII.13, Example 1], but alternatively we note that there is $t = t_k \in (0,+\infty)$ such that $t_k + g_k(n) = 0$ has no solutions for $n \in \mathbb{Z}$. So we let

$$w_k(n) := \frac{1}{t_k + g_k(n)}.$$

In any case, with either choice we certainly have $\psi \in \ell^2(\mathbb{Z})$ and (4.1) is clearly satisfied. As for (4.2), we calculate

$$\begin{aligned}
\sin(k)\frac{\cos(kn)}{\sin(kn)}\left(\frac{w(n+1)}{w(n)} - \frac{w(n-1)}{w(n)}\right) &= \sin(k)\frac{\cos(kn)}{\sin(kn)}\frac{g(n-1)-g(n+1)}{[t+g(n-1)][t+g(n+1)]}[t+g(n)]\\
&= \frac{-2\sin(k)\sin(2k)\sin(2kn)}{[t+g(n-1)][t+g(n+1)]}[t+g(n)]\\
&= \frac{-2\sin(k)\sin(2kn)}{n} + O(n^{-2}).
\end{aligned}$$

So (4.2) also holds. Note that this calculation follows from these useful relations:

$$g(n+1)-g(n) = \sin(2k) - 2\sin(k)\cos(2kn+k),$$

$$\frac{1}{[t+g(n+1)]} = \frac{1}{\sin(2k)n} + O(n^{-2}), \quad \text{and} \quad \frac{1}{[t+g(n-1)]} = \frac{1}{\sin(2k)n} + O(n^{-2}).$$

Letting $E = 2 - 2\cos(k)$, we then find that V is given by

$$\begin{aligned}V(n) &= \cos(k)\left(\frac{2t + g(n-1) + g(n+1)}{[t+g(n-1)][t+g(n+1)]}[t+g(n)] - 2\right) - \frac{2\sin(k)\sin(2k)\sin(2kn)[t+g(n)]}{[t+g(n-1)][t+g(n+1)]}\\ &= \cos(k)\left(\frac{g(n)-g(n-1)}{[t+g(n-1)]} - \frac{g(n+1)-g(n)}{[t+g(n+1)]}\right) - \frac{2\sin(k)\sin(2k)\sin(2kn)[t+g(n)]}{[t+g(n-1)][t+g(n+1)]}.\end{aligned}$$

By a calculation done above, we know the asymptotic behavior of the second term of this expression. Another calculation shows that the first term of this expression has the exact same asymptotic behavior as the second. Thus, we have found a potential having the property that $2 - 2\cos(k)$ is an eigenvalue of $\Delta + V$ with eigenvector given by $\psi(n) = \sin(kn)[t_k + \sin(2k)n - \sin(2kn)]^{-1}$. Moreover the potential has the asymptotic behavior

$$V(n) = -\frac{4\sin(k)\sin(2kn)}{n} + O_{k,t_k}(n^{-2}).$$

Part 2. We simply extend to two dimensions. The Schrödinger equation is rewritten as follows:

$$V(n,m) = (E-4) + \frac{\psi(n+1,m)}{\psi(n,m)} + \frac{\psi(n-1,m)}{\psi(n,m)} + \frac{\psi(n,m+1)}{\psi(n,m)} + \frac{\psi(n,m-1)}{\psi(n,m)}.$$

Try the Ansatz $\psi(n,m) = \sin(k_1 n)w_{k_1}(n)\sin(k_2 m)w_{k_2}(m)$, for some $k_1, k_2 \in (0,\pi)$. For simplicity, write $w_1(n)$ instead of $w_{k_1}(n)$, and $w_2(m)$ instead of $w_{k_2}(m)$. We get

$$\begin{aligned}V(n,m) = (E-4)&\\ &+ \cos(k_1)\left(\frac{w_1(n+1)+w_1(n-1)}{w_1(n)}\right) + \sin(k_1)\frac{\cos(k_1 n)}{\sin(k_1 n)}\left(\frac{w_1(n+1)-w_1(n-1)}{w_1(n)}\right)\\ &+ \cos(k_2)\left(\frac{w_2(m+1)+w_2(m-1)}{w_2(m)}\right) + \sin(k_2)\frac{\cos(k_2 m)}{\sin(k_2 m)}\left(\frac{w_2(m+1)-w_2(m-1)}{w_2(m)}\right).\end{aligned}$$

Let $E := 4 - 2\cos(k_1) - 2\cos(k_2)$, and

$$w_1(n) := (t_1 + g_1(n))^{-1}, \quad \text{where } g_1(n) := \sin(2k_1)n - \sin(2k_1 n),$$

$$w_2(m) := (t_2 + g_2(m))^{-1}, \quad \text{where } g_2(m) := \sin(2k_2)m - \sin(2k_2 m).$$

Here $t_1 = t_{k_1}$ and $t_2 = t_{k_2}$ are real numbers chosen so that $t_1 + g_1(n) \neq 0$ and $t_2 + g_2(m) \neq 0$ for all $n, m \in \mathbb{Z}$. The calculations of the first part show that V is given by

$$\begin{aligned}&V(n,m) =\\ &\cos(k_1)\left[\frac{g_1(n)-g_1(n-1)}{t_1+g_1(n-1)} - \frac{g_1(n+1)-g_1(n)}{t_1+g_1(n+1)}\right] - \frac{2\sin(k_1)\sin(2k_1)\sin(2k_1 n)[t_1+g_1(n)]}{[t_1+g_1(n-1)][t_1+g_1(n+1)]}\\ &+\cos(k_2)\left[\frac{g_2(m)-g_2(m-1)}{t_2+g_2(m-1)} - \frac{g_2(m+1)-g_2(m)}{t_2+g_2(m+1)}\right] - \frac{2\sin(k_2)\sin(2k_2)\sin(2k_2 m)[t_2+g_2(m)]}{[t_2+g_2(m-1)][t_2+g_2(m+1)]}.\end{aligned}$$

This potential has the property that $4 - 2\cos(k_1) - 2\cos(k_2)$ is an eigenvalue of $\Delta + V$ with eigenvector

$$\psi(n,m) = \sin(k_1 n)\sin(k_2 m)[t_{k_1} + \sin(2k_1)n - \sin(2k_1 n)]^{-1}[t_{k_2} + \sin(2k_2)m - \sin(2k_2 m)]^{-1}.$$

Moreover V has the asymptotic behavior

$$V(n,m) = -\frac{4\sin(k_1)\sin(2k_1 n)}{n} - \frac{4\sin(k_2)\sin(2k_2 m)}{m} + O_{k_1,t_{k_1}}(n^{-2}) + O_{k_2,t_{k_2}}(m^{-2}).$$

Part 3. We still have to prove that the eigenvalue $E := 4 - 2\cos(k_1) - 2\cos(k_2)$ is a threshold of $H = \Delta + V$. But V satisfies Hypothesis 1, and the eigenvector ψ has slow decay at infinity. So we conclude by Theorem 1.5 that this eigenvalue is unmistakably a threshold. If $H_1(k)$ denotes the one-dimensional Schrödinger operator of Part 1 and H denotes the two-dimensional operator of Part 2, then we have $H = H_1(k_1) \otimes \mathbf{1} + \mathbf{1} \otimes H_1(k_2)$. A basic result on the spectra of tensor products gives

$$\sigma(H) = \overline{\sigma(H_1(k_1)) + \sigma(H_1(k_2))} \supset [0, 8].$$

Thus $E \in [0,8] \subset \sigma_{\mathrm{ess}}(H)$. □

5. The one-dimensional case: exponential decay of eigenfunctions

In this section we deal with the one-dimensional Schrödinger operator H on $\mathcal{H} = \ell^2(\mathbb{Z})$. We follow the same definitions as in the Introduction and Section 3, but since $i = 1$, we will drop this subscript. We shall write S and S^* instead of S_i and S_i^*, N instead of N_i, etc...Consider an increasing function $F \in C^2([0,\infty))$ with bounded derivative away from the origin. This function induces a radial operator on $\mathcal{H}$ as in Section 3: $(Fu)(n) := F(\langle n \rangle)u(n)$ for all $u \in \mathcal{H}$.

Proposition 5.1. *Suppose that Hypothesis 1 holds for the potential V. Let F be as above, and suppose additionally that*

$$|xF''(x)| \leqslant C, \quad \text{for } x \text{ away from the origin.} \tag{5.1}$$

Suppose that $H\psi = E\psi$, with $\psi \in \mathcal{H}$. Let $\psi_F := e^F \psi$, and assume that $\psi_F \in \mathcal{H}$. Then $\psi_F \in \mathcal{D}(\sqrt{g_r - g_\ell}A')$ and there exist bounded operators W, M and G depending on F such that

$$\langle \psi_F, [H, A']\psi_F \rangle = -\left\|\sqrt{g_r - g_\ell}A'\psi_F\right\|^2 - \left\|\sqrt{\Delta(4-\Delta)}W\psi_F\right\|^2 + 2^{-1}\langle \psi_F, (M+G)\psi_F \rangle. \tag{5.2}$$

The exact expressions of W, M and G are given by (6.13), (6.14) and (6.15) respectively.

Proof. The proof is done in two steps. The first step consists in proving that

$$\begin{aligned}\langle \phi, [e^F A' e^F, \Delta]\phi \rangle = \langle \phi_F, [A', \Delta]\phi_F \rangle - \|\sqrt{g_r - g_\ell}A'\phi_F\|^2 \\ - \|\sqrt{\Delta(4-\Delta)}W\phi_F\|^2 + 2^{-1}\langle \phi_F, (M+G)\phi_F \rangle.\end{aligned} \tag{5.3}$$

The proof of this is in the Appendix starting from (6.12). That F' is bounded away from the origin ensures that W and $(g_r - g_\ell)$ are bounded. The additional assumption (5.1) ensures that $(\tau^*\varphi_r - \varphi_r)N$ and like terms are bounded. The second step is the same as that of Proposition 3.1, and the proof is identical. □

Lemma 5.2. *Suppose that $H\psi = E\psi$ with $\psi \in \ell^2(\mathbb{Z})$. Let F be a general function as above, and assume that $\psi_F := e^F\psi \in \ell^2(\mathbb{Z})$. Define the operator*

$$H_F := e^F H e^{-F}. \tag{5.4}$$

Then H_F is bounded, $H_F\psi_F = E\psi_F$ and there exist bounded operators C_F and R_F such that

$$H_F = C_F H + (2 - 2C_F) + 2^{-1}R_F, \quad \text{where} \tag{5.5}$$

$$C_F := 2^{-1}\left(e^{F - \tau F} + e^{F - \tau^* F}\right) \quad \text{and} \tag{5.6}$$

$$\begin{aligned}R_F := V(2 - 2C_F) + (\tau\varphi_r - \varphi_r)(S^* - S) + (\varphi_\ell - \tau^*\varphi_\ell)(S^* - S) \\ + (g_r - g_\ell)A' - 2^{-1}(g_r - g_\ell)(S^* + S).\end{aligned} \tag{5.7}$$

Proof. Because F' is bounded away from the origin, both $e^F S e^{-F}\phi = S e^{\tau^* F - F}\phi$ and $e^F S^* e^{-F}\phi = S^* e^{\tau F - F}\phi$ belong to $\ell^2(\mathbb{Z})$ whenever $\phi \in \ell^2(\mathbb{Z})$. Thus H_F is bounded, and $H_F \psi_F = E\psi_F$ follows immediately. Now

$$H_F = 2 + V - e^{F-\tau F} S - e^{F-\tau^* F} S^*.$$

Rewriting this relation in two different ways, we have

$$H_F = e^{F-\tau F} H + (2+V)(1 - e^{F-\tau F}) + (e^{F-\tau F} - e^{F-\tau^* F})S^*,$$
$$H_F = e^{F-\tau^* F} H + (2+V)(1 - e^{F-\tau^* F}) + (e^{F-\tau^* F} - e^{F-\tau F})S.$$

Adding these two relations gives

$$2H_F = 2C_F H + (2+V)(2 - 2C_F) + (e^{F-\tau F} - e^{F-\tau^* F})(S^* - S). \tag{5.8}$$

We further develop the third term on the right side:

$$\begin{aligned}(e^{F-\tau F} - e^{F-\tau^* F})(S^* - S) &= (\tau\varphi_r - \tau^*\varphi_\ell)(S^* - S) \\ &= (\tau\varphi_r - \varphi_r)(S^* - S) + (\varphi_\ell - \tau^*\varphi_\ell)(S^* - S) + (\varphi_r - \varphi_\ell)(S^* - S) \\ &= (\tau\varphi_r - \varphi_r)(S^* - S) + (\varphi_\ell - \tau^*\varphi_\ell)(S^* - S) \\ &\quad + (g_r - g_\ell)A' - 2^{-1}(g_r - g_\ell)(S^* + S) + (\varphi_r - \varphi_\ell)\mathbf{1}_{\{n=0\}}(S^* - S).\end{aligned}$$

Here, $\mathbf{1}_B$ is the projector onto $B \subset \mathbb{Z}$. Note that $(\varphi_r - \varphi_\ell)\mathbf{1}_{\{n=0\}} = 0$, and thus (5.5) is shown. □

We are now ready to prove the main result concerning the one-dimensional operator H:

Proof of Theorem 1.2, the first part. We first handle the case $E \neq 2$. Suppose that the statement of the theorem is false. Then $\theta_E = \theta_E(\alpha_0) = (E-2)/\cosh(\alpha_0) + 2 \in \Theta(H) \setminus \{+2\}$ for some $\alpha_0 \in [0, \infty)$, and there is an interval

$$\Sigma_0 := (\theta_E(\alpha_0) - 2\delta, \theta_E(\alpha_0) + 2\delta) \tag{5.9}$$

such that the Mourre estimate holds there, i.e.

$$E_{\Sigma_0}(H)[H, A']_\circ E_{\Sigma_0}(H) \geqslant \eta E_{\Sigma_0}(H) + K \tag{5.10}$$

for some $\eta > 0$ and some compact operator K. For the remainder of the proof, δ, η and K are fixed. If $\alpha_0 > 0$, choose $\alpha_1 > 0$ and $\gamma > 0$ such that

$$\alpha_1 < \alpha_0 < \alpha_1 + \gamma. \tag{5.11}$$

If however $\alpha_0 = 0$, let $\alpha_1 = 0$ and $\gamma > 0$. By continuity of the map $\theta_E(\alpha) = (E-2)/\cosh(\alpha) + 2$, $\theta_E(\alpha_1) \to \theta_E(\alpha_0)$ as $\alpha_1 \to \alpha_0$, so taking α_1 close enough to α_0 we obtain intervals

$$\Sigma_1 := (\theta_E(\alpha_1) - \delta, \theta_E(\alpha_1) + \delta) \subset \Sigma_0$$

with the inclusion remaining valid as $\alpha_1 \to \alpha_0$. Multiplying to the right and left of (5.10) by $E_{\Sigma_1}(H)$, we obtain

$$E_{\Sigma_1}(H)[H, A']_\circ E_{\Sigma_1}(H) \geqslant \eta E_{\Sigma_1}(H) + E_{\Sigma_1}(H) K E_{\Sigma_1}(H). \tag{5.12}$$

Later in the proof α_1 will be taken even closer to α_0 allowing γ to be as small as necessary in order to lead to a contradiction (in this limiting process, δ, η and K are fixed). Before delving into the details of the proof, we expose the strategy. For a suitable sequence of functions $\{F_s(x)\}_{s>0}$, let

$$\Psi_s := e^{F_s}\psi / \|e^{F_s}\psi\|. \tag{5.13}$$

With F_s and Ψ_s instead of F and ψ_F respectively, we apply Proposition 5.1 to conclude that

$$\limsup_{s\downarrow 0} \langle \Psi_s, [H, A']_\circ \Psi_s\rangle \leqslant \limsup_{s\downarrow 0} |\langle \Psi_s, 2^{-1}\big(M_{F_s} + G_{F_s}\big)\Psi_s\rangle|. \tag{5.14}$$

Notice how the the negativity of the first two terms on the right side of (5.2) was crucial. We have also written M_{F_s} and G_{F_s} instead of M and G to show the dependence on F_s. The first part of the proof consists in showing that

$$\limsup_{s\downarrow 0} \langle \Psi_s, [H, A']_\circ \Psi_s\rangle \leqslant \limsup_{s\downarrow 0} |\langle \Psi_s, 2^{-1}\big(M_{F_s} + G_{F_s}\big)\Psi_s\rangle| \leqslant c\epsilon_\gamma \tag{5.15}$$

for some $\epsilon_\gamma > 0$ satisfying $\epsilon_\gamma \to 0$ when $\gamma \to 0$. Here and thereafter, $c > 0$ denotes a constant independent of s, α_1 and γ. The second part of the proof consists in showing that

$$\limsup_{s\downarrow 0} \|(H - \theta_E(\alpha_1))\Psi_s\| \leqslant c\epsilon_\gamma. \tag{5.16}$$

Roughly speaking (5.16) says that Ψ_s has energy concentrated about $\theta_E(\alpha_1)$ and so localizing (5.15) about this energy will lead to

$$\limsup_{s\downarrow 0} \langle \Psi_s, E_{\Sigma_1}(H)[H, A']_\circ E_{\Sigma_1}(H)\Psi_s\rangle \leqslant c\epsilon_\gamma. \tag{5.17}$$

However, the Mourre estimate (5.12) holds on Σ_1. In the end, the contradiction will come from the fact that the Mourre estimate asserts that the left side of (5.17) is not that small.

We now begin in earnest the proof. Notice that $\psi \in \mathcal{D}(\vartheta_{\alpha_1})$ but $\psi \notin \mathcal{D}(\vartheta_{\alpha_1+\gamma})$. Let Υ_s be the interpolating function defined in (3.4), and for $s > 0$ let

$$F_s(x) := \alpha_1 x + \gamma\Upsilon_s(x). \tag{5.18}$$

As explained in the multi-dimensional case, F_s induces a radial potential as follows : $(F_s u)(n) := F_s(\langle n\rangle)u(n)$, for all $u \in \ell^2(\mathbb{Z})$. By (3.5), $e^{F_s}\psi \in \ell^2(\mathbb{Z})$ for all $s > 0$, but $\|e^{F_s}\psi\| \to \infty$ as $s \downarrow 0$. To ease the notation, we will be bounding various quantities by the same constant $c > 0$, a constant that is independent of α_1, γ, s and of position x (or n).

Part 1. We use Proposition 5.1 with F_s replacing F, and so we verify that F_s satisfies the hypotheses of that proposition. Since

$$F_s'(x) = \alpha_1 + \gamma\Upsilon_s'(x) \quad \text{and} \quad F_s''(x) = \gamma\Upsilon_s''(x),$$

indeed $|F_s'(x)| \leqslant c$, $|xF_s''(x)| \leqslant c$. Dividing (5.2) by $\|e^{F_s}\psi\|^2$ throughout we obtain (5.14) as claimed. To prove (5.15), we need two ingredients. First, for any bounded set $B \subset \mathbb{Z}$,

$$\lim_{s\downarrow 0} \sum_{n\in B} |\Psi_s(n)|^2 = 0. \tag{5.19}$$

In particular, Ψ_s converges weakly to zero. What's more, we also have for any $k \in \mathbb{N}$

$$\lim_{s\downarrow 0} \sum_{n\in B} |(S^k\Psi_s)(n)|^2 = 0, \quad \text{and} \quad \lim_{s\downarrow 0} \sum_{n\in B} |((S^*)^k\Psi_s)(n)|^2 = 0. \tag{5.20}$$

Now M_{F_s} and G_{F_s} are a finite sum of terms of the form $P_1(S, S^*)TP_2(S, S^*)$, where P_1 and P_2 are polynomials and the $T = T(n)$ are sequences. The second item to show is that,

$$|T(n)| \leqslant c(\langle n\rangle^{-1} + \epsilon_\gamma). \tag{5.21}$$

In other words we want smallness coming from decay in position n or from γ. Outside a sufficiently large bounded set, decay in position can be converted into smallness in γ by using (5.19) while $P_1(S, S^*)$ and $P_2(S, S^*)$ get absorbed in the process thanks to (5.20). Consider first $M = M_{F_s}$ given by (6.14). Applying the Mean Value Theorem (MVT) gives the uniform estimates in s

$$|\tau F_s - F_s| \quad \text{and} \quad |\tau^* F_s - F_s| \in O(1). \tag{5.22}$$

It follows that

$$|\varphi_\ell| \quad \text{and} \quad |\varphi_r| \in O(1), \quad \text{and} \quad |g_r - g_\ell| \in O(\langle n \rangle^{-1}).$$

To handle the term $(\tau^* \varphi_\ell - \varphi_\ell)$, define the function $f(x) := e^{F_s(\langle x-1 \rangle) - F_s(\langle x \rangle)}$. Then $(\tau^* \varphi_\ell - \varphi_\ell)(n) = f(n+1) - f(n)$. Applying twice the MVT gives

$$|(\tau^* \varphi_\ell - \varphi_\ell)(n)| \leqslant c(\langle n \rangle^{-3} + \gamma \langle n \rangle^{-1}).$$

The same estimate holds for the similar terms like $(\varphi_r - \tau\varphi_r)$, $(\tau^* \varphi_r - \varphi_r)$ and so forth. We turn our attention to $G = G_{F_s}$ given by (6.15). By (5.22), $|W_{F_s}| \in O(1)$. To estimate $(W_{F_s} - W_{\tau^* F_s})$, let $g(x) := \sqrt{\cosh(F_s(\langle x-1 \rangle) - F_s(\langle x \rangle)) - 1}$, so that $(W_{F_s} - W_{\tau^* F_s})(n) = g(n) - g(n+1)$. Moreover,

$$g'(x) = \frac{(F_s'(\langle x-1 \rangle) - F_s'(\langle x \rangle)) \sinh(F_s(\langle x-1 \rangle) - F_s(\langle x \rangle))}{2\sqrt{\cosh(F_s(\langle x-1 \rangle) - F_s(\langle x \rangle)) - 1}}.$$

If $\alpha_1 > 0$, then $|F_s(\langle x-1 \rangle) - F_s(\langle x \rangle)| \geqslant c' \alpha_1$ for some constant $c' > 0$ independent of x and s, and so $\cosh(F_s(\langle x-1 \rangle) - F_s(\langle x \rangle)) - 1$ is uniformly bounded from below by a positive number. Applying the MVT to $(F_s'(\langle x-1 \rangle) - F_x'(\langle x \rangle))$ yields the estimate

$$|(W_{F_s} - W_{\tau^* F_s})(n)| \leqslant c(\langle n \rangle^{-3} + \gamma \langle n \rangle^{-1}).$$

If however $\alpha_1 = 0$, then

$$|(\tau F_s - F_s)(n) - (F_s - \tau^* F_s)(n)| \leqslant c\gamma \langle n \rangle^{-1}. \tag{5.23}$$

By continuity of the function $x \mapsto \sqrt{\cosh(x) - 1}$ we have that for any $\epsilon_\gamma > 0$,

$$|W_{F_s} - W_{\tau^* F_s}| = |\sqrt{\cosh(\tau F_s - F_s) - 1} - \sqrt{\cosh(F_s - \tau^* F_s) - 1}| \leqslant \epsilon_\gamma$$

whenever (5.23) holds. A similar argument works for $(W_{F_s} - W_{\tau F_s})$. Thus (5.21) is proven, and this shows (5.15) when combined with the fact that Ψ_s converges weakly to zero.

Part 2. We now prove (5.16). Consider Lemma 5.2 with F_s instead of F. We claim that

$$\lim_{s \downarrow 0} \left\| (C_{F_s} H + 2 - E - 2C_{F_s}) \Psi_s \right\| = 0. \tag{5.24}$$

By (5.5) of Lemma 5.2, this is equivalent to showing that

$$\lim_{s \downarrow 0} \left\| R_{F_s} \Psi_s \right\| = 0.$$

Dividing each term in (5.2) by $\|e^{F_s} \psi\|^2$, we see that $\|\sqrt{g_r - g_\ell} A' \Psi_s\| \leqslant c$. Let χ_N denote the characteristic function of the set $\{n \in \mathbb{Z} : (g_r - g_\ell) < N^{-1}\}$. Then

$$\limsup_{s \downarrow 0} \|(g_r - g_\ell) A' \Psi_s\| \leqslant \limsup_{s \downarrow 0} N^{-\frac{1}{2}} \|\chi_N \sqrt{g_r - g_\ell} A' \Psi_s\| + \|(1 - \chi_N)(g_r - g_\ell) A' \Psi_s\| \leqslant c N^{-\frac{1}{2}}.$$

Here we used the fact that $1 - \chi_N$ has support in a fixed, bounded set as $s \downarrow 0$. Since N is arbitrary, this shows that $\|(g_r - g_\ell) A' \Psi_s\| \to 0$ as $s \downarrow 0$. The other terms of R_{F_s} are handled similarly. Note that for the term containing V we use the fact it goes to zero at infinity, and from Part 1, $(\tau\varphi_r - \varphi_r)$, $(\varphi_\ell - \tau^* \varphi_\ell)$ and $(g_r - g_\ell)$ also go to zero at infinity. Hence (5.24) is proved. Let $\kappa := \kappa(n) = \text{sign}(n)$. From the expression of F_s', we have the estimates :

$$|(F_s - \tau F_s)(n) - \kappa(n)\alpha_1| \leqslant c(\alpha_1 \langle n \rangle^{-1} + \gamma) \quad \text{and} \quad |(F_s - \tau^* F_s)(n) - (-\kappa(n)\alpha_1)| \leqslant c(\alpha_1 \langle n \rangle^{-1} + \gamma).$$

Therefore, outside a fixed bounded set we have

$$|(F_s - \tau F_s) - \kappa\alpha_1| \leqslant c\gamma \quad \text{and} \quad |(F_s - \tau^* F_s) - (-\kappa\alpha_1)| \leqslant c\gamma. \tag{5.25}$$

By continuity of the exponential function, we have for any $\epsilon_\gamma > 0$ that

$$|e^{F_s - \tau F_s} - e^{\kappa\alpha_1}| \leqslant \epsilon_\gamma \quad \text{and} \quad |e^{F_s - \tau^* F_s} - e^{-\kappa\alpha_1}| \leqslant \epsilon_\gamma$$

whenever the respective terms of (5.25) hold. It follows from (5.24) that

$$\limsup_{s\downarrow 0} \left\| \left[2^{-1}\left(e^{\alpha_1} + e^{-\alpha_1}\right) H + 2 - E - \left(e^{\alpha_1} + e^{-\alpha_1}\right)\right]\Psi_s \right\| \leqslant c\epsilon_\gamma.$$

Dividing this expression by $\cosh(\alpha_1)$ proves (5.16).

Part 3. By functional calculus and (5.16), we have

$$\limsup_{s\downarrow 0} \|E_{\mathbb{R}\setminus\Sigma_1}(H)\Psi_s\| \leqslant \limsup_{s\downarrow 0} \delta^{-1} \left\|E_{\mathbb{R}\setminus\Sigma_1}(H)\big(H - \theta_E(\alpha_1)\big)\Psi_s\right\| \leqslant c\epsilon_\gamma. \tag{5.26}$$

We have

$$\langle \Psi_s, E_{\Sigma_1}(H)[H, A']_\circ E_{\Sigma_1}(H)\Psi_s\rangle = \langle \Psi_s, [H, A']_\circ \Psi_s\rangle - f_1(s) - f_2(s), \quad \text{where} \tag{5.27}$$

$$f_1(s) = \langle \Psi_s, E_{\mathbb{R}\setminus\Sigma_1}(H)[H, A']_\circ E_{\Sigma_1}(H)\Psi_s\rangle, \quad \text{and} \quad f_2(s) = \langle \Psi_s, [H, A']_\circ E_{\mathbb{R}\setminus\Sigma_1}(H)\Psi_s\rangle.$$

By (5.26),

$$\max_{i=1,2} \limsup_{s\downarrow 0} |f_i(s)| \leqslant c\epsilon_\gamma.$$

This together with (5.15) and (5.27) implies

$$\limsup_{s\downarrow 0} \ \langle \Psi_s, E_{\Sigma_1}(H)[H, A']_\circ E_{\Sigma_1}(H)\Psi_s\rangle \leqslant c\epsilon_\gamma. \tag{5.28}$$

On the other hand, by the Mourre estimate (5.12), we have that

$$\langle \Psi_s, E_{\Sigma_1}(H)[H, A']_\circ E_{\Sigma_1}(H)\Psi_s\rangle \geqslant \eta\|E_{\Sigma_1}(H)\Psi_s\|^2 + \langle \Psi_s, E_{\Sigma_1}(H) K E_{\Sigma_1}(H)\Psi_s\rangle. \tag{5.29}$$

Thus, since Ψ_s converges weakly to zero and $E_{\Sigma_1}(H)KE_{\Sigma_1}(H)$ is compact, we have, using (5.26)

$$\liminf_{s\downarrow 0} \ \langle \Psi_s, E_{\Sigma_1}(H)[H, A']_\circ E_{\Sigma_1}(H)\Psi_s\rangle \geqslant \eta(1 - c\epsilon_\gamma^2). \tag{5.30}$$

Recall that $\epsilon_\gamma \to 0$ as $\gamma \to 0$. Taking first α_1 sufficiently close to α_0, we can then take γ small enough to see that (5.30) contradicts (5.28). The proof is complete for the case $E \neq 2$.

Part 4. Case $E = 2$: the proof is almost the same as before but a bit simpler. We briefly go over the proof to point out the small adjustments. Assuming the statement of the theorem to be false, we have that $2 \in \Theta(H)$, and also that $\psi \notin \mathcal{D}(\vartheta_\alpha)$ for some $\alpha \in (0, \infty)$. Since $\Theta(H)$ is open, there is an interval

$$\Sigma := (2 - \delta, 2 + \delta)$$

such that the Mourre estimate holds there, i.e.

$$E_\Sigma(H)[H, A']_\circ E_\Sigma(H) \geqslant \eta E_\Sigma(H) + K \tag{5.31}$$

for some $\eta > 0$ and some compact operator K. Let $\alpha_0 := \inf\{\alpha \geqslant 0 : \psi \notin \mathcal{D}(\vartheta_\alpha)\}$. As before, let α_1 and γ be such that $\alpha_1 < \alpha_0 < \alpha_1 + \gamma$ if $\alpha_0 > 0$; if $\alpha_0 = 0$, let $\alpha_1 = 0$. Let F_s and Ψ_s be defined as before (see (5.18) and (5.13)), so that Ψ_s has norm one but converges weakly to zero. The calculation of Part 1 shows that

$$\limsup_{s\downarrow 0} \ \langle \Psi_s, [H, A']_\circ \Psi_s\rangle \leqslant c\epsilon_\gamma,$$

whereas the calculation of Part 2 shows that

$$\lim_{s\downarrow 0} \|(H-2)\Psi_s\| \leqslant c\epsilon_\gamma.$$

The functional calculus then gives

$$\limsup_{s\downarrow 0} \|E_{\mathbb{R}\setminus\Sigma(H)}\Psi_s\| \leqslant \limsup_{s\downarrow 0} \delta^{-1}\|E_{\mathbb{R}\setminus\Sigma}(H)(H-2)\Psi_s\| \leqslant c\epsilon_\gamma.$$

As in Part 3, we get inequalities (5.28) and (5.30) with Σ instead of Σ_1. Taking α_1 very close to α_0 in order to take γ sufficiently small, these two inequalities disagree. The proof is complete. □

It remains to show however that

$$H\psi = E\psi, \quad \text{and} \quad \psi \in \mathcal{D}(\vartheta_\alpha) \quad \text{for all} \quad \alpha \geqslant 0 \quad \text{implies} \quad \psi = 0. \tag{5.32}$$

We slightly modify the notation we have been using so far. Let

$$F_\alpha(n) := \alpha|n| \quad \text{and} \quad \psi_\alpha(n) := e^{F_\alpha(n)}\psi(n) = e^{\alpha|n|}\psi(n), \quad \text{for all } n \in \mathbb{Z}. \tag{5.33}$$

Proof of Theorem 1.2, the second part. The proof is by contradiction, and the strategy is as follows: we assume that $\psi \neq 0$ and define $\Psi_\alpha := \psi_\alpha/\|\psi_\alpha\|$. It is not hard to see that Ψ_α converges weakly to zero as $\alpha \to +\infty$ (use the fact that the difference equation $H\psi = E\psi$ implies $\psi(n) \neq 0$ infinitely often). In the first part we apply Proposition 5.1 with F_α replacing F. In this case we can exactly compute terms to show that

$$\begin{aligned} 0 = \cosh(\alpha)^{-1}\langle \Psi_\alpha, [V, A']_\circ \Psi_\alpha\rangle + 2\tanh(\alpha)\|\sqrt{|N|}(S^*-S)\Psi_\alpha\|^2 \\ + \|\sqrt{\Delta(4-\Delta)}\Psi_\alpha\|^2 - \tanh(\alpha)\left(2\Psi_\alpha^2(0) + (\Psi_\alpha(-1)-\Psi_\alpha(1))^2\right). \end{aligned} \tag{5.34}$$

In the second part, we apply Lemma 5.2 again with F_α replacing F. We show that

$$\lim_{\alpha\to+\infty} \|\sqrt{\Delta(4-\Delta)}\Psi_\alpha\|^2 = \lim_{\alpha\to+\infty} \Re\,\langle \Psi_\alpha, \Delta(4-\Delta)\Psi_\alpha\rangle = 2. \tag{5.35}$$

The conclusion is then imminent: taking the limit $\alpha \to +\infty$ in (5.34), and recalling that $[V, A']_\circ$ exists as a bounded operator and Ψ_α converges weakly to zero leads to a contradiction.

Part 1. It follows from (6.2) and the limiting argument of Proposition 3.1 that

$$\langle \psi_\alpha, [H, A']_\circ \psi_\alpha\rangle = \langle \psi_\alpha, A'[e^F, \Delta]e^{-F}\psi_\alpha\rangle + \langle \psi_\alpha, e^{-F}[e^F, \Delta]A'\psi_\alpha\rangle.$$

All terms are computed exactly:

$$e^{(\tau F_\alpha - F_\alpha)(n)} = \begin{cases} e^{-\alpha} & \text{if } n \geqslant 1 \\ e^{\alpha} & \text{if } n \leqslant 0 \end{cases} \quad \text{and} \quad e^{(\tau^* F_\alpha - F_\alpha)(n)} = \begin{cases} e^{\alpha} & \text{if } n \geqslant 0 \\ e^{-\alpha} & \text{if } n \leqslant -1, \end{cases} \tag{5.36}$$

$$e^{(F_\alpha - \tau F_\alpha)(n)} = \begin{cases} e^{\alpha} & \text{if } n \geqslant 1 \\ e^{-\alpha} & \text{if } n \leqslant 0 \end{cases} \quad \text{and} \quad e^{(F_\alpha - \tau^* F_\alpha)(n)} = \begin{cases} e^{-\alpha} & \text{if } n \geqslant 0 \\ e^{\alpha} & \text{if } n \leqslant -1. \end{cases} \tag{5.37}$$

Let $\mathbf{1}_B$ be the projector onto $B \subset \mathbb{Z}$. Therefore

$$\begin{aligned} \varphi_r - \varphi_\ell &= 2\sinh(\alpha)\text{sign}(N)\mathbf{1}_{\{n\neq 0\}}, & \varphi_r + \varphi_\ell &= 2\left(\cosh(\alpha) - 1 + \sinh(\alpha)\mathbf{1}_{\{n=0\}}\right), \\ \tau^*\varphi_\ell - \varphi_\ell &= -2\sinh(\alpha)\mathbf{1}_{\{n=0\}}, & \varphi_\ell - \tau\varphi_\ell &= -2\sinh(\alpha)\mathbf{1}_{\{n=+1\}}, \\ \tau\varphi_r - \varphi_r &= -2\sinh(\alpha)\mathbf{1}_{\{n=0\}}, & \varphi_r - \tau^*\varphi_r &= -2\sinh(\alpha)\mathbf{1}_{\{n=-1\}}, \\ \tau^*\varphi_\ell - {\tau^*}^2\varphi_\ell &= 2\sinh(\alpha)\mathbf{1}_{\{n=-1\}}, & \tau\varphi_r - \tau^2\varphi_r &= 2\sinh(\alpha)\mathbf{1}_{\{n=+1\}}. \end{aligned}$$

Let $\mathcal{T} := A'[e^F, \Delta]e^{-F} + e^{-F}[e^F, \Delta]A'$. By (6.3) and (6.4), we have:

$$\begin{aligned}\mathcal{T} &= A'(-Se^F\varphi_r - S^*e^F\varphi_\ell)e^{-F} + e^{-F}(\varphi_r e^F S^* + \varphi_\ell e^F S)A' \\ &= -A'(S\varphi_r + S^*\varphi_\ell) + (\varphi_r S^* + \varphi_\ell S)A'.\end{aligned}$$

Plug in $A' = 2^{-1}(S^* + S) + N(S^* - S)$ and simplify to get $\mathcal{T} = \mathcal{T}_1 + \mathcal{T}_2$, where

$$\mathcal{T}_1 := 2^{-1}\left(-S^2\varphi_r + 3\varphi_r(S^*)^2 - (S^*)^2\varphi_\ell + 3\varphi_\ell S^2\right) - (\varphi_r + \varphi_\ell), \quad \text{and}$$

$$\mathcal{T}_2 := N\left(S^2\varphi_r + \varphi_r(S^*)^2 - (S^*)^2\varphi_\ell - \varphi_\ell S^2\right) - 2N(\varphi_r - \varphi_\ell).$$

We calculate $\mathcal{T}_1$:

$$\begin{aligned}\mathcal{T}_1 &= -2^{-1}(\varphi_r + \varphi_\ell)\left(2 - S^2 - (S^*)^2\right) - 2^{-1}\left(S^2\varphi_r + \varphi_r S^2 + (S^*)^2\varphi_\ell + \varphi_\ell(S^*)^2\right) \\ &\quad + \varphi_r(S^*)^2 + \varphi_\ell S^2 \\ &= -(\cosh(\alpha) - 1 + \sinh(\alpha)\mathbf{1}_{\{n=0\}})\Delta(4-\Delta) + (\varphi_r - \varphi_\ell)\left((S^*)^2 - S^2\right) \\ &\quad + 2^{-1}\left((\varphi_\ell - \tau^*\varphi_\ell)(S^*)^2 + (\tau^*\varphi_\ell - \tau^{*2}\varphi_\ell)(S^*)^2 + (\varphi_r - \tau\varphi_r)S^2 + (\tau\varphi_r - \tau^2\varphi_r)S^2\right) \\ &= \mathcal{T}_{1;1} + \mathcal{T}_{1;2}\end{aligned}$$

where

$$\mathcal{T}_{1;1} := -(\cosh(\alpha) - 1)\Delta(4-\Delta), \quad \text{and} \tag{5.38}$$

$$\begin{aligned}\mathcal{T}_{1;2} &:= -\sinh(\alpha)\mathbf{1}_{\{n=0\}}\Delta(4-\Delta) + 2\sinh(\alpha)\mathrm{sign}(N)\mathbf{1}_{\{n\neq0\}}((S^*)^2 - S^2) \\ &\quad + \sinh(\alpha)\left(\mathbf{1}_{\{n=0\}}(S^*)^2 + \mathbf{1}_{\{n=-1\}}(S^*)^2 + \mathbf{1}_{\{n=0\}}S^2 + \mathbf{1}_{\{n=1\}}S^2\right).\end{aligned}$$

We calculate $\mathcal{T}_2$:

$$\begin{aligned}\mathcal{T}_2 &= -N(\varphi_r - \varphi_\ell)\left(2 - S^2 - (S^*)^2\right) + N(S^2\varphi_r - \varphi_r S^2) + N(\varphi_\ell(S^*)^2 - (S^*)^2\varphi_\ell) \\ &= -N(\varphi_r - \varphi_\ell)\Delta(4-\Delta) + N\left(\tau^2\varphi_r - \tau\varphi_r + \tau\varphi_r - \varphi_r\right)S^2 \\ &\quad + N\left(\varphi_\ell - \tau^*\varphi_\ell + \tau^*\varphi_\ell - \tau^{*2}\varphi_\ell\right)(S^*)^2 \\ &= -2\sinh(\alpha)|N|\Delta(4-\Delta) \\ &\quad + 2\sinh(\alpha)N\left(-(\mathbf{1}_{\{n=1\}} + \mathbf{1}_{\{n=0\}})S^2 + (\mathbf{1}_{\{n=0\}} + \mathbf{1}_{\{n=-1\}})(S^*)^2\right) \\ &= -2\sinh(\alpha)|N|\Delta(4-\Delta) - 2\sinh(\alpha)\left(\mathbf{1}_{\{n=1\}}S^2 + \mathbf{1}_{\{n=-1\}}(S^*)^2\right).\end{aligned}$$

The following commutation formulae hold

$$S^*(\mathbf{1}_{\{n\neq0\}}\mathrm{sign}(N)) = [\mathbf{1}_{\{n\neq0\}}\mathrm{sign}(N) + \mathbf{1}_{\{n=0\}} + \mathbf{1}_{\{n=-1\}}]S^*, \tag{5.39}$$

$$S(\mathbf{1}_{\{n\neq0\}}\mathrm{sign}(N)) = [\mathbf{1}_{\{n\neq0\}}\mathrm{sign}(N) - \mathbf{1}_{\{n=0\}} - \mathbf{1}_{\{n=+1\}}]S. \tag{5.40}$$

Using

$$\begin{aligned}S|N| &= |N|S + \left(\mathbf{1}_{\{n=0\}} - \mathbf{1}_{\{n\neq0\}}\mathrm{sign}(N)\right)S, \\ S^*|N| &= |N|S^* + \left(\mathbf{1}_{\{n=0\}} + \mathbf{1}_{\{n\neq0\}}\mathrm{sign}(N)\right)S^*,\end{aligned}$$

one checks that

$$|N|\Delta(4-\Delta) = (S - S^*)|N|(S^* - S) - \mathbf{1}_{\{n=0\}}\Delta(4-\Delta) - \mathbf{1}_{\{n\neq0\}}\mathrm{sign}(N)(S^2 - (S^*)^2). \tag{5.41}$$

Therefore $\mathcal{T}_2 = \mathcal{T}_{2;1} + \mathcal{T}_{2;2}$, where

$$\mathcal{T}_{2;1} = -2\sinh(\alpha)(S - S^*)|N|(S^* - S), \quad \text{and} \tag{5.42}$$

$$\mathcal{T}_{2;2} = -2\sinh(\alpha)\left(\mathbf{1}_{\{n=1\}}S^2 + \mathbf{1}_{\{n=-1\}}(S^*)^2\right) + 2\sinh(\alpha)\left(\mathbf{1}_{\{n=0\}}\Delta(4-\Delta) + \mathbf{1}_{\{n\neq 0\}}\mathrm{sign}(N)(S^2-(S^*)^2)\right).$$

Finally, a calculation shows that

$$\mathcal{T}_{1;2} + \mathcal{T}_{2;2} = \sinh(\alpha)\left(2\mathbf{1}_{\{n=0\}} - \mathbf{1}_{\{n=-1\}}(S^*)^2 - \mathbf{1}_{\{n=1\}}S^2\right). \tag{5.43}$$

Note that

$$\langle\psi_\alpha, [H, A']_\circ\psi_\alpha\rangle = \langle\psi_\alpha, \mathcal{T}\psi_\alpha\rangle = \langle\psi_\alpha, (\mathcal{T}_{1;1} + \mathcal{T}_{2;1} + \mathcal{T}_{1;2} + \mathcal{T}_{2;2})\,\psi_\alpha\rangle.$$

Plugging in for $\mathcal{T}_{1;1}$, $\mathcal{T}_{2;1}$ and $\mathcal{T}_{1;2} + \mathcal{T}_{2;2}$ given by (5.38), (5.42) and (5.43) yields

$$\langle\psi_\alpha, [H, A']_\circ\psi_\alpha\rangle = -2\sinh(\alpha)\|\sqrt{|N|}(S^*-S)\psi_\alpha\|^2 - (\cosh(\alpha)-1)\langle\psi_\alpha, \Delta(4-\Delta)\psi_\alpha\rangle + \sinh(\alpha)\left(2\psi_\alpha^2(0) + (\psi_\alpha(-1)-\psi_\alpha(1))^2\right).$$

Cancelling $\langle\psi_\alpha, [\Delta, A']\psi_\alpha\rangle = \langle\psi_\alpha, \Delta(4-\Delta)\psi_\alpha\rangle$ on both sides and dividing throughout by $\cosh(\alpha)\|\psi_\alpha\|^2$ yields (5.34) as required.

Part 2. From (5.37),

$$2^{-1}(e^{F_\alpha - \tau F_\alpha} + e^{F_\alpha - \tau^* F_\alpha}) = \begin{cases}\cosh(\alpha) & \text{if } |n| \geqslant 1\\ e^{-\alpha} & \text{if } n = 0,\end{cases}$$

$$2^{-1}(e^{F_\alpha - \tau F_\alpha} - e^{F_\alpha - \tau^* F_\alpha}) = \sinh(\alpha)\mathbf{1}_{\{n\neq 0\}}\mathrm{sign}(N).$$

We apply (5.8) of Lemma 5.2:

$$H_{F_\alpha} = \cosh(\alpha)\Delta + \mathbf{1}_{\{n=0\}}(e^{-\alpha} - \cosh(\alpha))\Delta + V + 2(1-\cosh(\alpha)) + 2\mathbf{1}_{\{n=0\}}(\cosh(\alpha) - e^{-\alpha}) + \sinh(\alpha)\mathbf{1}_{\{n\neq 0\}}\mathrm{sign}(N)(S^*-S).$$

The goal is to square H_{F_α}. Divide throughout by $\cosh(\alpha)$ and let $c_\alpha := (e^{-\alpha}\cosh(\alpha)^{-1} - 1)$:

$$\cosh(\alpha)^{-1}H_{F_\alpha} = \Delta + c_\alpha\mathbf{1}_{\{n=0\}}\Delta + \cosh(\alpha)^{-1}V + 2(\cosh(\alpha)^{-1}-1) - 2c_\alpha\mathbf{1}_{\{n=0\}} \tag{5.44}$$

$$+ \tanh(\alpha)\mathbf{1}_{\{n\neq 0\}}\mathrm{sign}(N)(S^*-S). \tag{5.45}$$

Note that $\sup_{\alpha\geqslant 0}|c_\alpha| \leqslant 2$. Since (S^*-S) is antisymmetric, by (5.39) and (5.40), we see that $\mathbf{1}_{\{n\neq 0\}}\mathrm{sign}(N)(S^*-S)$ is antisymmetric up to a couple of rank one projectors. The same goes for $\Delta\mathbf{1}_{\{n\neq 0\}}\mathrm{sign}(N)(S^*-S)$ and $\mathbf{1}_{\{n\neq 0\}}\mathrm{sign}(N)(S^*-S)\Delta$. Therefore

$$\lim_{\alpha\to+\infty}\Re\,\langle\Psi_\alpha, [\mathbf{1}_{\{n\neq 0\}}\mathrm{sign}(N)(S^*-S)]\Psi_\alpha\rangle = 0,$$

$$\lim_{\alpha\to+\infty}\Re\,\langle\Psi_\alpha, \Delta[\mathbf{1}_{\{n\neq 0\}}\mathrm{sign}(N)(S^*-S)]\Psi_\alpha\rangle = 0,$$

$$\lim_{\alpha\to+\infty}\Re\,\langle\Psi_\alpha, [\mathbf{1}_{\{n\neq 0\}}\mathrm{sign}(N)(S^*-S)]\Delta\Psi_\alpha\rangle = 0.$$

We compute $\left[\tanh(\alpha)\mathbf{1}_{\{n\neq 0\}}\mathrm{sign}(N)(S^*-S)\right]^2$ using (5.39) and (5.40):

$$(5.45)^2 = \tanh^2(\alpha)\Big[\mathbf{1}_{\{n\neq 0\}}(S^2 + (S^*)^2 - 2) + \mathbf{1}_{\{n=-1\}}(1-(S^*)^2) + \mathbf{1}_{\{n=+1\}}(S^2-1)\Big].$$

Thus squaring $\cosh(\alpha)^{-1}H_{F_\alpha}$ given by (5.44)-(5.45) and recalling that $\Delta(4-\Delta) = 2 - S^2 - (S^*)^2$ we get

$$\cosh(\alpha)^{-2}H_{F_\alpha}^2 = \Delta(\Delta-4) + 4 - \tanh^2(\alpha)\Delta(4-\Delta) + P_\alpha,$$

where P_α is a bounded operator satisfying

$$\lim_{\alpha\to\infty}\Re\,\langle\Psi_\alpha, P_\alpha\Psi_\alpha\rangle = 0.$$

Rearranging and recalling that $H_{F_\alpha}\Psi_\alpha = E\Psi_\alpha$ yields (5.35) as required. □

6. Appendix : Technical calculations

The Appendix is devoted to proving the key relations (3.13) and (5.3) that appear in Propositions 3.1 and 5.1 respectively. Recall that for $B \subset \mathbb{Z}^d$, $\mathbf{1}_B$ denotes the projector onto B. We start with the proof of the multi-dimensional formula

$$\begin{aligned}\langle \phi, [e^F A' e^F, \Delta]\phi\rangle &= \langle \phi_F, [A', \Delta]\phi_F\rangle - 2\left\|\sqrt{g}A'\phi_F\right\|^2 \\ &\quad - \sum_{i=1}^{d} \left\|\sqrt{\Delta_i(4-\Delta_i)}W_i\phi_F\right\|^2 + 2^{-1}\langle \phi_F, (\mathcal{L}+\mathcal{M}+\mathcal{G})\phi_F\rangle,\end{aligned} \tag{6.1}$$

where $\phi \in \ell_0(\mathbb{Z}^d)$ and $\phi_F := e^F\phi$. To jump to the proof of the $1d$ relation, go to (6.12).

Proof. It is understood that the operators are calculated and the commutators developed against $\phi \in \ell_0(\mathbb{Z}^d)$, so we omit the ϕ for ease of notation. Usual commutation relations give

$$[e^F A' e^F, \Delta] = e^F[A', \Delta]e^F + e^F A'[e^F, \Delta] + [e^F, \Delta]A' e^F. \tag{6.2}$$

We now concentrate on the second and third terms on the right side of the latter relation. The goal is to pop out $e^F A' g A' e^F$ and control the remainder. As pointed out in [FH] and [CFKS], this is the key quantity to single out. The following commutators will be used repeatedly:

$$[e^F, S_i] = -(\tau_i e^F - e^F)S_i = S_i(\tau_i^* e^F - e^F) = -e^F\varphi_{\ell_i}S_i = S_i\varphi_{r_i}e^F, \tag{6.3}$$

$$[e^F, S_i^*] = -(\tau_i^* e^F - e^F)S_i^* = S_i^*(\tau_i e^F - e^F) = -e^F\varphi_{r_i}S_i^* = S_i^*\varphi_{\ell_i}e^F. \tag{6.4}$$

Part 1 : Creating $e^F A' g A' e^F$ in a first way. We have

$$\begin{aligned}
[e^F, \Delta_i] &= \varphi_{r_i}e^F S_i^* + \varphi_{\ell_i}e^F S_i \\
&= g_{r_i}N_i e^F S_i^* + \varphi_{r_i}\mathbf{1}_{\{n_i=0\}}e^F S_i^* + \varphi_{\ell_i}e^F S_i \\
&= g_{r_i}N_i e^F(S_i^* - S_i) + \varphi_{r_i}\mathbf{1}_{\{n_i=0\}}e^F(S_i^* - S_i) + \left(\varphi_{r_i} + \varphi_{\ell_i}\right)e^F S_i \\
&= g_{r_i}N_i(S_i^* - S_i)e^F + g_{r_i}N_i[e^F, (S_i^* - S_i)] + \varphi_{r_i}\mathbf{1}_{\{n_i=0\}}e^F(S_i^* - S_i) + \left(\varphi_{r_i} + \varphi_{\ell_i}\right)e^F S_i \\
&= gN_i(S_i^* - S_i)e^F + (g_{r_i} - g)N_i(S_i^* - S_i)e^F + \varphi_{r_i}\mathbf{1}_{\{n_i=0\}}(S_i^* - S_i)e^F \\
&\quad + \varphi_{r_i}[e^F, (S_i^* - S_i)] + \left(\varphi_{r_i} + \varphi_{\ell_i}\right)e^F S_i \\
&= gA_i' e^F - 2^{-1}g(S_i^* + S_i)e^F + (g_{r_i} - g)N_i(S_i^* - S_i)e^F + \varphi_{r_i}\mathbf{1}_{\{n_i=0\}}(S_i^* - S_i)e^F \\
&\quad + \varphi_{r_i}[e^F, (S_i^* - S_i)] + \left(\varphi_{r_i} + \varphi_{\ell_i}\right)e^F S_i.
\end{aligned}$$

$$\begin{aligned}
[e^F, \Delta_i] &= -S_i e^F\varphi_{r_i} - S_i^* e^F\varphi_{\ell_i} \\
&= -S_i e^F N_i g_{r_i} - S_i e^F\varphi_{r_i}\mathbf{1}_{\{n_i=0\}} - S_i^* e^F\varphi_{\ell_i} \\
&= (S_i^* - S_i)e^F N_i g_{r_i} + (S_i^* - S_i)e^F\varphi_{r_i}\mathbf{1}_{\{n_i=0\}} - S_i^* e^F\left(\varphi_{r_i} + \varphi_{\ell_i}\right) \\
&= e^F(S_i^* - S_i)N_i g_{r_i} + [(S_i^* - S_i), e^F]N_i g_{r_i} + (S_i^* - S_i)e^F\varphi_{r_i}\mathbf{1}_{\{n_i=0\}} - S_i^* e^F\left(\varphi_{r_i} + \varphi_{\ell_i}\right) \\
&= e^F(S_i^* - S_i)N_i g + e^F(S_i^* - S_i)N_i(g_{r_i} - g) + e^F(S_i^* - S_i)\varphi_{r_i}\mathbf{1}_{\{n_i=0\}} \\
&\quad - [e^F, (S_i^* - S_i)]\varphi_{r_i} - S_i^* e^F\left(\varphi_{r_i} + \varphi_{\ell_i}\right) \\
&= e^F A_i' g + 2^{-1}e^F(S_i^* + S_i)g + e^F(S_i^* - S_i)N_i(g_{r_i} - g) + e^F(S_i^* - S_i)\varphi_{r_i}\mathbf{1}_{\{n_i=0\}} \\
&\quad - [e^F, (S_i^* - S_i)]\varphi_{r_i} - S_i^* e^F\left(\varphi_{r_i} + \varphi_{\ell_i}\right).
\end{aligned}$$

Therefore we have obtained

$$e^F A'[e^F,\Delta] + [e^F,\Delta]A'e^F = 2e^F A' g A' e^F + e^F(L_r + M_r + G_r + H_r)e^F, \quad \text{where} \tag{6.5}$$

$$L_r := \sum_{i,j} A'_i (g_{r_j} - g) N_j (S_j^* - S_j) + (S_i^* - S_i) N_i (g_{r_i} - g) A'_j,$$

$$M_r := 2^{-1} \sum_{i,j} -A'_i g (S_j^* + S_j) + (S_i^* + S_i) g A'_j,$$

$$\begin{aligned} G_r := &\sum_{i,j} A'_i \left(\varphi_{r_j}[e^F,(S_j^* - S_j)]e^{-F} + \left(\varphi_{r_j} + \varphi_{\ell_j}\right) e^F S_j e^{-F}\right) \\ &- \sum_{i,j} \left(e^{-F}[e^F,(S_i^* - S_i)]\varphi_{r_i} + e^{-F} S_i^* e^F \left(\varphi_{r_i} + \varphi_{\ell_i}\right)\right) A'_j, \quad \text{and} \end{aligned}$$

$$H_r := \sum_{i,j} A'_i \varphi_{r_j} \mathbf{1}_{\{n_j=0\}} (S_j^* - S_j) + (S_i^* - S_i) \varphi_{r_i} \mathbf{1}_{\{n_i=0\}} A_j.$$

We split M_r as follows: $M_r = M_{r;1} + M_{r;2}$, where

$$M_{r;1} := 2^{-1} \sum_{i\neq j} -A'_i g (S_j^* + S_j) + (S_i^* + S_i) g A'_j,$$

$$M_{r;2} := 2^{-1} \sum_{i} -A'_i g (S_i^* + S_i) + (S_i^* + S_i) g A'_i = M_{r;2;1} + M_{r;2;2}, \quad \text{with}$$

$$M_{r;2;1} := 2^{-1} \sum_{i} -A'_i g_{r_i} (S_i^* + S_i) + (S_i^* + S_i) g_{r_i} A'_i,$$

$$M_{r;2;2} := 2^{-1} \sum_{i} -A'_i (g - g_{r_i}) (S_i^* + S_i) + (S_i^* + S_i)(g - g_{r_i}) A'_i.$$

We calculate $M_{r;1}$ by expanding A'_i and A'_j:

$$\begin{aligned} M_{r;1} &:= 2^{-1} \sum_{i\neq j} -N_i (S_i^* - S_i) g (S_j^* + S_j) + (S_i^* + S_i) g N_j (S_j^* - S_j) \\ &= 2^{-1} \sum_{i\neq j} -N_i \big[(\tau_i^* g) S_i^* - (\tau_i g) S_i\big](S_j^* + S_j) + \big[(\tau_i^*(g N_j)) S_i^* + (\tau_i (g N_j)) S_i\big](S_j^* - S_j) \\ &= \frac{1}{2} \sum_{i\neq j} N_i \big[\tau_i g - \tau_j g\big] S_i S_j + N_i \big[\tau_j^* g - \tau_i^* g\big] S_i^* S_j^* \\ &\quad + \big[N_i(\tau_j g - \tau_i^* g) + N_j(\tau_j g - \tau_i^* g)\big] S_i^* S_j.^{(\ddagger_2)} \end{aligned}$$

Again expanding A_i':

$$\begin{aligned}
M_{r;2;1} &= 2^{-1}\sum_i (S_i^*+S_i)g_{r_i}(S_i^*+S_i) - (S_i^*-S_i)\varphi_{r_i}\mathbf{1}_{\{n_i\neq 0\}}(S_i^*+S_i)\\
&\quad + 2^{-1}\sum_i (S_i^*+S_i)\varphi_{r_i}\mathbf{1}_{\{n_i\neq 0\}}(S_i^*-S_i)\\
&= \sum_i 2^{-1}(S_i^*+S_i)g_{r_i}(S_i^*+S_i) + S_i\varphi_{r_i}S_i^* - S_i^*\varphi_{r_i}S_i\\
&\quad + \big(S_i^*\varphi_{r_i}\mathbf{1}_{\{n_i=0\}}S_i - S_i\varphi_{r_i}\mathbf{1}_{\{n_i=0\}}S_i^*\big)\\
&= M_{r;2;1;1} + M_{r;2;1;2}, \quad \text{where}
\end{aligned}$$

$$M_{r;2;1;1} := \sum_i 2^{-1}(S_i^*+S_i)g_{r_i}(S_i^*+S_i) + (\tau_i\varphi_{r_i} - \tau_i^*\varphi_{r_i}),^{(\ddagger_1,\ddagger_3)}$$

$$M_{r;2;1;2} := \sum_i (\tau_i^*\varphi_{r_i})\mathbf{1}_{\{n_i=-1\}} - (\tau_i\varphi_{r_i})\mathbf{1}_{\{n_i=+1\}}.$$

We calulate G_r. We note that
(6.6)

$$(\tau_i\varphi_{r_i})\varphi_{\ell_i} = \varphi_{\ell_i}(\tau_i\varphi_{r_i}) = -(\tau_i\varphi_{r_i}+\varphi_{\ell_i}), \quad \text{and} \quad (\tau_i^*\varphi_{\ell_i})\varphi_{r_i} = \varphi_{r_i}(\tau_i^*\varphi_{\ell_i}) = -(\tau_i^*\varphi_{\ell_i}+\varphi_{r_i}).$$

$$\begin{aligned}
G_r &:= \sum_{i,j} A_i'\left(\varphi_{r_j}\big(S_j^*\varphi_{\ell_j} - S_j\varphi_{r_j}\big) + \big(\varphi_{r_j}+\varphi_{\ell_j}\big)S_j\big(\varphi_{r_j}+1\big)\right)\\
&\quad - \sum_{i,j}\left(\big(-\varphi_{r_i}S_i^* + \varphi_{\ell_i}S_i\big)\varphi_{r_i} + \big(\varphi_{r_i}+1\big)S_i^*\big(\varphi_{r_i}+\varphi_{\ell_i}\big)\right)A_j'\\
&= \sum_{i,j} A_i'\left(S_j^*(\tau_j\varphi_{r_j})\varphi_{\ell_j} - S_j(\tau_j^*\varphi_{r_j})\varphi_{r_j} + S_j(\tau_j^*\varphi_{r_j})(\varphi_{r_j}+1) + S_j(\tau_j^*\varphi_{\ell_j})(\varphi_{r_j}+1)\right)\\
&\quad + \sum_{i,j}\left(\varphi_{r_i}(\tau_i^*\varphi_{r_i})S_i^* - \varphi_{\ell_i}(\tau_i\varphi_{r_i})S_i - (\varphi_{r_i}+1)(\tau_i^*\varphi_{r_i})S_i^* - (\varphi_{r_i}+1)(\tau_i^*\varphi_{\ell_i})S_i^*\right)A_j'\\
&= \sum_{i,j} A_i'\left(-S_j^*(\varphi_{\ell_j}+\tau_j\varphi_{r_j}) + S_j(\tau_j^*\varphi_{r_j}-\varphi_{r_j})\right) + \sum_{i,j}\left((\varphi_{r_i}-\tau_i^*\varphi_{r_i})S_i^* + (\varphi_{\ell_i}+\tau_i\varphi_{r_i})S_i\right)A_j'\\
&= G_{r;1} + G_{r;2}, \quad \text{where}
\end{aligned}$$

$$G_{r;1} := \sum_{i,j} A_i'S_j(\tau_j^*\varphi_{r_j} - \varphi_{r_j}) + (\varphi_{r_i} - \tau_i^*\varphi_{r_i})S_i^*A_j',^{(\ddagger_3)}$$

$$G_{r;2} := \sum_{i,j} -A_i'S_j^*(\varphi_{\ell_j}+\tau_j\varphi_{r_j}) + (\varphi_{\ell_i}+\tau_i\varphi_{r_i})S_iA_j'.$$

To end this section we note that we are left to deal with $L_r + M_{r;2;1;2} + M_{r;2;2} + G_{r;2} + H_r$.

Part 2 : Creating $e^F A' g A' e^F$ a second way. We repeat the calculation with a variation.

$$\begin{aligned}
[e^F, \Delta_i] &= \varphi_{\ell_i} e^F S_i + \varphi_{r_i} e^F S_i^* \\
&= g_{\ell_i} N_i e^F S_i + \varphi_{\ell_i} \mathbf{1}_{\{n_i=0\}} e^F S_i + \varphi_{r_i} e^F S_i^* \\
&= -g_{\ell_i} N_i e^F (S_i^* - S_i) + \varphi_{\ell_i} \mathbf{1}_{\{n_i=0\}} e^F (S_i - S_i^*) + \big(\varphi_{r_i} + \varphi_{\ell_i}\big) e^F S_i^* \\
&= -g_{\ell_i} N_i (S_i^* - S_i) e^F - g_{\ell_i} N_i [e^F, (S_i^* - S_i)] + \varphi_{\ell_i} \mathbf{1}_{\{n_i=0\}} e^F (S_i - S_i^*) + \big(\varphi_{r_i} + \varphi_{\ell_i}\big) e^F S_i^* \\
&= g N_i (S_i^* - S_i) e^F - (g_{\ell_i} + g) N_i (S_i^* - S_i) e^F + \varphi_{\ell_i} \mathbf{1}_{\{n_i=0\}} (S_i - S_i^*) e^F \\
&\quad - \varphi_{\ell_i} [e^F, (S_i^* - S_i)] + \big(\varphi_{r_i} + \varphi_{\ell_i}\big) e^F S_i^* \\
&= g A_i' e^F - 2^{-1} g (S_i^* + S_i) e^F - (g_{\ell_i} + g) N_i (S_i^* - S_i) e^F + \varphi_{\ell_i} \mathbf{1}_{\{n_i=0\}} (S_i - S_i^*) e^F \\
&\quad - \varphi_{\ell_i} [e^F, (S_i^* - S_i)] + \big(\varphi_{r_i} + \varphi_{\ell_i}\big) e^F S_i^*.
\end{aligned}$$

$$\begin{aligned}
[e^F, \Delta_i] &= -S_i^* e^F \varphi_{\ell_i} - S_i e^F \varphi_{r_i} \\
&= -S_i^* e^F N_i g_{\ell_i} - S_i^* e^F \varphi_{\ell_i} \mathbf{1}_{\{n_i=0\}} - S_i e^F \varphi_{r_i} \\
&= -(S_i^* - S_i) e^F N_i g_{\ell_i} + (S_i - S_i^*) e^F \varphi_{\ell_i} \mathbf{1}_{\{n_i=0\}} - S_i e^F \big(\varphi_{r_i} + \varphi_{\ell_i}\big) \\
&= -e^F (S_i^* - S_i) N_i g_{\ell_i} - [(S_i^* - S_i), e^F] N_i g_{\ell_i} + (S_i - S_i^*) e^F \varphi_{\ell_i} \mathbf{1}_{\{n_i=0\}} - S_i e^F \big(\varphi_{r_i} + \varphi_{\ell_i}\big) \\
&= e^F (S_i^* - S_i) N_i g - e^F (S_i^* - S_i) N_i (g_{\ell_i} + g) + e^F (S_i - S_i^*) \varphi_{\ell_i} \mathbf{1}_{\{n_i=0\}} \\
&\quad + [e^F, (S_i^* - S_i)] \varphi_{\ell_i} - S_i e^F \big(\varphi_{r_i} + \varphi_{\ell_i}\big) \\
&= e^F A_i' g + 2^{-1} e^F (S_i^* + S_i) g - e^F (S_i^* - S_i) N_i (g_{\ell_i} + g) + e^F (S_i - S_i^*) \varphi_{\ell_i} \mathbf{1}_{\{n_i=0\}} \\
&\quad + [e^F, (S_i^* - S_i)] \varphi_{\ell_i} - S_i e^F \big(\varphi_{r_i} + \varphi_{\ell_i}\big)
\end{aligned}$$

Therefore we have obtained

$$e^F A' [e^F, \Delta] + [e^F, \Delta] A' e^F = 2 e^F A' g A' e^F + e^F (L_\ell + M_\ell + G_\ell + H_\ell) e^F, \quad \text{where} \tag{6.7}$$

$$L_\ell := -\sum_{i,j} A_i' (g_{\ell_j} + g) N_j (S_j^* - S_j) + (S_i^* - S_i) N_i (g_{\ell_i} + g) A_j',$$

$$M_\ell := 2^{-1} \sum_{i,j} -A_i' g (S_j^* + S_j) + (S_i^* + S_i) g A_j',$$

$$\begin{aligned}
G_\ell := &\sum_{i,j} A_i' \left(-\varphi_{\ell_j} [e^F, (S_j^* - S_j)] e^{-F} + \big(\varphi_{r_j} + \varphi_{\ell_j}\big) e^F S_j^* e^{-F}\right) \\
&+ \sum_{i,j} \left(e^{-F} [e^F, (S_i^* - S_i)] \varphi_{\ell_i} - e^{-F} S_i e^F \big(\varphi_{r_i} + \varphi_{\ell_i}\big)\right) A_j', \quad \text{and}
\end{aligned}$$

$$H_\ell := \sum_{i,j} A_i' \varphi_{\ell_j} \mathbf{1}_{\{n_j=0\}} (S_j - S_j^*) + (S_i - S_i^*) \varphi_{\ell_i} \mathbf{1}_{\{n_i=0\}} A_j'.$$

We split M_ℓ as follows: $M_\ell := M_{\ell;1} + M_{\ell;2}$, where

$$M_{\ell;1} := 2^{-1} \sum_{i \neq j} -A_i' g (S_j^* + S_j) + (S_i^* + S_i) g A_j',$$

$$M_{\ell;2} := 2^{-1} \sum_{i} -A_i' g (S_i^* + S_i) + (S_i^* + S_i) g A_i' = M_{\ell;2;1} + M_{\ell;2;2}, \quad \text{with}$$

$$M_{\ell;2;1} := 2^{-1} \sum_i A_i' g_{\ell_i} (S_i^* + S_i) - (S_i^* + S_i) g_{\ell_i} A_i',$$

$$M_{\ell;2;2} := 2^{-1} \sum_i -A_i' (g + g_{\ell_i})(S_i^* + S_i) + (S_i^* + S_i)(g + g_{\ell_i}) A_i'.$$

We calculate $M_{\ell;1}$ by expanding A_i' and A_j':

$$\begin{aligned}
M_{\ell;1} &= 2^{-1} \sum_{i \neq j} -N_i (S_i^* - S_i) g (S_j^* + S_j) + (S_i^* + S_i) g N_j (S_j^* - S_j) \\
&= 2^{-1} \sum_{i \neq j} -N_i \big[(\tau_i^* g) S_i^* - (\tau_i g) S_i\big](S_j^* + S_j) + \big[(\tau_i^* (g N_j)) S_i^* + (\tau_i (g N_j)) S_i\big](S_j^* - S_j) \\
&= \frac{1}{2} \sum_{i \neq j} N_i \big[\tau_i g - \tau_j g\big] S_i S_j + N_i \big[\tau_j^* g - \tau_i^* g\big] S_i^* S_j^* \\
&\quad + \big[N_i (\tau_j g - \tau_i^* g) + N_j (\tau_j g - \tau_i^* g)\big] S_i^* S_j .^{(\ddagger_2)}
\end{aligned}$$

Again expanding A_i':

$$\begin{aligned}
M_{\ell;2;1} &= 2^{-1} \sum_i -(S_i^* + S_i) g_{\ell_i} (S_i^* + S_i) + (S_i^* - S_i) \varphi_{\ell_i} \mathbf{1}_{\{n_i \neq 0\}} (S_i^* + S_i) \\
&\quad - 2^{-1} \sum_i (S_i^* + S_i) \varphi_{\ell_i} \mathbf{1}_{\{n_i \neq 0\}} (S_i^* - S_i) \\
&= \sum_i -2^{-1} (S_i^* + S_i) g_{\ell_i} (S_i^* + S_i) + S_i^* \varphi_{\ell_i} S_i - S_i \varphi_{\ell_i} S_i^* \\
&\quad + \big(S_i \varphi_{\ell_i} \mathbf{1}_{\{n_i = 0\}} S_i^* - S_i^* \varphi_{\ell_i} \mathbf{1}_{\{n_i = 0\}} S_i\big) \\
&= M_{\ell;2;1;1} + M_{\ell;2;1;2}, \quad \text{where}
\end{aligned}$$

$$M_{\ell;2;1;1} := \sum_i -2^{-1} (S_i^* + S_i) g_{\ell_i} (S_i^* + S_i) + (\tau_i^* \varphi_{\ell_i} - \tau_i \varphi_{\ell_i}),^{(\ddagger_1, \ddagger_3)}$$

$$M_{\ell;2;1;2} := \sum_i (\tau_i \varphi_{\ell_i}) \mathbf{1}_{\{n_i = +1\}} - (\tau_i^* \varphi_{\ell_i}) \mathbf{1}_{\{n_i = -1\}}.$$

We calculate G_ℓ:

$$\begin{aligned}
G_\ell &:= \sum_{i,j} A_i' \left(-\varphi_{\ell_j} \big(S_j^* \varphi_{\ell_j} - S_j \varphi_{r_j}\big) + \big(\varphi_{r_j} + \varphi_{\ell_j}\big) S_j^* \big(\varphi_{\ell_j} + 1\big)\right) \\
&\quad + \sum_{i,j} \left(\big(-\varphi_{r_i} S_i^* + \varphi_{\ell_i} S_i\big) \varphi_{\ell_i} - \big(\varphi_{\ell_i} + 1\big) S_i \big(\varphi_{r_i} + \varphi_{\ell_i}\big)\right) A_j' \\
&= \sum_{i,j} A_i' \left(-S_j^* (\tau_j \varphi_{\ell_j}) \varphi_{\ell_j} + S_j (\tau_j^* \varphi_{\ell_j}) \varphi_{r_j} + S_j^* (\tau_j \varphi_{r_j})(\varphi_{\ell_j} + 1) + S_j^* (\tau_j \varphi_{\ell_j})(\varphi_{\ell_j} + 1)\right) \\
&\quad + \sum_{i,j} \left(-\varphi_{r_i} (\tau_i^* \varphi_{\ell_i}) S_i^* + \varphi_{\ell_i} (\tau_i \varphi_{\ell_i}) S_i - (\varphi_{\ell_i} + 1)(\tau_i \varphi_{r_i}) S_i - (\varphi_{\ell_i} + 1)(\tau_i \varphi_{\ell_i}) S_i\right) A_j' \\
&= \sum_{i,j} A_i' \left(S_j^* (\tau_j \varphi_{\ell_j} - \varphi_{\ell_j}) - S_j (\tau_j^* \varphi_{\ell_j} + \varphi_{r_j})\right) + \sum_{i,j} \left((\varphi_{\ell_i} - \tau_i \varphi_{\ell_i}) S_i + (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}) S_i^*\right) A_j' \\
&= G_{\ell;1} + G_{\ell;2}, \quad \text{where}
\end{aligned}$$

$$G_{\ell;1} := \sum_{i,j} A_i' S_j^* (\tau_j \varphi_{\ell_j} - \varphi_{\ell_j}) + (\varphi_{\ell_i} - \tau_i \varphi_{\ell_i}) S_i A_j',^{(\ddagger_3)}$$

$$G_{\ell;2} := \sum_{i,j} -A_i' S_j (\tau_j^* \varphi_{\ell_j} + \varphi_{r_j}) + (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}) S_i^* A_j'.$$

Note that we are left to deal with $L_\ell + M_{\ell;2;1;2} + M_{\ell;2;2} + G_{\ell;2} + H_\ell$.

Part 3 : Adding the terms of Parts 1 and 2. Take the average of (6.5) and (6.7):

$$\begin{aligned}[e^F A' e^F, \Delta] &= e^F [A', \Delta] e^F + 2 e^F A' g A' e^F \\ &\quad + 2^{-1} e^F \left(L_r + L_\ell + M_r + M_\ell + G_r + G_\ell + H_r + H_\ell\right) e^F. \end{aligned} \tag{6.8}$$

Applying $\phi \in \ell_0(\mathbb{Z}^d)$ to this equation and taking inner products leads to (6.1). We go into details. The terms that still have to be dealt with are $L_r + M_{r;2;1;2} + M_{r;2;2} + G_{r;2} + H_r$ from the first part and $L_\ell + M_{\ell;2;1;2} + M_{\ell;2;2} + G_{\ell;2} + H_\ell$ from the second part. Since

$$(\tau_i^* \varphi_{r_i} - \tau_i^* \varphi_{\ell_i}) \mathbf{1}_{\{n_i = -1\}} \phi = (\tau_i \varphi_{\ell_i} - \tau_i \varphi_{r_i}) \mathbf{1}_{\{n_i = +1\}} \phi = 0, \quad \text{and} \quad (\varphi_{r_i} - \varphi_{\ell_i}) \mathbf{1}_{\{n_i = 0\}} \phi = 0,$$

it follows that

$$(M_{r;2;1;2} + M_{\ell;2;1;2}) \phi = 0, \quad \text{and} \quad (H_r + H_\ell) \phi = 0.$$

We add L_r and L_ℓ and define this to be $\mathcal{L}$:

$$\begin{aligned}\mathcal{L} := L_r + L_\ell &= \sum_{i,j} A_i' [(g_{r_j} - g) - (g_{\ell_j} + g)] N_j (S_j^* - S_j) \\ &\quad + \sum_{i,j} (S_i^* - S_i) N_i [(g_{r_i} - g) - (g_{\ell_i} + g)] A_j'.^{(\ddagger_4)} \end{aligned} \tag{6.9}$$

We add $M_{r;2;2}$ and $M_{\ell;2;2}$:

$$M_{r;2;2} + M_{\ell;2;2} = 2^{-1} \sum_i A_i' [(g_{r_i} - g) - (g_{\ell_i} + g)] (S_i^* + S_i) - (S_i^* + S_i) [(g_{r_i} - g) - (g_{\ell_i} + g)] A_i'.^{(\ddagger_4)}$$

We can now define $\mathcal{M}$:

$$\mathcal{M} := M_r + M_\ell = M_{r;1} + M_{r;2;1;1} + M_{\ell;1} + M_{\ell;2;1;1} + (M_{r;2;2} + M_{\ell;2;2}). \tag{6.10}$$

The final step is to add $G_{r;2}$ and $G_{\ell;2}$:

$$\begin{aligned} G_{r;2} + G_{\ell;2} &= \sum_{i,j} -A_i S_j^* (\varphi_{\ell_j} + \tau_j \varphi_{r_j}) + (\varphi_{\ell_i} + \tau_i \varphi_{r_i}) S_i A_j \\ &\quad + \sum_{i,j} -A_i S_j (\tau_j^* \varphi_{\ell_j} + \varphi_{r_j}) + (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}) S_i^* A_j \\ &= - \sum_{i,j} [2^{-1} (S_i^* + S_i) + N_i (S_i^* - S_i)] S_j^* (\varphi_{\ell_j} + \tau_j \varphi_{r_j}) \\ &\quad + \sum_{i,j} (\varphi_{\ell_i} + \tau_i \varphi_{r_i}) S_i [-2^{-1} (S_j^* + S_j) + (S_j^* - S_j) N_j] \\ &\quad - \sum_{i,j} [2^{-1} (S_i^* + S_i) + N_i (S_i^* - S_i)] S_j (\tau_j^* \varphi_{\ell_j} + \varphi_{r_j}) \\ &\quad + \sum_{i,j} (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}) S_i^* [-2^{-1} (S_j^* + S_j) + (S_j^* - S_j) N_j] \\ &= G_1 + G_2 + G_3 + G_4 + G_5 + G_6, \quad \text{where} \end{aligned}$$

$$G_1 := \sum_{i,j} -N_i S_i^* S_j^* (\varphi_{\ell_j} + \tau_j \varphi_{r_j}) + (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}) S_i^* S_j^* N_j,$$

$$G_2 := \sum_{i,j} N_i S_i S_j (\tau_j^* \varphi_{\ell_j} + \varphi_{r_j}) - (\varphi_{\ell_i} + \tau_i \varphi_{r_i}) S_i S_j N_j,$$

$$G_3 := \sum_{i,j} N_i S_i S_j^* (\varphi_{\ell_j} + \tau_j \varphi_{r_j}) - N_i S_i^* S_j (\tau_j^* \varphi_{\ell_j} + \varphi_{r_j}) - (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}) S_i^* S_j N_j + (\varphi_{\ell_i} + \tau_i \varphi_{r_i}) S_i S_j^* N_j,$$

$$G_4 := -2^{-1} \sum_{i,j} S_i^* S_j^* (\varphi_{\ell_j} + \tau_j \varphi_{r_j}) + (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}) S_i^* S_j^*,$$

$$G_5 := -2^{-1} \sum_{i,j} (\varphi_{\ell_i} + \tau_i \varphi_{r_i}) S_i S_j + S_i S_j (\tau_j^* \varphi_{\ell_j} + \varphi_{r_j}),$$

$$G_6 := -2^{-1} \sum_{i,j} S_i S_j^* (\varphi_{\ell_j} + \tau_j \varphi_{r_j}) + (\varphi_{\ell_i} + \tau_i \varphi_{r_i}) S_i S_j^* + S_i^* S_j (\tau_j^* \varphi_{\ell_j} + \varphi_{r_j}) + (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}) S_i^* S_j.$$

We calculate G_i for $i = 1...6$. $G_1 = G_{1;1} + G_{1;2} + G_{1;3}$, with

$$G_{1;1} := \sum_{i,j} [(\tau_j^* \varphi_{\ell_j} - \tau_i^* \tau_j^* \varphi_{\ell_j}) + (\varphi_{r_j} - \tau_i^* \varphi_{r_j})] N_i S_i^* S_j^*,^{(\ddagger_3)}$$

$$G_{1;2} := \sum_{i \neq j} (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}) S_i^* S_j^* \quad \text{and} \quad G_{1;3} := 2 \sum_i (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}) (S_i^*)^2.$$

$$G_2 = G_{2;1} + G_{2;2} + G_{2;3}, \quad \text{where}$$

$$G_{2;1} := \sum_{i,j} [(\tau_i \varphi_{\ell_j} - \varphi_{\ell_j}) + (\tau_i \tau_j \varphi_{r_j} - \tau_j \varphi_{r_j})] N_i S_i S_j,^{(\ddagger_3)}$$

$$G_{2;2} := \sum_{i \neq j} (\varphi_{\ell_i} + \tau_i \varphi_{r_i}) S_i S_j \quad \text{and} \quad G_{2;3} := 2 \sum_i (\varphi_{\ell_i} + \tau_i \varphi_{r_i}) (S_i)^2.$$

$$\begin{aligned}
G_3 = &\sum_{i \neq j} N_i S_i S_j^* (\varphi_{\ell_j} + \tau_j \varphi_{r_j}) - N_i S_i^* S_j (\tau_j^* \varphi_{\ell_j} + \varphi_{r_j}) \\
&- (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}) S_i^* S_j N_j + (\varphi_{\ell_i} + \tau_i \varphi_{r_i}) S_i S_j^* N_j \\
&+ \sum_i N_i (\varphi_{\ell_i} + \tau_i \varphi_{r_i}) - N_i (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}) - (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}) N_i + (\varphi_{\ell_i} + \tau_i \varphi_{r_i}) N_i \\
= &\sum_{i \neq j} (\tau_i \tau_j^* \varphi_{\ell_j} + \tau_i \varphi_{r_j}) N_i S_i S_j^* - (\tau_i^* \varphi_{\ell_j} + \tau_i^* \tau_j \varphi_{r_j}) N_i S_i^* S_j \\
&+ \sum_{i \neq j} -(\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}) N_j S_i^* S_j + (\varphi_{\ell_i} + \tau_i \varphi_{r_i}) N_j S_i S_j^* \\
&+ \sum_{i \neq j} (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}) S_i^* S_j + (\varphi_{\ell_i} + \tau_i \varphi_{r_i}) S_i S_j^* + 2 \sum_i [(\varphi_{\ell_i} - \tau_i^* \varphi_{\ell_i}) + (\tau_i \varphi_{r_i} - \varphi_{r_i})] N_i \\
= &\, G_{3;1} + G_{3;2} + G_{3;3}, \quad \text{where}
\end{aligned}$$

$$G_{3;1} := \sum_{i \neq j} [(\tau_i \tau_j^* \varphi_{\ell_j} - \tau_j^* \varphi_{\ell_j}) + (\tau_i \varphi_{r_j} - \varphi_{r_j})] N_i S_i S_j^* + [(\varphi_{\ell_j} - \tau_i^* \varphi_{\ell_j}) + (\tau_j \varphi_{r_j} - \tau_i^* \tau_j \varphi_{r_j})] N_i S_i^* S_j,^{(\ddagger_3)}$$

$$G_{3;2} := \sum_{i \neq j} (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}) S_i^* S_j + (\varphi_{\ell_i} + \tau_i \varphi_{r_i}) S_i S_j^*,$$

$$G_{3;3} := 2\sum_i [(\varphi_{\ell_i} - \tau_i^* \varphi_{\ell_i}) + (\tau_i \varphi_{r_i} - \varphi_{r_i})] N_i.^{(\ddagger_3)}$$

$$G_4 = -2^{-1} \sum_{i,j} [(\tau_i^* \tau_j^* \varphi_{\ell_j} + \tau_i^* \varphi_{r_j}) + (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i})] S_i^* S_j^* = G_{4;1} + G_{4;2}, \quad \text{with}$$

$$G_{4;1} := -2^{-1} \sum_{i \neq j} [(\tau_i^* \tau_j^* \varphi_{\ell_j} + \tau_i^* \varphi_{r_j}) + (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i})] S_i^* S_j^*,$$

$$G_{4;2} := -2^{-1} \sum_i [(\tau_i^* \tau_i^* \varphi_{\ell_i} + \tau_i^* \varphi_{r_i}) + (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i})] (S_i^*)^2.$$

$$G_5 = -2^{-1} \sum_{i,j} [(\varphi_{\ell_i} + \tau_i \varphi_{r_i}) + (\tau_i \varphi_{\ell_j} + \tau_i \tau_j \varphi_{r_j})] S_i S_j = G_{5;1} + G_{5;2}, \quad \text{with}$$

$$G_{5;1} = -2^{-1} \sum_{i \neq j} [(\varphi_{\ell_i} + \tau_i \varphi_{r_i}) + (\tau_i \varphi_{\ell_j} + \tau_i \tau_j \varphi_{r_j})] S_i S_j,$$

$$G_{5;2} = -2^{-1} \sum_i [(\varphi_{\ell_i} + \tau_i \varphi_{r_i}) + (\tau_i \varphi_{\ell_i} + \tau_i \tau_i \varphi_{r_i})] (S_i)^2.$$

$$G_6 = -2^{-1} \sum_{i,j} [(\tau_i \tau_j^* \varphi_{\ell_j} + \tau_i \varphi_{r_j}) + (\varphi_{\ell_i} + \tau_i \varphi_{r_i})] S_i S_j^* + [(\tau_i^* \varphi_{\ell_j} + \tau_i^* \tau_j \varphi_{r_j}) + (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i})] S_i^* S_j$$
$$= G_{6;1} + G_{6;2}, \quad \text{with}$$

$$G_{6;1} := -2^{-1} \sum_{i \neq j} [(\tau_i \tau_j^* \varphi_{\ell_j} + \tau_i \varphi_{r_j}) + (\varphi_{\ell_i} + \tau_i \varphi_{r_i})] S_i S_j^* + [(\tau_i^* \varphi_{\ell_j} + \tau_i^* \tau_j \varphi_{r_j}) + (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i})] S_i^* S_j,$$

$$G_{6;2} := -\sum_i (\varphi_{\ell_i} + \tau_i \varphi_{r_i}) + (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}).$$

We add $G_{1;2}$ and $G_{4;1}$:

$$G_{1;2} + G_{4;1} = \sum_{i \neq j} (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i}) S_i^* S_j^* - 2^{-1} \sum_{i \neq j} [(\tau_i^* \tau_j^* \varphi_{\ell_j} + \tau_i^* \varphi_{r_j}) + (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i})] S_i^* S_j^*$$
$$= 2^{-1} \sum_{i \neq j} [(\tau_j^* \varphi_{\ell_j} - \tau_i^* \tau_j^* \varphi_{\ell_j}) + (\varphi_{r_j} - \tau_i^* \varphi_{r_j})] S_i^* S_j^*.^{(\ddagger_3)}$$

We add $G_{1;3}$ and $G_{4;2}$:

$$G_{1;3} + G_{4;2} = 2\sum_i (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i})(S_i^*)^2 - 2^{-1} \sum_i [(\tau_i^* \tau_i^* \varphi_{\ell_i} + \tau_i^* \varphi_{r_i}) + (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i})] (S_i^*)^2$$
$$= G_7 + G_8, \quad \text{where}$$

$$G_7 := 2^{-1} \sum_i [(\tau_i^* \varphi_{\ell_i} - \tau_i^* \tau_i^* \varphi_{\ell_i}) + (\varphi_{r_i} - \tau_i^* \varphi_{r_i})] (S_i^*)^{2\ (\ddagger_3)} \quad \text{and} \quad G_8 := \sum_i (\tau_i^* \varphi_{\ell_i} + \varphi_{r_i})(S_i^*)^2.$$

We add $G_{2;2}$ and $G_{5;1}$:

$$G_{2;2} + G_{5;1} = \sum_{i \neq j} (\varphi_{\ell_i} + \tau_i \varphi_{r_i}) S_i S_j - 2^{-1} \sum_{i \neq j} [(\varphi_{\ell_i} + \tau_i \varphi_{r_i}) + (\tau_i \varphi_{\ell_j} + \tau_i \tau_j \varphi_{r_j})] S_i S_j$$
$$= 2^{-1} \sum_{i \neq j} [(\varphi_{\ell_j} - \tau_i \varphi_{\ell_j}) + (\tau_j \varphi_{r_j} - \tau_i \tau_j \varphi_{r_j})] S_i S_j.^{(\ddagger_3)}$$

We add $G_{2;3}$ and $G_{5;2}$:

$$\begin{aligned}G_{2;3}+G_{5;2} &= 2\sum_i(\varphi_{\ell_i}+\tau_i\varphi_{r_i})(S_i)^2 - 2^{-1}\sum_i[(\varphi_{\ell_i}+\tau_i\varphi_{r_i})+(\tau_i\varphi_{\ell_i}+\tau_i\tau_i\varphi_{r_i})](S_i)^2\\ &= G_9+G_{10},\quad \text{where}\end{aligned}$$

$$G_9 := 2^{-1}\sum_i[(\varphi_{\ell_i}-\tau_i\varphi_{\ell_i})+(\tau_i\varphi_{r_i}-\tau_i\tau_i\varphi_{r_i})](S_i)^2\ ^{(\ddagger_3)} \quad \text{and} \quad G_{10} := \sum_i(\varphi_{\ell_i}+\tau_i\varphi_{r_i})(S_i)^2.$$

We add $G_{3;2}$ and $G_{6;1}$:

$$G_{3;2}+G_{6;1} = -2^{-1}\sum_{i\neq j}[(\tau_i\tau_j^*\varphi_{\ell_j}-\tau_j^*\varphi_{\ell_j})+(\tau_i\varphi_{r_j}-\varphi_{r_j})+(\tau_j^*\varphi_{\ell_i}-\varphi_{\ell_i})+(\tau_j^*\tau_i\varphi_{r_i}-\tau_i\varphi_{r_i})]S_iS_j^*.^{(\ddagger_3)}$$

We are left to deal with $G_{6;2}$, G_8 and G_{10}:

$$\begin{aligned}G_8+G_{10}+G_{6;2} &= \sum_i(\tau_i^*\varphi_{\ell_i}+\varphi_{r_i})S_i^*S_i^* + (\varphi_{\ell_i}+\tau_i\varphi_{r_i})S_iS_i - (\varphi_{\ell_i}+\tau_i\varphi_{r_i}) - (\tau_i^*\varphi_{\ell_i}+\varphi_{r_i})\\ &= \sum_i(\tau_i^*\varphi_{\ell_i}+\varphi_{r_i})((S_i^*)^2-1)+(\varphi_{\ell_i}+\tau_i\varphi_{r_i})((S_i)^2-1)\\ &= \sum_i[(\tau_i^*\varphi_{\ell_i}-\varphi_{\ell_i})+(\varphi_{r_i}-\tau_i\varphi_{r_i})]((S_i^*)^2-1)\\ &\quad +(\varphi_{\ell_i}+\tau_i\varphi_{r_i})((S_i^*)^2+S_i^2-2)\\ &= G_{11}+G_{12},\quad \text{where}\end{aligned}$$

$$G_{11} := \sum_i[(\tau_i^*\varphi_{\ell_i}-\varphi_{\ell_i})+(\varphi_{r_i}-\tau_i\varphi_{r_i})]((S_i^*)^2-1)^{(\ddagger_3)}$$

and

$$G_{12} := -2\sum_i(\cosh(\tau_iF-F)-1)\Delta_i(4-\Delta_i).$$

Let $W_{F;i} := \sqrt{\cosh(\tau_iF-F)-1}$. Commuting $W_{F;i}$ with Δ_i gives

$$W_{F;i}\Delta_i = \Delta_iW_{F;i} + S_i\big(W_{F;i}-\tau_i^*W_{F;i}\big) + S_i^*\big(W_{F;i}-\tau_iW_{F;i}\big).$$

Thus

$$W_{F;i}^2\Delta_i(4-\Delta_i) = W_{F;i}\Delta_i(4-\Delta_i)W_{F;i} + R_{F;i},\quad \text{where}$$

$$\begin{aligned}R_{F;i} := &-W_{F;i}\Delta_iS_i\big(W_{F;i}-\tau_i^*W_{F;i}\big) - W_{F;i}\Delta_iS_i^*\big(W_{F;i}-\tau_iW_{F;i}\big)\\ &+W_{F;i}S_i\big(W_{F;i}-\tau_i^*W_{F;i}\big)(4-\Delta_i)+W_{F;i}S_i^*\big(W_{F;i}-\tau_iW_{F;i}\big)(4-\Delta_i)^{\ddagger_5}.\end{aligned}$$

A final accounting job gives the expression of $\mathcal{G}$:

$$\begin{aligned}\mathcal{G} := &\ G_{r;1}+G_{\ell;1}+G_{1;1}+G_{2;1}+G_{3;1}+G_{3;3}+(G_{1;2}+G_{4;1})\\ &+G_7+(G_{2;2}+G_{5;1})+G_9+(G_{3;2}+G_{6;1})+G_{11}-2\sum_i R_{F;i},\end{aligned}\tag{6.11}$$

or equivalently, $\mathcal{G} = G_r + G_\ell + 2\sum_i W_{F;i}\Delta_i(4-\Delta_i)W_{F;i}$. □

* * *

We now turn to the proof of relation (5.3) that is key in Proposition 5.1. Here $d = 1$. For convenience we rewrite the relation we want to show. For $\phi \in \ell_0(\mathbb{Z})$, $\phi_F := e^F \phi$:

$$\langle \phi, [e^F A' e^F, \Delta]\phi \rangle = \langle \phi_F, [A', \Delta]\phi_F \rangle - \big\| \sqrt{g_r - g_\ell} A' \phi_F \big\|^2 - \big\| \sqrt{\Delta(4-\Delta)} W \phi_F \big\|^2 + 2^{-1}\langle \phi_F, (M+G)\phi_F \rangle, \quad \text{where} \tag{6.12}$$

$$W = W_F := \sqrt{\cosh(\tau F - F) - 1}, \tag{6.13}$$

$$M = M_F := 2^{-1}(S^* + S)(g_r - g_\ell)(S^* + S) + \big[(\tau^*\varphi_\ell - \varphi_\ell) + (\varphi_\ell - \tau\varphi_\ell) + (\tau\varphi_r - \varphi_r) + (\varphi_r - \tau^*\varphi_r)\big], \quad \text{and} \tag{6.14}$$

(6.15)

$$\begin{aligned} G = G_F := {} & A'S(\tau^*\varphi_r - \varphi_r) + (\varphi_r - \tau^*\varphi_r)S^*A' + A'S^*(\tau\varphi_\ell - \varphi_\ell) + (\varphi_\ell - \tau\varphi_\ell)SA' \\ & + \big[(\tau^*\varphi_\ell - \tau^{*2}\varphi_\ell) + (\varphi_r - \tau^*\varphi_r)\big] N S^{*2} + \big[(\tau^2\varphi_r - \tau\varphi_r) + (\tau\varphi_\ell - \varphi_\ell)\big] N S^2 \\ & + \frac{1}{2}\big[(\tau^*\varphi_\ell - \tau^{*2}\varphi_\ell) + (\varphi_r - \tau^*\varphi_r)\big](S^*)^2 + \frac{1}{2}\big[(\tau\varphi_r - \tau^2\varphi_r) + (\varphi_\ell - \tau\varphi_\ell)\big] S^2 \\ & + 2\big[(\varphi_\ell - \tau^*\varphi_\ell) + (\tau\varphi_r - \varphi_r)\big] N + \big[(\tau^*\varphi_\ell - \varphi_\ell) + (\varphi_r - \tau\varphi_r)\big]((S^*)^2 - 1) \\ & + 2W_F \Delta S\big(W_F - W_{\tau^* F}\big) + 2W_F \Delta S^*\big(W_F - W_{\tau F}\big) \\ & - 2W_F S\big(W_F - W_{\tau^* F}\big)(4 - \Delta) - 2W_F S^*\big(W_F - W_{\tau F}\big)(4 - \Delta). \end{aligned}$$

Proof of (6.12). For the most part, the proof of this relation is the same as that of (6.1) when $d \geqslant 1$. However, the main difference is that here we do not introduce the function $g(n) := F'(\langle n \rangle)/\langle n \rangle$. We go over the proof done just above and point out the differences. As before we start with

$$[e^F A' e^F, \Delta] = e^F [A', \Delta] e^F + e^F A' [e^F, \Delta] + [e^F, \Delta] A' e^F$$

and develop the last two terms of this relation.

Part 1 : Creating $e^F A' g_r A' e^F$.

$$[e^F, \Delta] = g_r A' e^F - \frac{1}{2} g_r (S^* + S) e^F + \varphi_r \mathbf{1}_{\{n=0\}} (S^* - S) e^F + \varphi_r [e^F, (S^* - S)] + \big(\varphi_r + \varphi_\ell\big) e^F S.$$

$$[e^F, \Delta] = e^F A' g_r + \frac{1}{2} e^F (S^* + S) g_r + e^F (S^* - S) \varphi_r \mathbf{1}_{\{n=0\}} - [e^F, (S^* - S)]\varphi_r - S^* e^F \big(\varphi_r + \varphi_\ell\big).$$

Therefore we have obtained

$$e^F A' [e^F, \Delta] + [e^F, \Delta] A' e^F = 2 e^F A' g_r A' e^F + e^F (M_r + G_r + H_r) e^F, \quad \text{where} \tag{6.16}$$

$$M_r := -2^{-1} A' g_r (S^* + S) + 2^{-1} (S^* + S) g_r A',$$

$$\begin{aligned} G_r := {} & A' \varphi_r [e^F, (S^* - S)] e^{-F} + A' \big(\varphi_r + \varphi_\ell\big) e^F S e^{-F} \\ & - e^{-F} [e^F, (S^* - S)] \varphi_r A' - e^{-F} S^* e^F \big(\varphi_r + \varphi_\ell\big) A', \quad \text{and} \end{aligned}$$

$$H_r := A' \varphi_r \mathbf{1}_{\{n=0\}} (S^* - S) + (S^* - S) \varphi_r \mathbf{1}_{\{n=0\}} A'.$$

We calculate M_r:

$$\begin{aligned} M_r &= -\frac{1}{2}\left(-\frac{1}{2}(S^*+S)+(S^*-S)N\right)g_r(S^*+S)+\frac{1}{2}(S^*+S)\,g_r\left(\frac{1}{2}(S^*+S)+N(S^*-S)\right)\\ &= 2^{-1}(S^*+S)g_r(S^*+S)-2^{-1}(S^*-S)\,\varphi_r\mathbf{1}_{\{n\neq 0\}}(S^*+S)\\ &\quad+2^{-1}(S^*+S)\,\varphi_r\mathbf{1}_{\{n\neq 0\}}(S^*-S)\\ &= 2^{-1}(S^*+S)g_r(S^*+S)+(S\varphi_rS^*-S^*\varphi_rS)+\big(S^*\varphi_r\mathbf{1}_{\{n=0\}}S-S\varphi_r\mathbf{1}_{\{n=0\}}S^*\big)\\ &= M_{r;1}+M_{r;2},\quad \text{where} \end{aligned}$$

$M_{r;1} := 2^{-1}(S^*+S)g_r(S^*+S)+\big[(\tau\varphi_r-\varphi_r)+(\varphi_r-\tau^*\varphi_r)\big]$ and $M_{r;2} := \varphi_r(0)\left(\mathbf{1}_{\{n=-1\}}-\mathbf{1}_{\{n=1\}}\right)$.

Part 2 : Creating $e^FA'g_\ell A'e^F$.

$$[e^F,\Delta]=-g_\ell A'e^F+\frac{1}{2}g_\ell(S^*+S)e^F-\varphi_\ell\mathbf{1}_{\{n=0\}}(S^*-S)e^F-\varphi_\ell[e^F,(S^*-S)]+\big(\varphi_r+\varphi_\ell\big)e^FS^*.$$

$$[e^F,\Delta]=-e^FA'g_\ell-\frac{1}{2}e^F(S^*+S)g_\ell-e^F(S^*-S)\varphi_\ell\mathbf{1}_{\{n=0\}}-[(S^*-S),e^F]\varphi_\ell-Se^F\big(\varphi_r+\varphi_\ell\big).$$

Therefore we have obtained

$$e^FA'[e^F,\Delta]+[e^F,\Delta]A'e^F=-2e^FA'g_\ell A'e^F+e^F(M_\ell+G_\ell+H_\ell)e^F,\quad \text{where} \tag{6.17}$$

$$M_\ell := 2^{-1}A'g_\ell(S^*+S)-2^{-1}(S^*+S)g_\ell A',$$

$$\begin{aligned} G_\ell &:= -A'\varphi_\ell[e^F,(S^*-S)]e^{-F}+A'\big(\varphi_r+\varphi_\ell\big)e^FS^*e^{-F}\\ &\quad+e^{-F}[e^F,(S^*-S)]\varphi_\ell A'-e^{-F}Se^F\big(\varphi_r+\varphi_\ell\big)A',\quad \text{and} \end{aligned}$$

$$H_\ell := -A'\varphi_\ell\mathbf{1}_{\{n=0\}}(S^*-S)-(S^*-S)\varphi_\ell\mathbf{1}_{\{n=0\}}A'.$$

We calculate M_ℓ:

$$M_\ell = M_{\ell;1}+M_{\ell;2},\quad \text{where}$$

$M_{\ell;1} := -2^{-1}(S^*+S)g_\ell(S^*+S)+\big[(\tau^*\varphi_\ell-\varphi_\ell)+(\varphi_\ell-\tau\varphi_\ell)\big]$ and $M_{\ell;2} := \varphi_\ell(0)\left(\mathbf{1}_{\{n=1\}}-\mathbf{1}_{\{n=-1\}}\right)$.

Part 3 : Adding the terms of Parts 1 and 2. Take the average of (6.16) and (6.17) to get :

$$[e^FA'e^F,\Delta]=e^F[A',\Delta]e^F+e^FA'(g_r-g_\ell)A'e^F+2^{-1}e^F\left(M_r+M_\ell+G_r+G_\ell+H_r+H_\ell\right)e^F.$$

Applying $\phi\in\ell_0(\mathbb{Z})$ to this equation and taking inner products will yield (6.12). Let us elaborate exactly how this is achieved. First, let

$$M := M_r+M_\ell = M_{r;1}+M_{\ell;1}.$$

The latter equality holds because $(M_{r;2}+M_{\ell;2})\phi=0$. Second, note that G_r, G_ℓ, H_r and H_ℓ are exactly the same as in the preceding proof when $i=j=1$, which corresponds to $d=1$. These terms are handled in the same way. In particular $(H_r+H_\ell)\phi=0$. Finally, we investigate G. Referring to the preceding proof with $i=j=1$, let

$$G := G_{r;1}+G_{\ell;1}+G_{1;1}+G_{2;1}+G_{3;3}+G_7+G_9+G_{11}-2R_{F;1}.$$

Terms that do not contribute here are: $G_{3;1}$, $G_{1;2}+G_{4;1}$, $G_{2;2}+G_{5;1}$, $G_{3;2}+G_{6;1}$. We warn the careful reader that G is not simply G_r+G_ℓ, because somewhere hidden in $G_{r;2}+G_{\ell;2}$ is the term $-2W\Delta(4-\Delta)W$ which needs to be extracted. After taking inner products, this term ultimately produces $-\|\sqrt{\Delta(4-\Delta)}W\phi_F\|^2$. Alternatively, $G = G_r + G_\ell + 2W\Delta(4-\Delta)W$. □

We also note that

(6.18)
$$\begin{aligned}G_r + G_\ell &= G_{r;1} + G_{\ell;1} + G_{1;1} + G_{2;1} + G_{3;3} + G_7 + G_9 + G_{11} + G_{12}\\ &= 2\big[(\tau^*\varphi_\ell - \tau^{*2}\varphi_\ell) + (\varphi_r - \tau^*\varphi_r)\big]NS^{*2} - 2\big[(\tau\varphi_r - \tau^2\varphi_r) + (\varphi_\ell - \tau\varphi_\ell)\big]NS^2\\ &\quad + 2\big[(\varphi_\ell - \tau\varphi_\ell) + (\tau^*\varphi_r - \varphi_r) + (\varphi_\ell - \tau^*\varphi_\ell) + (\tau\varphi_r - \varphi_r)\big]N\\ &\quad + \big[(\tau^*\varphi_\ell - \tau^{*2}\varphi_\ell) + 2(\varphi_r - \tau^*\varphi_r)\big]S^{*2} + \big[(\tau\varphi_r - \tau^2\varphi_r) + 2(\varphi_\ell - \tau\varphi_\ell)\big]S^2\\ &\quad + \big[(\tau\varphi_\ell - \varphi_\ell) + (\tau^*\varphi_r - \varphi_r)\big] + \big[(\tau^*\varphi_\ell - \varphi_\ell) + (\varphi_r - \tau\varphi_r)\big](S^{*2} - 1)\\ &\quad - 2(\cosh(\tau F - F) - 1)\Delta(4-\Delta).\end{aligned}$$

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PROPAGATION ESTIMATES FOR ONE COMMUTATOR REGULARITY

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ABSTRACT. In the abstract framework of Mourre theory, the propagation of states is understood in terms of a conjugate operator A. A powerful estimate has long been known for Hamiltonians having a good regularity with respect to A thanks to the limiting absorption principle (LAP). We study the case where H has less regularity with respect to A, specifically in a situation where the LAP and the absence of singularly continuous spectrum have not yet been established. We show that in this case the spectral measure of H is a Rajchman measure and we derive some propagation estimates. One estimate is an application of minimal escape velocities, while the other estimate relies on an improved version of the RAGE formula. Based on several examples, including continuous and discrete Schrödinger operators, it appears that the latter propagation estimate is a new result for multi-dimensional Hamiltonians.

1. INTRODUCTION

In quantum mechanics one is often interested in knowing the long-time behavior of a given state of a system. It is well-known that there exist states that to tend to remain localized in a region of space, called *bound* states, while there are states that tend to drift away from all bounded regions of space, called *scattering* states. The present article is concerned with the study of the latter. In particular, a propagation estimate is derived and serves to rigorously describe the long-time propagation, or behavior of these states. A classical way of obtaining a propagation estimate is by means of some resolvent estimates, or a Limiting Absorption Principle (LAP). The LAP is a powerful weighted estimate of the resolvent of an operator which implies a propagation estimate for scattering states as well as the absence of singular continuous spectrum for the system.

The theory of Mourre was introduced by E. Mourre in [M] and aims at showing a LAP. Among others, we refer to [CGH, FH, GGM, HS1, JMP, S, G, GJ1] and to the book [ABG] for the development of the theory. In a nutshell, Mourre theory studies the properties of a self-adjoint operator H, the Hamiltonian of the system, with the help of another self-adjoint operator A, referred to as a *conjugate operator* to H. The standard Mourre theory relies on three hypotheses on the commutator of H and A which are, loosely speaking, that

(M1) $[H, \mathrm{i}A]$ be positive,
(M2) $[H, \mathrm{i}A]$ be H-bounded,
(M3) $[[H, \mathrm{i}A], \mathrm{i}A]$ be H-bounded.

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The main theory goes as follows:

$$\underbrace{(\mathrm{M1}) + (\mathrm{M2})} + (\mathrm{M3}) \Longrightarrow \text{Resolvent estimates (LAP)} \Longrightarrow \text{Propagation estimates}$$

$$\Downarrow \qquad\qquad\qquad\qquad\qquad\qquad \Longrightarrow \text{No singular continuous spectrum.}$$

Absence of eigenvalues.

The purpose of the paper is to show that (M1) + (M2') $\Longrightarrow$ Weaker propagation estimates, where (M2') is slightly stronger than (M2).

We set up notation and basic notions. For arbitrary Hilbert spaces $\mathcal{F}$ and $\mathcal{G}$, denote the bounded operators from $\mathcal{F}$ to $\mathcal{G}$ by $\mathcal{B}(\mathcal{F},\mathcal{G})$ and the compact operators from $\mathcal{F}$ to $\mathcal{G}$ by $\mathcal{K}(\mathcal{F},\mathcal{G})$. When $\mathcal{F} = \mathcal{G}$, we shall abbreviate $\mathcal{B}(\mathcal{G}) := \mathcal{B}(\mathcal{G},\mathcal{G})$ and $\mathcal{K}(\mathcal{G}) := \mathcal{K}(\mathcal{G},\mathcal{G})$. When $\mathcal{G} \subset \mathcal{H}$, denote $\mathcal{G}^*$ the antidual of $\mathcal{G}$, when we identify $\mathcal{H}$ to its antidual $\mathcal{H}^*$ by the Riesz isomorphism Theorem. Fix self-adjoint operators H and A on a separable complex Hilbert space $\mathcal{H}$, with domains $\mathcal{D}(H)$ and $\mathcal{D}(A)$ respectively. In Mourre theory, regularity classes are defined and serve to describe the level of regularity that A has with respect to H. The most important of these classes are defined in Section 2, but we mention that they are typically distinct in applications and always satisfy the following inclusions

$$\mathcal{C}^2(A) \subset \mathcal{C}^{1,1}(A) \subset \mathcal{C}^{1,\mathrm{u}}(A) \subset \mathcal{C}^1(A). \tag{1.1}$$

Of these, $\mathcal{C}^1(A)$ is the class with the least regularity, whereas $\mathcal{C}^2(A)$ is the class with the strongest regularity. Indeed if $H \in \mathcal{C}^1(A)$, then the commutator $[H, \mathrm{i}A]$ extends to an operator in $\mathcal{B}(\mathcal{D}(H), \mathcal{D}(H)^*)$ and is denoted $[H, \mathrm{i}A]_\circ$; whereas if $H \in \mathcal{C}^2(A)$, then in addition the iterated commutator $[[H, \mathrm{i}A], \mathrm{i}A]$ extends to an operator in $\mathcal{B}(\mathcal{D}(H), \mathcal{D}(H)^*)$ and is denoted by $[[H, \mathrm{i}A]_\circ, \mathrm{i}A]_\circ$ (see Section 2). As the $\mathcal{C}^{1,\mathrm{u}}(A)$ class plays a key role in this article we recall here its definition. We say that H belongs to the $\mathcal{C}^{1,\mathrm{u}}(A)$ class if the map $t \mapsto e^{-\mathrm{i}tA}(H+\mathrm{i})^{-1}e^{\mathrm{i}tA}$ is of class $\mathcal{C}^1(\mathbb{R}; \mathcal{B}(\mathcal{H}))$, with $\mathcal{B}(\mathcal{H})$ endowed with the norm operator topology. The standard example of operators belonging to the aforementioned classes is the following.

Example 1.1 (Continuous Schrödinger operators)**.** *Let H_0 be the self-adjoint realization of the Laplace operator $-\Delta$ in $L^2(\mathbb{R}^d)$. Let Q be the operator of multiplication by $x = (x_1, ..., x_d) \in \mathbb{R}^d$, and let $P := -\mathrm{i}\nabla$. Set*

$$H := H_0 + V_{\mathrm{sr}}(Q) + V_{\mathrm{lr}}(Q),$$

where $V_{\mathrm{sr}}(x)$ and $V_{\mathrm{lr}}(x)$ are real-valued functions that belong to $L^\infty(\mathbb{R}^d)$. Thus $V_{\mathrm{sr}}(Q)$ and $V_{\mathrm{lr}}(Q)$ are bounded self-adjoint operators on $L^2(\mathbb{R}^d)$ and they are respectively the short- and long-range perturbations. Suppose that $\lim V_{\mathrm{sr}}(x) = \lim V_{\mathrm{lr}}(x) = 0$ *as $\|x\| \to +\infty$. Then $V_{\mathrm{sr}}(Q)$ and $V_{\mathrm{lr}}(Q)$ are H_0-form relatively compact operators. This notably implies that $\sigma_{\mathrm{ess}}(H) = [0, +\infty)$ by the Theorem of Weyl on relative compactness. Let $A := (Q \cdot P + P \cdot Q)/2$ be the so-called generator of dilations. It is the standard conjugate operator to H. For the long-range perturbation, further assume that $x \cdot \nabla V_{\mathrm{lr}}(x)$ is a well-defined function. Table 1 displays Hamiltonians belonging to each of the classes introduced in (1.1). The idea is clear: stronger decaying bounds on the potential imply stronger regularity. We study this example in Section 4 and prove the information reported in Table 1.*

Let $E_{\mathcal{I}}(H)$ be the spectral projector of H on a bounded interval $\mathcal{I} \subset \mathbb{R}$. Assuming $H \in \mathcal{C}^1(A)$, we say that the *Mourre estimate* holds for H on $\mathcal{I}$ if there is $c > 0$ and $K \in \mathcal{K}(\mathcal{H})$ such that

$$E_{\mathcal{I}}(H)[H, \mathrm{i}A]_\circ E_{\mathcal{I}}(H) \geqslant cE_{\mathcal{I}}(H) + K, \tag{1.2}$$

In addition, if $\langle x\rangle V_{\rm sr}(x)$ *and* $x\cdot\nabla V_{\rm lr}(x)$ *are*	*Then* H *belongs to*
$L^\infty(\mathbb{R}^d)$	$\mathcal{C}^1(A)$
$L^\infty(\mathbb{R}^d)$ *and* $o(1)$	$\mathcal{C}^{1,\mathrm{u}}(A)$
$L^\infty(\mathbb{R}^d)$ *and* $o(\langle x\rangle^{-\varepsilon})$*, for some* $\varepsilon>0$	$\mathcal{C}^{1,1}(A)$
$L^\infty(\mathbb{R}^d)$ *and* $O(\langle x\rangle^{-1})$	$\mathcal{C}^2(A)$

Table 1. Regularity of Hamiltonian H w.r.t. a bound on the decay of the potential at infinity

in the form sense on $\mathcal{H}\times\mathcal{H}$. The Mourre estimate (1.2) is the precise formulation of the positivity assumption (M1) alluded to at the very beginning. The Mourre estimate is localized in energy, hence it allows to infer information about the system at specific energies. Let $\mu^A(H)$ be the set of points where a Mourre estimate holds for H, i.e.

$$\mu^A(H):=\{\lambda\in\mathbb{R}:\exists c>0, K\in\mathcal{K}(\mathcal{H})\text{ and }\mathcal{I}\text{ open for which (1.2) holds for }H\text{ on }\mathcal{I}\text{ and }\lambda\in\mathcal{I}\},$$

In [M], Mourre assumes roughly $H\in\mathcal{C}^2(A)$ and the estimate (1.2) with $K=0$ to prove the following LAP on any compact sub-interval $\mathcal{J}\subset\mathcal{I}$:

$$\sup_{x\in\mathcal{J},\ y>0}\|\langle A\rangle^{-s}(H-x-\mathrm{i}y)^{-1}\langle A\rangle^{-s}\|<+\infty, \tag{1.3}$$

for all $s>1/2$. Here $\langle A\rangle:=\sqrt{1+A^2}$. We remark that if the Mourre estimate holds on $\mathcal{I}$ with $K=0$, then $\mathcal{I}$ is void of eigenvalues, as a result of the Virial Theorem [ABG, Proposition 7.2.10]. Estimate (1.3) can be shown to yield the following Kato-type propagation estimate:

$$\sup_{\substack{\psi\in\mathcal{H}\\ \|\psi\|\leqslant 1}}\int_{-\infty}^{\infty}\|\langle A\rangle^{-s}e^{-\mathrm{i}tH}E_{\mathcal{J}}(H)\psi\|^2dt<+\infty, \tag{1.4}$$

which in turn implies the absence of singular continuous spectrum on $\mathcal{J}$, e.g. [RS4, Section XIII.7]. The main improvement of this result is done in [ABG]. The same LAP is derived assuming only $H\in\mathcal{C}^{1,1}(A)$ and the estimate (1.2). It is further shown that this class is optimal in the general abstract framework. Precisely in [ABG, Appendix 7.B], there is an example of $H\in\mathcal{C}^{1,\mathrm{u}}(A)$ for which no LAP holds. However, other types of propagation estimates were subsequently derived for $H\in\mathcal{C}^{1,\mathrm{u}}(A)$, see [HSS, Ri] for instance. One major motivation for wanting to obtain dynamical estimates for this class was (and still is) to have a better understanding of the nature of the continuous spectrum of H. The aim of this article is to provide new propagation estimates for this class of operators. We also provide a simple criterion to check if an operator belongs to the $\mathcal{C}^{1,\mathrm{u}}(A)$ class.

Let $P_{\mathrm{c}}(H)$ and $P_{\mathrm{ac}}(H)$ respectively denote the spectral projectors onto the continuous and absolutely continuous subspaces of H. Our first result is the following:

Theorem 1.2. *Let H and A be self-adjoint operators in a separable Hilbert space $\mathcal{H}$ with $H\in\mathcal{C}^{1,\mathrm{u}}(A)$. Assume that $\mathcal{I}\subset\mathbb{R}$ is a compact interval for which $\lambda\in\mu^A(H)$ for all $\lambda\in\mathcal{I}$. Suppose moreover that $\ker(H-\lambda)\subset\mathcal{D}(A)$ for all $\lambda\in\mathcal{I}$. Then for all $\psi\in\mathcal{H}$ and all $s>0$,*

$$\lim_{t\to+\infty}\|\langle A\rangle^{-s}e^{-\mathrm{i}tH}P_{\mathrm{c}}(H)E_{\mathcal{I}}(H)\psi\|=0. \tag{1.5}$$

Moreover, if W is H-relatively compact, then

$$\lim_{t\to+\infty}\|We^{-\mathrm{i}tH}P_{\mathrm{c}}(H)E_{\mathcal{I}}(H)\psi\|=0. \tag{1.6}$$

In particular, if H has no eigenvalues in $\mathcal{I}$ and $\psi \in \mathcal{H}$, then the spectral measure $\Omega \mapsto \langle \psi, E_{\Omega \cap \mathcal{I}}(H)\psi \rangle$ is a Rajchman measure, i.e., its Fourier transform tends to zero at infinity.

Remark 1.1. *The last part of the Theorem follows by taking $W = \langle \psi, \cdot \rangle \psi$. If H has no eigenvalues in $\mathcal{I}$, then $P_{\mathrm{c}}(H)E_{\mathcal{I}}(H) = E_{\mathcal{I}}(H)$ and so by the Spectral Theorem,*

$$We^{-\mathrm{i}tH}P_{\mathrm{c}}(H)E_{\mathcal{I}}(H)\psi = \psi \times \langle \psi, e^{-\mathrm{i}tH}E_{\mathcal{I}}(H)\psi \rangle = \psi \times \int_{\mathbb{R}} e^{-\mathrm{i}tx} d\mu_{(\psi, E_{\mathcal{I}}(H)\psi)}(x).$$

The spectral measure μ satisfies $\Omega \mapsto \mu_{(\psi, E_{\mathcal{I}}(H)\psi)}(\Omega) = \langle \psi, E_{\Omega}(H)E_{\mathcal{I}}(H)\psi \rangle = \langle \psi, E_{\Omega \cap \mathcal{I}}(H)\psi \rangle$.

Remark 1.2. *The separability condition on the Hilbert space is used for the proof of (1.6), because the compact operator W is approximated in norm by finite rank operators.*

Remark 1.3. *Perhaps a few words about the condition $\ker(H - \lambda) \subset \mathcal{D}(A)$. In general, it is satisfied if H has a high regularity with respect to A. Although in the present framework it is not granted, it can be valid even if $H \in \mathcal{C}^1(A)$ only, as seen in [JM].*

This result is new to us. However, it is not strong enough to imply the absence of singular continuous spectrum for H. Indeed, there exist Rajchman measures whose support is a set of Hausdorff dimension zero, see [B]. We refer to [L] for a review of Rajchman measures. The proof of this result is an application of the minimal escape velocities obtained in [Ri]. The latter is a continuation of [HSS]. We refer to those articles for historical references.

We have several comments to do concerning the various propagation estimates listed above. First, it appears in practice that $\langle A \rangle^{-s}E_{\mathcal{I}}(H)$ is not always a compact operator, and so (1.5) is not a particular case of (1.6). The compactness issue of $\langle A \rangle^{-s}E_{\mathcal{I}}(H)$ is discussed in Section 7, where we study several examples including continuous and discrete Schrödinger operators. In all of these examples, it appears that $\langle A \rangle^{-s}E_{\mathcal{I}}(H)$ is compact in dimension one, but not in higher dimensions. Second, note that (1.4) implies (1.5). Indeed, the integrand of (1.4) is a $L^1(\mathbb{R})$ function with bounded derivative (and hence uniformly continuous on $\mathbb{R}$). Such functions must go to zero at infinity. On the other hand, it is an open question to know if (1.4) is true when $H \in \mathcal{C}^{1,\mathrm{u}}(A)$. Third, we point out that (1.6) is a consequence of the Riemann-Lebesgue Lemma (see (1.10) below) when $\psi = P_{\mathrm{ac}}(H)\psi$. This can be seen by writing the state in (1.6) as $W(H+\mathrm{i})^{-1}e^{-\mathrm{i}tH}P_{\mathrm{c}}(H)E_{\mathcal{I}}(H)(H+\mathrm{i})\psi$ and noting that $W(H+\mathrm{i})^{-1} \in \mathcal{K}(\mathcal{H})$ and $E_{\mathcal{I}}(H)(H+\mathrm{i}) \in \mathcal{B}(\mathcal{H})$.

Propagation estimates (1.5) and (1.6) cannot hold uniformly on the unit sphere of states in $\mathcal{H}$, for if they did, they would imply that the norm of a time-constant operator goes to zero as t goes to infinity. Moving forward, we seek a propagation estimate uniform on the unit sphere and go deeper into the hypotheses. Let $\mathcal{H}$ be a Hilbert space. Let H_0 be a self-adjoint operator on $\mathcal{H}$, with domain $\mathcal{D}(H_0)$. We use standard notation and set $\mathcal{H}^2 := \mathcal{D}(H_0)$ and $\mathcal{H}^1 := \mathcal{D}(\langle H_0 \rangle^{1/2})$, the form domain of H_0. Also, $\mathcal{H}^{-2} := \mathcal{D}(H_0)^*$, and $\mathcal{H}^{-1} := \mathcal{D}(\langle H_0 \rangle^{1/2})^*$. The following continuous and dense embeddings hold:

$$\mathcal{H}^2 \subset \mathcal{H}^1 \subset \mathcal{H} = \mathcal{H}^* \subset \mathcal{H}^{-1} \subset \mathcal{H}^{-2}. \tag{1.7}$$

These are Hilbert spaces with the appropriate graph norms. We split the assumptions into two categories: the spectral and the regularity assumptions. We start with the former.

Spectral Assumptions:

- A1 : H_0 is a semi-bounded operator with form domain $\mathcal{H}^1$.
- A2 : V defines a symmetric quadratic form on $\mathcal{H}^1$.
- A3 : $V \in \mathcal{K}(\mathcal{H}^1, \mathcal{H}^{-1})$.

Importantly, these assumptions allow us to define the perturbed Hamiltonian H. Indeed, A1 - A3 imply, by the KLMN Theorem ([RS2, Theorem X.17]), that $H := H_0 + V$ in the form sense is a semi-bounded self-adjoint operator with domain $\mathcal{D}(\langle H\rangle^{1/2}) = \mathcal{H}^1$. Furthermore, we have by Weyl's Theorem that $\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(H_0)$.

Before proceeding with the other assumptions, let us take a moment to recall two well-known propagation estimates that typically hold under these few assumptions. The first estimate is the RAGE Theorem due to Ruelle [Ru], Amrein and Georgescu [AG] and Enss [E]. It states that for any self-adjoint operator H and any $W \in \mathcal{B}(\mathcal{H})$ that is H-relatively compact, and any $\psi \in \mathcal{H}$,

$$\lim_{T\to\pm\infty} \frac{1}{T} \int_0^T \|W P_{\text{c}}(H) e^{-\text{i}tH}\psi\|^2 dt = 0. \tag{1.8}$$

We refer to the appendix B for an observation on this Theorem. Let us go back to Example 1.1, the case of the Schrödinger operators. Assuming only that the short- and long-range potentials be bounded and go to zero at infinity, we see that A1 - A3 hold. Thus $H := H_0 + V_{\text{sr}}(Q) + V_{\text{lr}}(Q)$ is self-adjoint. Moreover $\mathbf{1}_\Sigma(Q)$ is a bounded operator that is H-relatively compact whenever $\Sigma \subset \mathbb{R}^d$ is a compact set. Hence, in this example, the above spectral assumptions and the RAGE Theorem combine to yield the following very meaningful propagation estimate:

$$\lim_{T\to\pm\infty} \frac{1}{T} \int_0^T \|\mathbf{1}_\Sigma(Q) P_{\text{c}}(H) e^{-\text{i}tH}\psi\|^2 dt = 0. \tag{1.9}$$

In words, the scattering state $P_{\text{c}}(H)\psi$ escapes all compact sets averagely in time. The second standard estimate we wish to recall is the Riemann-Lebesgue Lemma, see e.g. [RS3, Lemma 2]. It states that for any self-adjoint operator H and any $W \in \mathcal{B}(\mathcal{H})$ that is H-relatively compact, and any $\psi \in \mathcal{H}$,

$$\lim_{t\to\pm\infty} \|W P_{\text{ac}}(H) e^{-\text{i}tH}\psi\| = 0. \tag{1.10}$$

In particular, this estimate implies that the Fourier transform of the spectral measure

$$\Omega \mapsto \langle \psi, E_\Omega(H) P_{\text{ac}}(H)\psi\rangle = \mu_{(\psi, P_{\text{ac}}(H)\psi)}(\Omega)$$

goes to zero at infinity, i.e.

$$\int_{\mathbb{R}} e^{-\text{i}tx} d\mu_{(\psi, P_{\text{ac}}(H)\psi)}(x) \to 0 \quad \text{as} \quad t \to \pm\infty.$$

Applying the Riemann-Lebesgue Lemma to Example 1.1 gives for all compact sets $\Sigma \subset \mathbb{R}^d$,

$$\lim_{t\to\pm\infty} \|\mathbf{1}_\Sigma(Q) P_{\text{ac}}(H) e^{-\text{i}tH}\psi\| = 0. \tag{1.11}$$

Thus, the scattering state $P_{\text{ac}}(H)\psi$ escapes all compact sets in the long run. In contrast, a basic argument such as the one given in the Appendix A as well as estimates like (1.4) or (1.5) indicate that the scattering states tend to concentrate in regions where the conjugate operator A is prevalent. We continue with the assumptions concerning the operator H.

Regularity Assumptions: There is a self-adjoint operator A on $\mathcal{H}$ such that

- A4 : $e^{\text{i}tA}\mathcal{H}^1 \subset \mathcal{H}^1$ for all $t \in \mathbb{R}$.

- A5 : $H_0 \in \mathcal{C}^2(A; \mathcal{H}^1, \mathcal{H}^{-1})$.
- A6 : $V \in \mathcal{C}^{1,\mathrm{u}}(A; \mathcal{H}^1, \mathcal{H}^{-1})$.
- A6′ : $V \in \mathcal{C}^1(A; \mathcal{H}^1, \mathcal{H}^{-1})$ and $[V, \mathrm{i}A]_\circ \in \mathcal{K}(\mathcal{H}^1, \mathcal{H}^{-1})$.

First we note that $\mathcal{C}^\sharp(A; \mathcal{H}^1, \mathcal{H}^{-1}) \subset \mathcal{C}^\sharp(A)$ for $\sharp \in \{1; 1,\mathrm{u}; 2\}$. We refer to Section 2 for a complete description of these classes. While A4 and A5 are standard assumptions to apply Mourre theory, A6 is significantly weaker. It causes H to have no more than the $\mathcal{C}^{1,\mathrm{u}}(A; \mathcal{H}^1, \mathcal{H}^{-1})$ regularity, in which case the LAP is not always true, as mentioned previously. Proposition 2.1 proves the equivalence between A6 and A6′. In many applications, A6′ is more convenient to check than A6.

Let $\mu^A(H_0)$ be the set of points where a Mourre estimate holds for H_0. The assumptions mentioned above imply that $\mu^A(H) = \mu^A(H_0)$, by Lemma 3.3. The uniform propagation estimate derived in this paper is the following:

Theorem 1.3. *Suppose A1 through A6. Let $\lambda \in \mu^A(H)$ be such that $\ker(H - \lambda) \subset \mathcal{D}(A)$. Then there exists a bounded open interval $\mathcal{I}$ containing λ such that for all $s > 1/2$,*

$$\lim_{T \to \pm\infty} \sup_{\substack{\psi \in \mathcal{H} \\ \|\psi\| \leqslant 1}} \frac{1}{T} \int_0^T \|\langle A \rangle^{-s} P_{\mathrm{c}}(H) E_{\mathcal{I}}(H) e^{-\mathrm{i}tH} \psi\|^2 \, dt = 0. \tag{1.12}$$

This formula is to be compared with (1.4), (1.5) and (1.8). First note that (1.4) implies (1.12). Also, on the one hand, (1.12) without the supremum is a trivial consequence of (1.5). On the other hand, if (1.5) held uniformly on the unit sphere, then it would imply (1.12). But we saw that this is not the case. So the main gain in Theorem 1.3 over Theorem 1.2 is the supremum. Let us further comment the supremum in (1.12). This is because one can in fact take the supremum in the RAGE formula, as explained in the Appendix B. The parallel with the RAGE formula (see Theorem B.1) raises an important concern however. The novelty of the propagation estimate (1.12) depends critically on the non-compactness of the operator $\langle A \rangle^{-s} E_{\mathcal{I}}(H)$. As mentioned previously, it appears that $\langle A \rangle^{-s} E_{\mathcal{I}}(H)$ is not always compact. Theorem 1.3 therefore appears to be a new result for multi-dimensional Hamiltonians.

To summarize, the various propagation estimates discussed in the Introduction are listed in Table 2 according to the regularity of the potential V. Sufficient regularity for the free operator H_0 is implicit. In this table, question marks indicate open problems and R.-L. stands for Riemann-Lebesgue.

V is of class	RAGE formula	R.-L. formula	Prop. estimates (1.5) and (1.6)	Prop. estimate (1.12)	Kato - type Prop. estimate	LAP
$\mathcal{C}^1(A)$	✓	✓	?	?	?	?
$\mathcal{C}^{1,\mathrm{u}}(A)$	✓	✓	✓	✓	?	?
$\mathcal{C}^{1,1}(A)$	✓	✓	✓	✓	✓	✓
$\mathcal{C}^2(A)$	✓	✓	✓	✓	✓	✓

TABLE 2. Regularity of Hamiltonian H w.r.t. a bound on the decay of the potential at infinity

We underline that the LAP has been derived for several specific systems where the Hamiltonian H belongs to a regularity class as low as $\mathcal{C}^1(A)$, and sometimes even lower (see for example [DMR], [GJ2], [JM] and [Ma1] to name a few). In all these cases, a strong propagation estimate of type (1.4) and absence of singular continuous spectrum follow. We also note that the derivation of the propagation estimate (1.12) is in fact very similar to the derivation of a weighted Mourre estimate which is used in the proof of a LAP for Hamiltonians with oscillating potentials belonging to the $\mathcal{C}^1(A)$ class, see [G] and [GJ2].

The article is organized as follows: in Section 2, we review the classes of regularity in Mourre theory and in particular prove the equivalence between A6 and A6′. In Section 3, we discuss the Mourre estimate and justify that under the assumptions of Theorem 1.3, H and H_0 share the same set of points where a Mourre estimate holds. In Section 4, we give examples of continuous and discrete Schrödinger operators that fit the assumptions of Theorems 1.2 and 1.3. In Section 5, we prove Theorem 1.2 and in Section 6, we prove Theorem 1.3. In Section 7, we discuss the compactness of the operator $\langle A\rangle^{-s}E_{\mathcal{I}}(H)$. In Appendix A, we provide a simple argument as to why we expect scattering states to evolve in the direction where the conjugate operator prevails. In Appendix B we make the observation that one may in fact take a supremum in the RAGE Theorem. Finally, in Appendix C we review facts about almost analytic extensions of smooth functions that are used in the proof of the uniform propagation estimate.

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2. The classes of regularity in Mourre theory

We define the classes of regularity that were introduced in (1.1). Let $T \in \mathcal{B}(\mathcal{H})$ and A be a self-adjoint operator on the Hilbert space $\mathcal{H}$. Consider the map

$$\mathbb{R} \ni t \mapsto e^{-\mathrm{i}tA}Te^{\mathrm{i}tA} \in \mathcal{B}(\mathcal{H}). \tag{2.1}$$

Let $k \in \mathbb{N}$. If the map is of class $\mathcal{C}^k(\mathbb{R};\mathcal{B}(\mathcal{H}))$, with $\mathcal{B}(\mathcal{H})$ endowed with the strong operator topology, we say that $T \in \mathcal{C}^k(A)$; whereas if the map is of class $\mathcal{C}^k(\mathbb{R};\mathcal{B}(\mathcal{H}))$, with $\mathcal{B}(\mathcal{H})$ endowed with the operator norm topology, we say that $T \in \mathcal{C}^{k,\mathrm{u}}(A)$. Note that $\mathcal{C}^{k,\mathrm{u}}(A) \subset \mathcal{C}^k(A)$ is immediate from the definitions. If $T \in \mathcal{C}^1(A)$, then the derivative of the map (2.1) at $t = 0$ is denoted $[T, \mathrm{i}A]_\circ$ and belongs to $\mathcal{B}(\mathcal{H})$. Also, if $T_1, T_2 \in \mathcal{B}(\mathcal{H})$ belong to the $\mathcal{C}^1(A)$ class, then so do $T_1 + T_2$ and T_1T_2. We say that $T \in \mathcal{C}^{1,1}(A)$ if

$$\int_0^1 \Big\| [[T, e^{\mathrm{i}tA}]_\circ, e^{\mathrm{i}tA}]_\circ \Big\| t^{-2} dt < \infty.$$

The proof that $\mathcal{C}^2(A) \subset \mathcal{C}^{1,1}(A) \subset \mathcal{C}^{1,\mathrm{u}}(A)$ is given in [ABG, Section 5]. This yields (1.1).

Now let T be a self-adjoint operator (possibly unbounded), with spectrum $\sigma(T)$. Let $z \in \mathbb{C} \setminus \sigma(T)$. We say that $T \in \mathcal{C}^\sharp(A)$ if $(z-T)^{-1} \in \mathcal{C}^\sharp(A)$, for $\sharp \in \{k; k,\mathrm{u}; 1,1\}$. This definition does not depend on the choice of $z \in \mathbb{C} \setminus \sigma(T)$, and furthermore if T is bounded and self-adjoint then the two definitions coincide, see [ABG, Lemma 6.2.1]. If $T \in \mathcal{C}^1(A)$, one shows that $[T, \mathrm{i}A]_\circ \in \mathcal{B}(\mathcal{D}(T), \mathcal{D}(T)^*)$ and that the following formula holds:

$$[(z-T)^{-1}, \mathrm{i}A]_\circ = (z-T)^{-1}[T, \mathrm{i}A]_\circ(z-T)^{-1}. \tag{2.2}$$

These definitions can be refined. Let $\mathcal{G}$ and $\mathcal{H}$ be Hilbert spaces verifying the following continuous and dense embeddings $\mathcal{G} \subset \mathcal{H} = \mathcal{H}^* \subset \mathcal{G}^*$, where we have identified $\mathcal{H}$ with its antidual $\mathcal{H}^*$ by the Riesz isomorphism Theorem. Let A be a self-adjoint operator on $\mathcal{H}$, and suppose that the semi-group $\{e^{\mathrm{i}tA}\}_{t\in\mathbb{R}}$ stabilizes $\mathcal{G}$. Then by duality it stabilizes $\mathcal{G}^*$. Let T be a self-adjoint operator on $\mathcal{H}$ belonging to $\mathcal{B}(\mathcal{G},\mathcal{G}^*)$ and consider the map

$$\mathbb{R} \ni t \mapsto e^{-\mathrm{i}tA} T e^{\mathrm{i}tA} \in \mathcal{B}(\mathcal{G},\mathcal{G}^*). \tag{2.3}$$

If this map is of class $\mathcal{C}^k(\mathbb{R};\mathcal{B}(\mathcal{G},\mathcal{G}^*))$, with $\mathcal{B}(\mathcal{G},\mathcal{G}^*)$ endowed with the strong operator topology, we say that $T \in \mathcal{C}^k(A;\mathcal{G},\mathcal{G}^*)$; whereas if the map is of class $\mathcal{C}^k(\mathbb{R};\mathcal{B}(\mathcal{G},\mathcal{G}^*))$, with $\mathcal{B}(\mathcal{G},\mathcal{G}^*)$ endowed with the norm operator topology, we say that $T \in \mathcal{C}^{k,\mathrm{u}}(A;\mathcal{G},\mathcal{G}^*)$. If $T \in \mathcal{C}^1(A;\mathcal{G},\mathcal{G}^*)$, then the derivative of map (2.3) at $t=0$ is denoted by $[T,\mathrm{i}A]_\circ$ and belongs to $\mathcal{B}(\mathcal{G},\mathcal{G}^*)$. Moreover, by [ABG, Proposition 5.1.6], $T \in \mathcal{C}^\sharp(A;\mathcal{G},\mathcal{G}^*)$ if and only if $(z-T)^{-1} \in \mathcal{C}^\sharp(A;\mathcal{G}^*,\mathcal{G})$ for all $z \in \mathbb{C}\setminus\sigma(T)$ and $\sharp \in \{k;k,\mathrm{u}\}$. This notably implies that $\mathcal{C}^\sharp(A;\mathcal{G},\mathcal{G}^*) \subset \mathcal{C}^\sharp(A)$.

In the setting of Theorem 1.3, $\mathcal{G} = \mathcal{H}^1 := \mathcal{D}(\langle H_0\rangle^{1/2})$, and T stands for H_0, V or H. In all cases $T \in \mathcal{B}(\mathcal{H}^1,\mathcal{H}^{-1})$. We also assume that $\{e^{\mathrm{i}tA}\}_{t\in\mathbb{R}}$ stabilizes $\mathcal{H}^1$, see A4. Consider the map

$$\mathbb{R} \ni t \mapsto \langle H_0\rangle^{-1/2} e^{-\mathrm{i}tA} T e^{\mathrm{i}tA} \langle H_0\rangle^{-1/2} \in \mathcal{B}(\mathcal{H}). \tag{2.4}$$

The latter operator belongs indeed to $\mathcal{B}(\mathcal{H})$ since the domains concatenate as follows:

$$\underbrace{\langle H_0\rangle^{-1/2}}_{\in\mathcal{B}(\mathcal{H}^{-1},\mathcal{H})} \underbrace{e^{-\mathrm{i}tA}}_{\in\mathcal{B}(\mathcal{H}^{-1},\mathcal{H}^{-1})} \underbrace{T}_{\in\mathcal{B}(\mathcal{H}^{1},\mathcal{H}^{-1})} \underbrace{e^{\mathrm{i}tA}}_{\in\mathcal{B}(\mathcal{H}^{1},\mathcal{H}^{1})} \underbrace{\langle H_0\rangle^{-1/2}}_{\in\mathcal{B}(\mathcal{H},\mathcal{H}^{1})}.$$

We remark that $T \in \mathcal{C}^k(A;\mathcal{H}^1,\mathcal{H}^{-1})$ is equivalent to the map (2.4) being of class $\mathcal{C}^k(\mathbb{R};\mathcal{B}(\mathcal{H}))$, with $\mathcal{B}(\mathcal{H})$ endowed with the strong operator topology; whereas $T \in \mathcal{C}^{k,\mathrm{u}}(A;\mathcal{H}^1,\mathcal{H}^{-1})$ is equivalent to the map being of class $\mathcal{C}^k(\mathbb{R};\mathcal{B}(\mathcal{H}))$, with $\mathcal{B}(\mathcal{H})$ endowed with the norm operator topology.

In many applications, the free operator H_0 has a nice regularity with respect to the conjugate operator A, i.e. $H_0 \in \mathcal{C}^k(A;\mathcal{G},\mathcal{G}^*)$ for some $k \geqslant 2$ and for some $\mathcal{G} \subset \mathcal{H}$. However, the perturbation V typically doesn't have very much regularity w.r.t. A and showing that V is of class $\mathcal{C}^{1,\mathrm{u}}(A;\mathcal{G},\mathcal{G}^*)$ directly from the definition is usually not very practical. To ease the difficulty we provide the following criterion. Its proof is inspired by [Ge, Lemma 8.5].

Proposition 2.1. *Suppose that $T \in \mathcal{K}(\mathcal{H}^1,\mathcal{H}^{-1}) \cap \mathcal{C}^1(A;\mathcal{H}^1,\mathcal{H}^{-1})$. Then $T \in \mathcal{C}^{1,\mathrm{u}}(A;\mathcal{H}^1,\mathcal{H}^{-1})$ if and only if $[T,\mathrm{i}A]_\circ \in \mathcal{K}(\mathcal{H}^1,\mathcal{H}^{-1})$.*

Remark 2.1. *The proof actually shows that if $T \in \mathcal{B}(\mathcal{H}^1,\mathcal{H}^{-1}) \cap \mathcal{C}^1(A;\mathcal{H}^1,\mathcal{H}^{-1})$ and $[T,\mathrm{i}A]_\circ \in \mathcal{K}(\mathcal{H}^1,\mathcal{H}^{-1})$, then $T \in \mathcal{C}^{1,\mathrm{u}}(A;\mathcal{H}^1,\mathcal{H}^{-1})$. Thus the compactness of T is needed only for the reverse implication in Proposition 2.1.*

Remark 2.2. *Adapting the proof of Proposition 2.1, one can see that the results of Proposition 2.1 and Remark 2.1 are still valid if $\mathcal{K}(\mathcal{H}^1,\mathcal{H}^{-1})$ (resp. $\mathcal{C}^1(A;\mathcal{H}^1,\mathcal{H}^{-1})$, resp. $\mathcal{C}^{1,\mathrm{u}}(A;\mathcal{H}^1,\mathcal{H}^{-1})$, resp. $\mathcal{B}(\mathcal{H}^1,\mathcal{H}^{-1})$) is replaced by $\mathcal{K}(\mathcal{H})$ (resp. $\mathcal{C}^1(A)$, resp. $\mathcal{C}^{1,\mathrm{u}}(A)$, resp. $\mathcal{B}(\mathcal{H})$).*

Proof. We start with the easier of the two implications, namely $T \in \mathcal{C}^{1,\mathrm{u}}(A;\mathcal{H}^1,\mathcal{H}^{-1})$ implies $[T,\mathrm{i}A]_\circ \in \mathcal{K}(\mathcal{H}^1,\mathcal{H}^{-1})$. Let

$$\mathbb{R} \ni t \mapsto \Lambda(t) := \langle H_0\rangle^{-1/2} e^{-\mathrm{i}tA} T e^{\mathrm{i}tA} \langle H_0\rangle^{-1/2} \in \mathcal{B}(\mathcal{H}).$$

To say that $T \in \mathcal{C}^{1,\mathrm{u}}(A; \mathcal{H}^1, \mathcal{H}^{-1})$ is equivalent to Λ being of class $\mathcal{C}^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$, with $\mathcal{B}(\mathcal{H})$ endowed with the norm operator topology. Since

$$\langle H_0\rangle^{-1/2}[T, \mathrm{i}A]_\circ \langle H_0\rangle^{-1/2} = \lim_{t\to 0} \frac{\Lambda(t) - \Lambda(0)}{t}$$

holds w.r.t. the operator norm on $\mathcal{B}(\mathcal{H})$ and $\Lambda(t) - \Lambda(0)$ is equal to

$$\underbrace{\langle H_0\rangle^{-1/2} e^{-\mathrm{i}tA} \langle H_0\rangle^{1/2}}_{\in\, \mathcal{B}(\mathcal{H})} \underbrace{\langle H_0\rangle^{-1/2} T \langle H_0\rangle^{-1/2}}_{\in\, \mathcal{K}(\mathcal{H})} \underbrace{\langle H_0\rangle^{1/2} e^{\mathrm{i}tA} \langle H_0\rangle^{-1/2}}_{\in\, \mathcal{B}(\mathcal{H})} - \underbrace{\langle H_0\rangle^{-1/2} T \langle H_0\rangle^{-1/2}}_{\in\, \mathcal{K}(\mathcal{H})},$$

we see that $\langle H_0\rangle^{-1/2}[T, \mathrm{i}A]_\circ \langle H_0\rangle^{-1/2} \in \mathcal{K}(\mathcal{H})$ as a norm limit of compact operators. Hence $[T, \mathrm{i}A]_\circ \in \mathcal{K}(\mathcal{H}^1, \mathcal{H}^{-1})$.

We now show the reverse implication. We have to show that the map Λ is of class $\mathcal{C}^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$. This is the case if and only if Λ is differentiable with continuous derivative at $t = 0$. Let

$$\ell(t) := \langle H_0\rangle^{-1/2} e^{-\mathrm{i}tA} [T, \mathrm{i}A]_\circ e^{\mathrm{i}tA} \langle H_0\rangle^{-1/2} \in \mathcal{B}(\mathcal{H}).$$

The following equality holds strongly in $\mathcal{H}$ for all $t > 0$ due to the fact that $T \in \mathcal{C}^1(A, \mathcal{H}^1, \mathcal{H}^{-1})$:

$$\frac{\Lambda(t) - \Lambda(0)}{t} - \ell(0) = \frac{1}{t} \int_0^t \langle H_0\rangle^{-1/2} \left(e^{-\mathrm{i}\tau A}[T, \mathrm{i}A]_\circ e^{\mathrm{i}\tau A} - [T, \mathrm{i}A]_\circ\right) \langle H_0\rangle^{-1/2} d\tau. \tag{2.5}$$

Let us estimate the integrand:

$$\begin{aligned}
&\left\|\langle H_0\rangle^{-1/2} \left(e^{-\mathrm{i}\tau A}[T, \mathrm{i}A]_\circ e^{\mathrm{i}\tau A} - [T, \mathrm{i}A]_\circ\right) \langle H_0\rangle^{-1/2}\right\| \\
&\leqslant \left\|\langle H_0\rangle^{-1/2} \left(e^{-\mathrm{i}\tau A}[T, \mathrm{i}A]_\circ e^{\mathrm{i}\tau A} - e^{-\mathrm{i}\tau A}[T, \mathrm{i}A]_\circ\right) \langle H_0\rangle^{-1/2}\right\| \\
&\quad + \left\|\langle H_0\rangle^{-1/2} \left(e^{-\mathrm{i}\tau A}[T, \mathrm{i}A]_\circ - [T, \mathrm{i}A]_\circ\right) \langle H_0\rangle^{-1/2}\right\| \\
&\leqslant \Bigg\| \underbrace{\langle H_0\rangle^{-1/2} e^{-\mathrm{i}\tau A} \langle H_0\rangle^{1/2}}_{\|\cdot\| \leqslant 1} \underbrace{\langle H_0\rangle^{-1/2}[T, \mathrm{i}A]_\circ \langle H_0\rangle^{-1/2}}_{\in\, \mathcal{K}(\mathcal{H})} \underbrace{\left(\langle H_0\rangle^{1/2} e^{\mathrm{i}\tau A} \langle H_0\rangle^{-1/2} - I\right)}_{\xrightarrow{s} 0} \Bigg\| \\
&\quad + \Bigg\| \underbrace{\left(\langle H_0\rangle^{-1/2} e^{-\mathrm{i}\tau A} \langle H_0\rangle^{1/2} - I\right)}_{\xrightarrow{s} 0} \underbrace{\langle H_0\rangle^{-1/2}[T, \mathrm{i}A]_\circ \langle H_0\rangle^{-1/2}}_{\in\, \mathcal{K}(\mathcal{H})} \Bigg\|.
\end{aligned} \tag{2.6}$$

Thus the integrand of (2.5) converges in norm to zero as t goes to zero. It follows that the l.h.s. of (2.5) converges in norm to zero, showing that $\Lambda'(0) = \ell(0)$. It easily follows that $\Lambda'(t) = \ell(t)$ for all $t \in \mathbb{R}$. Again invoking (2.6) shows that Λ' is continuous at $t = 0$, completing the proof. □

3. A few words about the Mourre estimate

This section is based on the content of [ABG, Section 7.2], where the results are presented for a self-adjoint operator $T \in \mathcal{C}^1(A)$, which (we recall) contains the $\mathcal{C}^1(A; \mathcal{G}, \mathcal{G}^*)$ class. Let T be a self-adjoint operator on $\mathcal{H}$ with domain $\mathcal{D}(T) \subset \mathcal{H}$. Let $\mathcal{G}$ be a subspace such that

$$\mathcal{D}(T) \subset \mathcal{G} \subset \mathcal{D}(\langle T\rangle^{1/2}) \subset \mathcal{H} = \mathcal{H}^* \subset \mathcal{D}(\langle T\rangle^{1/2})^* \subset \mathcal{G}^* \subset \mathcal{D}(T)^*.$$

If $T \in \mathcal{C}^1(A, \mathcal{G}, \mathcal{G}^*)$, then in particular $[T, \mathrm{i}A]_\circ \in \mathcal{B}(\mathcal{G}, \mathcal{G}^*)$. If $\mathcal{I} \subset \mathbb{R}$ is a bounded interval, then $E_{\mathcal{I}}(T) \in \mathcal{B}(\mathcal{H}, \mathcal{G})$ and by duality $E_{\mathcal{I}}(T) \in \mathcal{B}(\mathcal{G}^*, \mathcal{H})$. We say that the *Mourre estimate* holds for T w.r.t. A on the bounded interval $\mathcal{I}$ if there exist $c > 0$ and $K \in \mathcal{K}(\mathcal{H})$ such that

$$E_{\mathcal{I}}(T)[T, \mathrm{i}A]_\circ E_{\mathcal{I}}(T) \geqslant c E_{\mathcal{I}}(T) + K \tag{3.1}$$

in the form sense on $\mathcal{H}\times\mathcal{H}$. Note that both the l.h.s. and r.h.s. of (3.1) are well-defined bounded operators on $\mathcal{H}$. For reminder, if this estimate holds, then the total multiplicity of eigenvalues of T in $\mathcal{I}$ is finite by [ABG, Corollary 7.2.11], whereas if the estimate holds with $K=0$, then $\mathcal{I}$ is void of eigenvalues, as a result of the Virial Theorem [ABG, Proposition 7.2.10]. We let $\mu^A(T)$ be the collection of points belonging to neighborhood for which the Mourre estimate holds, i.e.

$$\mu^A(T) := \{\lambda \in \mathbb{R} : \exists c>0, K\in\mathcal{K}(\mathcal{H}) \text{ and } \mathcal{I} \text{ open for which (3.1) holds for } T \text{ on } \mathcal{I} \text{ and } \lambda\in\mathcal{I}\}.$$

This is an open set. It is natural to introduce a function defined on $\mu^A(T)$ which gives the best constant $c>0$ that can be achieved in the Mourre estimate, i.e. for $\lambda\in\mu^A(T)$, let

$$\varrho_T^A(\lambda) := \sup_{\mathcal{I}\ni\lambda}\big\{\sup\{c\in\mathbb{R} : E_{\mathcal{I}}(T)[T,\mathrm{i}A]_\circ E_{\mathcal{I}}(T) \geqslant cE_{\mathcal{I}}(T)+K, \text{ for some } K\in\mathcal{K}(\mathcal{H})\}\big\}.$$

Equivalent definitions and various properties of the ϱ_T^A function are given in [ABG, Section 7.2]. One very useful result that we shall use is the following:

Proposition 3.1. [ABG, Proposition 7.2.7] *Suppose that T has a spectral gap and that $T\in\mathcal{C}^1(A)$. Let $R(\varsigma) := (\varsigma - T)^{-1}$, where ς is a real number in the resolvent set of T. Then*

$$\varrho_T^A(\lambda) = (\varsigma-\lambda)^2 \varrho^A_{R(\varsigma)}((\varsigma-\lambda)^{-1}). \tag{3.2}$$

In particular, T is conjugate to A at λ if and only if $R(\varsigma)$ is conjugate to A at $(\varsigma-\lambda)^{-1}$.

As a side note, this Proposition is stated without proof in [ABG], so we indicate to the reader that it may be proven following the same lines as that of [ABG, Proposition 7.2.5] together with the following Lemma, which is the equivalent of [ABG, Proposition 7.2.1]. Denote $\mathcal{I}(\lambda;\varepsilon)$ the open interval of radius ε centered at λ.

Lemma 3.2. *Suppose that $T\in\mathcal{C}^1(A)$. If $\lambda\notin\sigma_{\mathrm{ess}}(H)$, then $\varrho_T^A(\lambda)=+\infty$. If $\lambda\in\sigma_{\mathrm{ess}}(H)$, then $\varrho_T^A(\lambda)$ is finite and given by*

$$\varrho_T^A(\lambda) = \lim_{\varepsilon\to 0^+}\inf\big\{\langle\psi,[T,\mathrm{i}A]_\circ\psi\rangle : \psi\in\mathcal{H}, \|\psi\|=1 \text{ and } E_{\mathcal{I}(\lambda;\varepsilon)}(T)\psi=\psi\big\}.$$

Furthermore, there is a sequence $(\psi_n)_{n=1}^\infty$ of vectors such that $\psi_n\in\mathcal{H}$, $\|\psi_n\|\equiv 1$, $\langle\psi_n,\psi_m\rangle=\delta_{nm}$, $E_{\mathcal{I}(\lambda;1/n)}\psi_n=\psi_n$ and $\lim_{n\to\infty}\langle\psi_n,[T,\mathrm{i}A]_\circ\psi_n\rangle = \varrho_T^A(\lambda)$.

We will be employing formula (3.2) in the proof of the main result of this paper, but for the moment we apply it to show that under the assumptions of Theorem 1.3, H and H_0 share the same points where a Mourre estimate hold. The remark is done after [ABG, Theorem 7.2.9]. Let $R(z) := (z-T)^{-1}$ and $R_0(z) := (z-T_0)^{-1}$.

Lemma 3.3. *Let T_0, T and A be self-adjoint operators on $\mathcal{H}$. Let T_0 have a spectral gap, and suppose that $T,T_0\in\mathcal{C}^{1,\mathrm{u}}(A)$. If $R(\mathrm{i})-R_0(\mathrm{i})\in\mathcal{K}(\mathcal{H})$ then $\mu^A(T)=\mu^A(T_0)$.*

Remark 3.1. The assumptions of Theorem 1.3 fulfill the requirements of this Lemma, with $(T_0,T)=(H_0,H)$. Indeed, $\mathcal{D}(\langle H\rangle^{1/2})=\mathcal{D}(\langle H_0\rangle^{1/2})$ implies the compactness of $R(\mathrm{i})-R_0(\mathrm{i})$:

$$R(\mathrm{i})-R_0(\mathrm{i}) = R(\mathrm{i})VR_0(\mathrm{i}) = \underbrace{R(\mathrm{i})\langle H\rangle^{1/2}}_{\in\mathcal{B}(\mathcal{H})}\underbrace{\langle H\rangle^{-1/2}\langle H_0\rangle^{1/2}}_{\in\mathcal{B}(\mathcal{H})}\underbrace{\langle H_0\rangle^{-1/2}V\langle H_0\rangle^{-1/2}}_{\in\mathcal{K}(\mathcal{H}) \text{ by A3}}\underbrace{\langle H_0\rangle^{1/2}R_0(\mathrm{i})}_{\in\mathcal{B}(\mathcal{H})}.$$

Proof. Firstly, the assumption that $R(\mathrm{i}) - R_0(\mathrm{i})$ is compact implies $\sigma_{\mathrm{ess}}(T_0) = \sigma_{\mathrm{ess}}(T)$. Because T_0 has a spectral gap, $\sigma_{\mathrm{ess}}(T_0) = \sigma_{\mathrm{ess}}(T) \neq \mathbb{R}$, and therefore there exists $\varsigma \in \mathbb{R} \setminus (\sigma(T) \cup \sigma(T_0))$. For all $z, z' \in \mathbb{R} \setminus (\sigma(T) \cup \sigma(T_0))$, the following identity holds:

$$R(z) - R_0(z) = [I + (z' - z)R(z)][R(z') - R_0(z')][I + (z' - z)R_0(z)].$$

Thus $R(\varsigma) - R_0(\varsigma)$ is compact. To simplify the notation onwards, let $R_0 := R_0(\varsigma)$ and $R := R(\varsigma)$.

Secondly, if $\lambda \in \mu^A(T_0)$, then $(\varsigma - \lambda)^{-1} \in \mu^A(R_0)$ by Proposition 3.1, and so there is an open interval $\mathcal{I} \ni (\varsigma - \lambda)^{-1}$, $c > 0$ and a compact K such that

$$E_{\mathcal{I}}(R_0)[R_0, \mathrm{i}A]_\circ E_{\mathcal{I}}(R_0) \geqslant c E_{\mathcal{I}}(R_0) + K.$$

Applying to the right and left by $\theta(R_0)$, where $\theta \in \mathcal{C}_c^\infty(\mathbb{R})$ is a bump function supported and equal to one in a neighborhood of $(\varsigma - \lambda)^{-1}$, we get

$$\theta(R_0)[R_0, \mathrm{i}A]_\circ \theta(R_0) \geqslant c\theta^2(R_0) + \text{compact}.$$

By the Helffer-Sjötrand formula and the fact that $R(z) - R_0(z)$ is compact for all $z \in \mathbb{C} \setminus \mathbb{R}$, we see that $\theta(R) - \theta(R_0)$ is compact, and likewise for $\theta^2(R) - \theta^2(R_0)$. Note also that $R_0 - R \in \mathcal{C}^{1,\mathrm{u}}(A)$ and so by Remark 2.2, $[R_0 - R, \mathrm{i}A]_\circ \in \mathcal{K}(\mathcal{H})$. Thus exchanging R_0 for R, $\theta(R_0)$ for $\theta(R)$, and $\theta^2(R_0)$ for $\theta^2(R)$ in the previous inequality, we have

$$\theta(R)[R, \mathrm{i}A]_\circ \theta(R) \geqslant c\theta^2(R) + \text{compact}.$$

Let $\mathcal{I}' \subset \theta^{-1}(\{1\})$. Applying $E_{\mathcal{I}'}(R)$ to the left and right of this equation shows that the Mourre estimate holds for R in a neighborhood of $(\varsigma - \lambda)^{-1}$. Thus $\lambda \in \mu^A(T)$ by Proposition 3.1, and this shows $\mu^A(T_0) \subset \mu^A(T)$. Exchanging the roles of T and T_0 shows the reverse inclusion. □

4. Examples of Schrödinger operators

4.1. **The case of continuous Schrödinger operators.** Our first application is to continuous Schrödinger operators. The setting has already been described in Example 1.1 for the most part. For an integer $d \geqslant 1$, let $\mathcal{H} := L^2(\mathbb{R}^d)$. The free operator is the Laplacian, i.e. $H_0 := -\Delta = -\sum_{i=1}^d \partial^2/\partial x_i^2$ with domain the Sobolev space $\mathcal{H}^2 := \mathcal{H}^2(\mathbb{R}^d)$. Then H_0 is a positive operator with purely absolutely continuous spectrum and $\sigma(H_0) = [0, +\infty)$. Let Q be the operator of multiplication by $x = (x_1, ..., x_d) \in \mathbb{R}^d$, and let $P := -\mathrm{i}\nabla$. Set

$$H := H_0 + V_{\mathrm{sr}}(Q) + V_{\mathrm{lr}}(Q),$$

where $V_{\mathrm{sr}}(x)$ and $V_{\mathrm{lr}}(x)$ are real-valued functions belonging to $L^\infty(\mathbb{R}^d)$, satisfying $V_{\mathrm{sr}}(x)$, $V_{\mathrm{lr}}(x) = o(1)$ at infinity. Then $V_{\mathrm{sr}}(Q)$ and $V_{\mathrm{lr}}(Q)$ are bounded self-adjoint operators in $\mathcal{H}$ and H_0-form relatively compact operators, i.e. $V_{\mathrm{sr}}(Q), V_{\mathrm{lr}}(Q) \in \mathcal{K}(\mathcal{H}^1, \mathcal{H}^{-1})$, where $\mathcal{H}^1$ denotes the form domain of H_0. The latter is a direct consequence of the following standard fact:

Proposition 4.1. *Let f, g be bounded Borel measurable functions on $\mathbb{R}^d$ which vanish at infinity. Then $g(Q)f(P) \in \mathcal{K}(L^2(\mathbb{R}^d))$.*

Assumptions A1 - A3 are verified. We add that $\sigma_{\mathrm{ess}}(H) = [0, +\infty)$ by the Theorem of Weyl on relative compactness. Moving forward, we use the following result:

Proposition 4.2. [ABG, p. 258] *Let T and A be self-adjoint operators in a Hilbert space $\mathcal{H}$ and denote $\mathcal{H}^1 := \mathcal{D}(\langle T\rangle^{1/2})$, the form domain of T, and $\mathcal{H}^{-1} := (\mathcal{H}^1)^*$. Suppose that $e^{\mathrm{i}tA}\mathcal{H}^1 \subset \mathcal{H}^1$. Then the following are equivalent:*

(1) $T \in \mathcal{C}^1(A; \mathcal{H}^1, \mathcal{H}^{-1})$

(2) The form $[T, \mathrm{i}A]$ defined on $\mathcal{D}(T) \cap \mathcal{D}(A)$ extends to an operator in $\mathcal{B}(\mathcal{H}^1, \mathcal{H}^{-1})$.

Remark 4.1. *The form $[T, \mathrm{i}A]$ is defined for $\psi, \phi \in \mathcal{D}(T) \cap \mathcal{D}(A)$ as follows :*

$$\langle \psi, [T, \mathrm{i}A]\phi\rangle := \langle T^*\psi, \mathrm{i}A\phi\rangle - \langle A^*\psi, \mathrm{i}T\phi\rangle = \langle T\psi, \mathrm{i}A\phi\rangle - \langle A\psi, \mathrm{i}T\phi\rangle.$$

The last equality holds because T and A are assumed to be self-adjoint.

Let $A := (Q \cdot P + P \cdot Q)/2$ be the generator of dilations which is essentially self-adjoint on the Schwartz space $\mathcal{S}(\mathbb{R}^d)$. The relation

$$(e^{\mathrm{i}tA}\psi)(x) = e^{td/2}\psi(e^t x), \quad \text{for all } \psi \in L^2(\mathbb{R}^d), x \in \mathbb{R}^d$$

implies that $\{e^{\mathrm{i}tA}\}_{t\in\mathbb{R}}$ stabilizes $\mathcal{H}^2(\mathbb{R}^d)$, and thus $\mathcal{H}^\theta(\mathbb{R}^d)$ for all $\theta \in [-2, 2]$ by duality and interpolation. Thus A4 holds. A straightforward computation gives

$$\langle \psi, [H_0, \mathrm{i}A]\phi\rangle = \langle \psi, 2H_0\phi\rangle$$

for all $\psi, \phi \in \mathcal{H}^2 \cap \mathcal{D}(A)$. Let $\mathcal{H}^1 := \mathcal{D}(\langle H_0\rangle^{1/2})$. We see that $[H_0, \mathrm{i}A]$ extends to operator in $\mathcal{B}(\mathcal{H}^1, \mathcal{H}^{-1})$, thereby implying that $H_0 \in \mathcal{C}^1(A; \mathcal{H}^1, \mathcal{H}^{-1})$ by Proposition 4.2. The extension of $[H_0, \mathrm{i}A]$ is in fact $[H_0, \mathrm{i}A]_\circ$. An easy induction gives $H_0 \in \mathcal{C}^k(A; \mathcal{H}^1, \mathcal{H}^{-1})$ for all $k \in \mathbb{N}$. In particular, A5 is fulfilled. The strict Mourre estimate holds for H_0 with respect to A on all intervals $\mathcal{I}$ verifying $\overline{\mathcal{I}} \subset (0, +\infty)$. In particular, $\mu^A(H_0) = (0, +\infty)$.

We now examine the commutator between the potentials $V_{\mathrm{sr}}(Q) + V_{\mathrm{lr}}(Q)$ and A. For the long-range potential, we now additionally assume that $x \cdot \nabla V_{\mathrm{lr}}(x)$ exists as a function and belongs to $L^\infty(\mathbb{R}^d)$. A computation gives

$$\langle \psi, [V_{\mathrm{lr}}(Q), \mathrm{i}A]\phi\rangle = -\langle \psi, Q \cdot \nabla V_{\mathrm{lr}}(Q)\phi\rangle,$$

for all $\psi, \phi \in \mathcal{D}(A)$. In particular, this shows that $[V_{\mathrm{lr}}(Q), \mathrm{i}A]$ extends to an operator in $\mathcal{B}(\mathcal{H}^1, \mathcal{H}^{-1})$, and by Proposition 4.2, this implies that $V_{\mathrm{lr}}(Q) \in \mathcal{C}^1(A; \mathcal{H}^1, \mathcal{H}^{-1})$. Furthermore, $[V_{\mathrm{lr}}(Q), \mathrm{i}A]_\circ = -Q \cdot \nabla V_{\mathrm{lr}}(Q)$. If $x \cdot \nabla V_{\mathrm{lr}}(x) = o(1)$ at infinity is further assumed, then $\langle H_0\rangle^{-1/2} Q \cdot \nabla V_{\mathrm{lr}}(Q)\langle H_0\rangle^{-1/2} \in \mathcal{K}(L^2(\mathbb{R}^d))$ by Proposition 4.1, i.e. $[V_{\mathrm{lr}}(Q), \mathrm{i}A]_\circ \in \mathcal{K}(\mathcal{H}^1, \mathcal{H}^{-1})$. In this case, we have that $V_{\mathrm{lr}}(Q) \in \mathcal{C}^{1,\mathrm{u}}(A; \mathcal{H}^1, \mathcal{H}^{-1})$ by Proposition 2.1.

We now analyze the commutator with the short range potential, and additionally assume that $\langle x\rangle V_{\mathrm{sr}}(x) \in L^\infty(\mathbb{R}^d)$. For $\psi, \phi \in \mathcal{D}(A)$, we have

$$\begin{aligned}\langle \psi, [V_{\mathrm{sr}}(Q), \mathrm{i}A]\phi\rangle &= \langle V_{\mathrm{sr}}(Q)\psi, \mathrm{i}A\phi\rangle + \langle \mathrm{i}A\psi, V_{\mathrm{sr}}(Q)\phi\rangle \\ &= \langle \langle Q\rangle V_{\mathrm{sr}}(Q)\psi, \langle Q\rangle^{-1}(\mathrm{i}Q \cdot P + d/2)\phi\rangle + \langle \langle Q\rangle^{-1}(\mathrm{i}Q \cdot P + d/2)\psi, \langle Q\rangle V_{\mathrm{sr}}(Q)\phi\rangle.\end{aligned}$$

We handle the operator in the first inner product on the r.h.s. of the previous equation. Note that $\langle Q\rangle^{-1}(\mathrm{i}Q \cdot P + d/2) \in \mathcal{B}(\mathcal{H}^1, \mathcal{H})$ and $\langle Q\rangle V_{\mathrm{sr}}(Q) \in \mathcal{B}(\mathcal{H}, \mathcal{H}^{-1})$. Thus

$$\langle Q\rangle V_{\mathrm{sr}}(Q) \times \langle Q\rangle^{-1}(\mathrm{i}Q \cdot P + d/2) \tag{4.1}$$

belongs to $\mathcal{B}(\mathcal{H}^1, \mathcal{H}^{-1})$. The operator in the second inner product on the r.h.s. of the previous equation also belongs to $\mathcal{B}(\mathcal{H}^1, \mathcal{H}^{-1})$, because it is the adjoint of (4.1). We conclude that $[V_{\mathrm{sr}}(Q), \mathrm{i}A]$ extends to an operator in $\mathcal{B}(\mathcal{H}^1, \mathcal{H}^{-1})$, and by Proposition 4.2, this implies that $V_{\mathrm{sr}}(Q) \in \mathcal{C}^1(A; \mathcal{H}^1, \mathcal{H}^{-1})$. The extension of $[V_{\mathrm{sr}}(Q), \mathrm{i}A]$ is precisely $[V_{\mathrm{sr}}(Q), \mathrm{i}A]_\circ$. If $x \cdot \nabla V_{\mathrm{sr}}(x) = o(1)$ at infinity is further assumed, then $\langle H_0\rangle^{-1/2}\langle Q\rangle V_{\mathrm{sr}}(Q) \in \mathcal{K}(L^2(\mathbb{R}^d))$ by

Proposition 4.1, i.e. $\langle Q\rangle V_{\mathrm{sr}}(Q) \in \mathcal{K}(\mathcal{H}, \mathcal{H}^{-1})$. So (4.1) and its adjoint belong to $\mathcal{K}(\mathcal{H}^1, \mathcal{H}^{-1})$. Thus $[V_{\mathrm{lr}}(Q), \mathrm{i}A]_\circ \in \mathcal{K}(\mathcal{H}^1, \mathcal{H}^{-1})$ and $V_{\mathrm{sr}}(Q) \in \mathcal{C}^{1,\mathrm{u}}(A; \mathcal{H}^1, \mathcal{H}^{-1})$ follows from Proposition 2.1.

The above calculations along with Theorems 1.2 and 1.3 yield the following specific result for continuous Schrödinger operators:

Theorem 4.3. *Let $H := H_0 + V_{\mathrm{sr}}(Q) + V_{\mathrm{lr}}(Q)$ and A be as above, namely*

(1) $H_0 = -\Delta$ and $A = (Q \cdot P + P \cdot Q)/2$ in $L^2(\mathbb{R}^d)$,
(2) $V_{\mathrm{sr}}(x)$ and $V_{\mathrm{lr}}(x)$ are real-valued functions in $L^\infty(\mathbb{R}^d)$,
(3) $\lim V_{\mathrm{sr}}(x) = \lim V_{\mathrm{lr}}(x) = 0$ as $\|x\| \to +\infty$,
(4) $\lim \langle x\rangle V_{\mathrm{sr}}(x) = 0$ as $\|x\| \to +\infty$, and
(5) $x \cdot \nabla V_{\mathrm{lr}}(x)$ exists as a function, belongs to $L^\infty(\mathbb{R}^d)$, and $\lim x \cdot \nabla V_{\mathrm{lr}}(x) = 0$ as $\|x\| \to +\infty$.

Then $V_{\mathrm{sr}}(Q)$ and $V_{\mathrm{lr}}(Q)$ belong to $\mathcal{C}^{1,\mathrm{u}}(A; \mathcal{H}^1, \mathcal{H}^{-1})$. In particular $H \in \mathcal{C}^{1,\mathrm{u}}(A)$. Moreover, $\mu^A(H) = \mu^A(H_0) = (0, +\infty)$, by Lemma 3.3. Finally, for all $\lambda \in (0, +\infty)$ there is a bounded open interval $\mathcal{I}$ containing λ such that for all $s > 1/2$ and $\psi \in \mathcal{H}$, the propagation estimates (1.5), (1.6) and (1.12) hold.

Remark 4.2. *Notice that the condition $\ker(H - \lambda) \subset \mathcal{D}(A)$ that appears in the formulation of Theorems 1.2 and 1.3 is totally absent here. This is because under the assumptions $\lim \langle x\rangle V_{\mathrm{sr}}(x) = \lim x \cdot \nabla V_{\mathrm{lr}}(x) = 0$ as $\|x\| \to +\infty$, it is well-known from research in the sixties that the continuous Schrödinger operator H does not have any eigenvalues in $[0, +\infty)$, see articles by Kato [K2], Simon [Si] and Agmon [A].*

4.2. **The case of discrete Schrödinger operators.** Our second application is to discrete Schrödinger operators. For an integer $d \geqslant 1$, let $\mathcal{H} := \ell^2(\mathbb{Z}^d)$ The free operator is the discrete Laplacian, i.e. $H_0 := \Delta \in \mathcal{B}(\mathcal{H})$, where

$$(\Delta\psi)(n) := \sum_{m:\|m-n\|=1} \psi(n) - \psi(m). \tag{4.2}$$

Here we have equipped $\mathbb{Z}^d$ with the following norm: for $n = (n_1, ..., n_d)$, $\|n\| := \sum_{i=1}^d |n_i|$. It is well-known that Δ is a bounded positive operator on $\mathcal{H}$ with purely absolutely continuous spectrum, and $\sigma(\Delta) = \sigma_{\mathrm{ac}}(\Delta) = [0, 4d]$. Let V be a bounded real-valued function on $\mathbb{Z}^d$ such that $V(n) \to 0$ as $\|n\| \to \infty$. Then V induces a bounded self-adjoint compact operator on $\mathcal{H}$ as follows, $(V\psi)(n) := V(n)\psi(n)$. Recall that a multiplication operator V on $\ell^2(\mathbb{Z}^d)$ is compact if and only if $V(n) \to 0$ as $\|n\| \to \infty$. Assumptions A1 - A3 are verified. Set $H := H_0 + V$. Then H is a bounded self-adjoint operator and $\sigma_{\mathrm{ess}}(H) = [0, 4d]$.

To write the conjugate operator, we need more notation. Let $S = (S_1, ..., S_d)$, where, for $1 \leqslant i \leqslant d$, S_i is the shift operator given by

$$(S_i\psi)(n) := \psi(n_1, ..., n_i - 1, ..., n_d), \quad \text{for all } n \in \mathbb{Z}^d \text{ and } \psi \in \mathcal{H}.$$

Let $N = (N_1, ..., N_d)$, where, for $1 \leqslant i \leqslant d$, N_i is the position operator given by

$$(N_i\psi)(n) := n_i\psi(n), \quad \text{with domain} \quad \mathcal{D}(N_i) := \left\{\psi \in \mathcal{H} : \sum_{n\in\mathbb{Z}^d} |n_i\psi(n)|^2 < \infty\right\}.$$

The conjugate operator, denoted by A, is the closure of the following operator

$$A_0 := \frac{\mathrm{i}}{2}\sum_{i=1}^d (S_i - S_i^*)N_i + N_i(S_i - S_i^*), \quad \text{with domain} \quad \mathcal{D}(A_0) := \ell_0(\mathbb{Z}^d), \tag{4.3}$$

the sequences with compact support. The operator A is self-adjoint, see [BS] and [GGo]. That $\{e^{\mathrm{i}tA}\}_{t\in\mathbb{R}}$ stabilizes the form domain of H_0 is a triviality, because $\mathcal{D}(H_0) = \mathcal{H}$. So Assumption A4 is true.

Next, we study the commutator between H_0 and A. A calculation shows that

$$\langle\psi, [H_0, \mathrm{i}A]\psi\rangle = \langle\psi, \sum_{i=1}^{d} \Delta_i(4 - \Delta_i)\psi\rangle, \tag{4.4}$$

for all $\psi \in \ell_0(\mathbb{Z}^d)$. Here $\Delta_i := 2 - S_i - S_i^*$. Since H_0 is a bounded self-adjoint operator, (4.4) implies that $H_0 \in \mathcal{C}^1(A)$, thanks to a simple criterion for such operators, see [ABG, Lemma 6.2.9] and [ABG, Theorem 6.2.10]. We could also have invoked Proposition 4.2, but that is a bit of an overkill. An easy induction shows that $H_0 \in \mathcal{C}^k(A)$ for all $k \in \mathbb{N}$. In particular, Assumption A5 holds. By (4.4) and [ABG, Theorem 8.3.6], we have that

$$\mu^A(H_0) = [0, 4d] \setminus \{4k : k = 0, ..., d\}. \tag{4.5}$$

Let us now study the commutator between V and A. Let $\tau_i V$ be the shifted potential acting as follows:

$$[(\tau_i V)\psi](n) := V(n_1, ..., n_i - 1, ..., n_d)\psi(n), \quad \text{for all } \psi \in \mathcal{H}.$$

Define $\tau_i^* V$ correspondingly. A straightforward computation gives

$$\langle\psi, [V, \mathrm{i}A]\psi\rangle = \sum_{i=1}^{d} \Big\langle \psi, \Big((2^{-1} + N_i)(V - \tau_i^* V)S_i^* + (2^{-1} - N_i)(V - \tau_i V)S_i\Big)\psi \Big\rangle,$$

for all $\psi \in \ell_0(\mathbb{Z}^d)$. If $\sup_{n\in\mathbb{Z}^d} |n_i(V - \tau_i V)(n)| < +\infty$ is assumed for all $1 \leqslant i \leqslant d$, we see that $V \in \mathcal{C}^1(A)$. The bounded extension of the form $[V, \mathrm{i}A]$ is precisely $[V, \mathrm{i}A]_\circ$. If $\lim |n_i(V - \tau_i V)(n)| = 0$ as $\|n\| \to +\infty$ for all $1 \leqslant i \leqslant d$ is further assumed, then $[V, \mathrm{i}A]_\circ \in \mathcal{K}(\mathcal{H})$. This is equivalent to $V \in \mathcal{C}^{1,\mathrm{u}}(A)$, by Remark 2.2. Thus A6 is fulfilled.

The above calculations along with Theorems 1.2 and 1.3 yield the following specific result for discrete Schrödinger operators:

Theorem 4.4. *Let $H := H_0 + V$ and A be as above, namely*

(1) H_0 is given by (4.2) and A is the closure of (4.3),
(2) $V(n)$ is a bounded real-valued function defined on $\mathbb{Z}^d$,
(3) $\lim V(n) = 0$ as $\|n\| \to +\infty$, and
(4) $\lim |n_i(V - \tau_i V)(n)| = 0$ as $\|n\| \to +\infty$ for all $1 \leqslant i \leqslant d$.

Then V belongs to $\mathcal{C}^{1,\mathrm{u}}(A)$. In particular $H \in \mathcal{C}^{1,\mathrm{u}}(A)$. Moreover, $\mu^A(H) = \mu^A(H_0) = [0, 4d] \setminus \{4k : k = 0, ..., d\}$, by Lemma 3.3 and (4.5). Finally, for all $\lambda \in \mu^A(H)$ there is a bounded open interval $\mathcal{I}$ containing λ such that for all $s > 1/2$ and $\psi \in \mathcal{H}$, the propagation estimates (1.5), (1.6) and (1.12) hold.

Remark 4.3. *As in the continuous operator case, the condition* $\ker(H - \lambda) \subset \mathcal{D}(A)$ *holds here for all $\lambda \in \mu^A(H)$. Indeed, if $\psi \in \ker(H - \lambda)$ and $\lambda \in \mu^A(H)$, then for all $p \geqslant 0$ there is $c_p > 0$ such that $|\psi(n)| \leqslant c_p\langle n\rangle^{-p}$, $n \in \mathbb{Z}^d$. This is a consequence of* [Ma2, Theorem 1.5] *for instance. Under Assumptions (3) and (4), the absence of positive eigenvalues holds for one-dimensional discrete Schrödinger operators, by* [Ma2, Theorem 1.3]*. To our knowledge, the absence of positive eigenvalues under Assumptions (3) and (4) is an open problem for multi-dimensional discrete Schrödinger operators on $\mathbb{Z}^d$.*

5. Proof of Theorem 1.2

We start with an improvement of [GJ1, Proposition 2.1].

Lemma 5.1. *For $\phi, \varphi \in \mathcal{D}(A)$, the rank one operator $|\phi\rangle\langle\varphi| : \psi \mapsto \langle\varphi, \psi\rangle\phi$ is of class $\mathcal{C}^{1,\mathrm{u}}(A)$.*

Proof. First, by [ABG, Lemma 6.2.9], $|\phi\rangle\langle\varphi| \in \mathcal{C}^1(A)$ if and only if the sesquilinear form

$$\mathcal{D}(A) \ni \psi \mapsto \langle\psi, [|\phi\rangle\langle\varphi|, A]\psi\rangle := \langle\langle\phi, \psi\rangle\varphi, A\psi\rangle - \langle A\psi, \langle\varphi|\psi\rangle\phi\rangle$$

is continuous for the topology induced by $\mathcal{H}$. Since

$$\langle\psi, [|\phi\rangle\langle\varphi|, A]\psi\rangle = \langle\psi, \phi\rangle\langle A\varphi, \psi\rangle - \langle\psi, A\phi\rangle\langle\varphi, \psi\rangle = \langle\psi, (|\phi\rangle\langle A\varphi| - |A\phi\rangle\langle\varphi|)\,\psi\rangle,$$

we see that $|\phi\rangle\langle\varphi| \in \mathcal{C}^1(A)$ and $[|\phi\rangle\langle\varphi|, A]_\circ = |\phi\rangle\langle A\varphi| - |A\phi\rangle\langle\varphi|$, which is a bounded operator of rank at most two. Apply Proposition 2.1, more specifically Remark 2.2, to obtain the result. □

Next, we quote for convenience the result of [Ri] that we use in the proof of Theorem 1.2.

Theorem 5.2. [Ri, Theorem 1] *Let H and A be self-adjoint operators in $\mathcal{H}$ with $H \in \mathcal{C}^{1,\mathrm{u}}(A)$. Assume that there exist an open interval $J \subset \mathbb{R}$ and $c > 0$ such that $\eta(H)[H, \mathrm{i}A]_\circ\eta(H) \geqslant c \cdot \eta^2(H)$ for all real $\eta \in \mathcal{C}_\mathrm{c}^\infty(J)$. Let a and t be real numbers. Then for each real $\eta \in \mathcal{C}_\mathrm{c}^\infty(J)$ and for each $v < c$ one has uniformly in a,*

$$\|E_{(-\infty, a+vt]}(A)e^{-\mathrm{i}tH}\eta(H)E_{[a,+\infty)}(A)\| \to 0 \quad \textit{as} \quad t \to +\infty.$$

We are now ready to prove Theorem 1.2.

Proof of Theorem 1.2. Let $\mathcal{I} \subset \mathbb{R}$ be a compact interval as in the statement of Theorem 1.2, that is, for all $\lambda \in \mathcal{I}$, $\lambda \in \mu^A(H)$ and $\ker(H - \lambda) \subset \mathcal{D}(A)$. Let $\lambda \in \mathcal{I}$ be given, and assume that a Mourre estimate holds with $K \in \mathcal{K}(\mathcal{H})$ in a neighborhood J of λ.
Step 1: This step is a remark due to Serge Richard. In this step, we assume that λ is not an eigenvalue of H. In this case, from the Mourre estimate, we may derive a strict Mourre estimate on a possibly smaller neighborhood of λ, because $E_J(H)KE_J(H)$ converges in norm to zero as the support of J shrinks to zero around λ. So, without loss of generality, there is an open interval J containing λ and $c > 0$ such that a strict Mourre estimate holds for H on J, i.e.

$$E_J(H)[H, \mathrm{i}A]_\circ E_J(H) \geqslant cE_J(H).$$

In particular, J does not contain any eigenvalue of H. We look to apply [Ri, Theorem 1]. Let $\psi \in \mathcal{H}$, and assume without loss of generality that $\|\psi\| = 1$. Fix $v \in (0, c)$ and let $a \in \mathbb{R}$. Let $\eta \in \mathcal{C}_c^\infty(J)$ be such that $\max_{x\in J}|\eta(x)| \leqslant 1$, so that $\|\eta(H)\| \leqslant 1$. Note also that $\|\langle A\rangle^{-s}\| \leqslant 1$ for all $s > 0$. Then

$$\begin{aligned}
\|\langle A\rangle^{-s}e^{-\mathrm{i}tH}\eta(H)\psi\| &\leqslant \|\langle A\rangle^{-s}e^{-\mathrm{i}tH}\eta(H)E_{(-\infty,a)}(A)\psi\| + \|\langle A\rangle^{-s}e^{-\mathrm{i}tH}\eta(H)E_{[a,+\infty)}(A)\psi\| \\
&\leqslant \|E_{(-\infty,a)}(A)\psi\| + \|\langle A\rangle^{-s}E_{(-\infty,a+vt]}(A)e^{-\mathrm{i}tH}\eta(H)E_{[a,+\infty)}(A)\psi\| \\
&\quad + \|\langle A\rangle^{-s}E_{(a+vt,+\infty)}(A)e^{-\mathrm{i}tH}\eta(H)E_{[a,+\infty)}(A)\psi\| \\
&\leqslant \|E_{(-\infty,a)}(A)\psi\| + \|E_{(-\infty,a+vt]}(A)e^{-\mathrm{i}tH}\eta(H)E_{[a,+\infty)}(A)\| \\
&\quad + \|\langle A\rangle^{-s}E_{(a+vt,+\infty)}(A)\|
\end{aligned}$$

Let $\varepsilon > 0$ be given. Choose a so that $\|E_{(-\infty,a)}(A)\psi\| \leqslant \varepsilon/3$. Then take t large enough so that the other two terms on the r.h.s. of the previous inequality are each less than $\varepsilon/3$. The second one is controlled by [Ri, Theorem 1] and the third one by functional calculus. Then $\|\langle A\rangle^{-s}e^{-\mathrm{i}tH}\eta(H)\psi\| \leqslant \varepsilon$. Thus

$$\lim_{t\to+\infty} \|\langle A\rangle^{-s}e^{-\mathrm{i}tH}\eta(H)\psi\| = 0.$$

By taking a sequence $\eta_k \in \mathcal{C}_c^\infty(J)$ that converges pointwise to the characteristic function of J, we infer from the previous limit that

$$\lim_{t\to+\infty} \|\langle A\rangle^{-s}e^{-\mathrm{i}tH}E_J(H)\psi\| = 0.$$

Finally, as there are no eigenvalues of H in J, $E_J(H) = E_J(H)P_\mathrm{c}(H)$ and we have

$$\lim_{t\to+\infty} \|\langle A\rangle^{-s}e^{-\mathrm{i}tH}E_J(H)P_\mathrm{c}(H)\psi\| = 0. \tag{5.1}$$

Step 2: In this step, $\lambda \in \mathcal{I}$ is assumed to be an eigenvalue of H. By adding a constant to H, we may assume that $\lambda \neq 0$. By assumption, there is an interval J containing λ, $c > 0$ and $K \in \mathcal{K}(\mathcal{H})$ such that

$$E_J(H)[H, \mathrm{i}A]_\circ E_J(H) \geqslant cE_J(H) + K.$$

As the point spectrum of H is finite in J, we further choose J so that it contains only one eigenvalue of H, namely λ. Furthermore, the interval J is chosen so that $0 \notin J$. Denote $P = P_{\{\lambda\}}(H)$ and $P^\perp := 1 - P_{\{\lambda\}}(H)$. Also let $H' := HP^\perp$. Then

$$P^\perp E_J(H)[H, \mathrm{i}A]_\circ E_J(H)P^\perp \geqslant cE_J(H)P^\perp + P^\perp E_J(H)KE_J(H)P^\perp.$$

Functional calculus yields $P^\perp E_J(H) = E_J(HP^\perp)$ – this is where the technical point $0 \notin J$ is required. Moreover, $P^\perp E_J(H)KE_J(H)P^\perp$ converges in norm to zero as the size of the interval J shrinks to zero around λ. Therefore there is $c' > 0$ and an open interval J' containing λ, with $J' \subset J$, such that

$$E_{J'}(H')[H', \mathrm{i}A]_\circ E_{J'}(H') \geqslant c'E_{J'}(H').$$

In other words, a strict Mourre estimate holds for H' on J'. Now $H' := HP^\perp = H - HP$. Note that P is a finite sum of rank one projectors because $\lambda \in \mu^A(H)$. Thanks to the assumption $\ker(H - \lambda) \subset \mathcal{D}(A)$, we have by Lemma 5.1 that $P \in \mathcal{C}^{1,\mathrm{u}}(A)$. Thus $H' \in \mathcal{C}^{1,\mathrm{u}}(A)$. Performing the same calculation as in Step 1 with (H', J') instead of (H, J) gives

$$\lim_{t\to+\infty} \|\langle A\rangle^{-s}e^{-\mathrm{i}tH'}E_{J'}(H')\psi\| = 0.$$

Since $e^{-\mathrm{i}tH'}E_{J'}(H') = e^{-\mathrm{i}tH}E_{J'}(H)P^\perp$, we have

$$\lim_{t\to+\infty} \|\langle A\rangle^{-s}e^{-\mathrm{i}tH}E_{J'}(H)P^\perp\psi\| = 0.$$

The only eigenvalue of H belonging to J' is λ, so $E_{J'}(H)P^\perp = E_{J'}(H)P_\mathrm{c}(H)$. Thus

$$\lim_{t\to+\infty} \|\langle A\rangle^{-s}e^{-\mathrm{i}tH}E_{J'}(H)P_\mathrm{c}(H)\psi\| = 0. \tag{5.2}$$

Step 3: In this way, for each $\lambda \in \mathcal{I}$, we obtain an open interval J_λ or J'_λ containing λ such that (5.1) or (5.2) holds true, depending on whether λ is an eigenvalue of H or not. To conclude, as

$$\left(\bigcup_{\substack{\lambda\in\mathcal{I},\\ \lambda\in\sigma_{\mathrm{c}}(H)}} J_\lambda\right)\bigcup\left(\bigcup_{\substack{\lambda\in\mathcal{I},\\ \lambda\in\sigma_{\mathrm{pp}}(H)}} J'_\lambda\right)$$

is an open cover of $\mathcal{I}$, we may choose a finite sub-cover. If $\{J_i\}_{i=1}^n$ denotes this sub-cover, we may further shrink these intervals so that $J_i\cap J_j=\emptyset$ for $i\neq j$, $\overline{\cup J_i}=\mathcal{I}$, and $\overline{J_i}\cap\overline{J_j}\in\sigma_{\mathrm{c}}(H)$ for i $\neq j$. Thus $E_{\mathcal{I}}(H)P_{\mathrm{c}}(H)=\sum_i^n E_{J_i}(H)P_{\mathrm{c}}(H)$. Then, by applying (5.1) and (5.2) we get

$$\lim_{t\to+\infty}\|\langle A\rangle^{-s}e^{-\mathrm{i}tH}E_{\mathcal{I}}(H)P_{\mathrm{c}}(H)\psi\|\leqslant\lim_{t\to+\infty}\sum_{i=1}^n\|\langle A\rangle^{-s}e^{-\mathrm{i}tH}E_{J_i}(H)P_{\mathrm{c}}(H)\psi\|=0.$$

This proves the estimate (1.5).

Step 4: We turn to the proof of (1.6). Since, A is self-adjoint, $\mathcal{D}(A)$ is dense in $\mathcal{H}$. Let $\{\phi_n\}_{n=1}^\infty\subset\mathcal{D}(A)$ be an orthonormal set. Let $W\in\mathcal{K}(\mathcal{H})$ and denote $F_N:=\sum_{n=1}^N\langle\phi_n,\cdot\rangle W\phi_n$. The proof of [RS1, Theorem VI.13] shows that $\|W-F_N\|\to0$ as $N\to+\infty$. Then

$$\begin{aligned}\|WP_{\mathrm{c}}(H)E_{\mathcal{I}}(H)e^{-\mathrm{i}tH}\psi\|&\leqslant\|(W-F_N)P_{\mathrm{c}}(H)E_{\mathcal{I}}(H)e^{-\mathrm{i}tH}\psi\|+\|F_NP_{\mathrm{c}}(H)E_{\mathcal{I}}(H)e^{-\mathrm{i}tH}\psi\|\\&\leqslant\underbrace{\|W-F_N\|}_{\to 0\text{ as }N\to+\infty}+\|F_N\langle A\rangle\|\underbrace{\|\langle A\rangle^{-1}P_{\mathrm{c}}(H)E_{\mathcal{I}}(H)e^{-\mathrm{i}tH}\psi\|}_{\to 0\text{ as }t\to+\infty}.\end{aligned}$$

The result follows by noting that $F_N\langle A\rangle$ is a bounded operator for each N. If W is H-relatively compact, use the fact that $E_{\mathcal{I}}(H)(H+\mathrm{i})$ is a bounded operator. □

6. Proof of Theorem 1.3

To prove the result, we will need the following fact:

Lemma 6.1. *Let T be a self-adjoint operator with $T\in\mathcal{C}^1(A)$. Let $\lambda\in\mu^A(T)$ and suppose that* $\ker(T-\lambda)\subset\mathcal{D}(A)$. *Then there is an interval $\mathcal{I}\subset\mu^A(T)$ containing λ such that $P_{\mathrm{c}}^\perp(T)E_{\mathcal{I}}(T)$ and $P_{\mathrm{c}}(T)\eta(T)$ are of class $\mathcal{C}^1(A)$ for all $\eta\in C_c^\infty(\mathbb{R})$ with supp$(\eta)\subset\mathcal{I}$.*

Proof. Since there are finitely many eigenvalues of T in a neighborhood of λ, there is a bounded interval $\mathcal{I}$ containing λ such that $\ker(T-\lambda')\subset\mathcal{D}(A)$ for all $\lambda'\in\mathcal{I}$. Then $P_{\mathrm{c}}^\perp(T)E_{\mathcal{I}}(T)$ is a finite rank operator and belongs to the class $\mathcal{C}^1(A)$ by Lemma 5.1. Moreover $T\in\mathcal{C}^1(A)$ implies $\eta(T)\in\mathcal{C}^1(A)$, by the Helffer-Sjöstrand formula. So $P_{\mathrm{c}}^\perp(T)E_{\mathcal{I}}(T)\eta(T)\in\mathcal{C}^1(A)$ as the product of two bounded operators in this class. Finally, $P_{\mathrm{c}}(T)\eta(T)=\eta(T)-P_{\mathrm{c}}^\perp(T)E_{\mathcal{I}}(T)\eta(T)$ is a difference of two bounded operators in $\mathcal{C}^1(A)$, so $P_{\mathrm{c}}(T)\eta(T)\in\mathcal{C}^1(A)$. □

Proof of Theorem 1.3. Since H_0 is semi-bounded and $\sigma_{\mathrm{ess}}(H)=\sigma_{\mathrm{ess}}(H_0)$, there is $\varsigma\in\mathbb{R}\setminus(\sigma(H)\cup\sigma(H_0))$. Denote the resolvents of H and H_0 respectively by $R(z):=(z-H)^{-1}$ and $R_0(z):=(z-H_0)^{-1}$. Also denote the spectral projector of $R(z)$ onto the continuous spectrum by $P_{\mathrm{c}}(R(z))$. We split the proof into four parts. First we translate the problem in terms of the resolvent $R(\varsigma)$. Second we show the following formula:

$$\begin{aligned}&P_{\mathrm{c}}(R(\varsigma))\theta(R(\varsigma))[R(\varsigma),\mathrm{i}\varphi(A/L)]_\circ\theta(R(\varsigma))P_{\mathrm{c}}(R(\varsigma))\geqslant\\&\qquad L^{-1}P_{\mathrm{c}}(R(\varsigma))\theta(R(\varsigma))\Big(C\langle A/L\rangle^{-2s}+K\Big)\theta(R(\varsigma))P_{\mathrm{c}}(R(\varsigma)),\end{aligned}\tag{6.1}$$

where θ is a smooth function compactly supported about $(\varsigma-\lambda)^{-1}$, φ is an appropriately chosen smooth bounded function, $L \in \mathbb{R}^{+}$ is sufficiently large, K is a compact operator uniformly bounded in L, $C > 0$, and $s \in (1/2, 1)$. θ, φ, C and s are independent of L. This formula is expressed in terms of the resolvent $R(\varsigma)$. Third, we look to convert it into a formula for H. We show that the latter formula implies the existence of an open interval J containing λ such that

$$\begin{aligned} P_{\mathrm{c}}(H)E_J(H)[R(\varsigma), \mathrm{i}\varphi(A/L)]_{\circ}E_J(H)P_{\mathrm{c}}(H) \geqslant \\ L^{-1}P_{\mathrm{c}}(H)E_J(H)\Big(C\langle A/L\rangle^{-2s}+K\Big)E_J(H)P_{\mathrm{c}}(H). \end{aligned} \tag{6.2}$$

We note that the operator K is the same in (6.1) and (6.2). Fourth, we insert the dynamics into the previous formula and average over time. We notably use the RAGE Theorem (B.1) to derive the desired formula, i.e.

$$\lim_{T\to\pm\infty} \sup_{\|\psi\|\leqslant 1} \frac{1}{T}\int_0^T \|\langle A\rangle^{-s}e^{-\mathrm{i}tH}P_{\mathrm{c}}(H)E_J(H)\psi\|^2 dt = 0. \tag{6.3}$$

Part 1: Let $\lambda \in \mu^A(H)$ be such that $\ker(H-\lambda) \subset \mathcal{D}(A)$. Then there are finitely many eigenvalues in a neighborhood of λ including multiplicity. We may find an interval $\mathcal{I} = (\lambda_0, \lambda_1)$ containing λ such that $\mathcal{I} \subset \mu^A(H)$ and for all $\lambda' \in \mathcal{I}$, $\ker(H-\lambda') \subset \mathcal{D}(A)$. Define

$$f : \mathbb{R}\setminus\{\varsigma\} \mapsto \mathbb{R}, \quad f : x \mapsto 1/(\varsigma - x). \tag{6.4}$$

Since eigenvalues of H located in $\mathcal{I}$ are in one-to-one correspondence with the eigenvalues of $R(\varsigma)$ located in $f(\mathcal{I}) = (f(\lambda_0), f(\lambda_1))$, it follows that $f(\mathcal{I})$ is an interval containing $f(\lambda)$ such that $f(\mathcal{I}) \subset \mu^A(R(\varsigma))$ and $\ker(R(\varsigma)-\lambda') \subset \mathcal{D}(A)$ for all $\lambda' \in f(\mathcal{I})$. Note the use of Proposition 3.1.

To simplify the notation in what follows, we let $R := R(\varsigma)$, $R_0 := R_0(\varsigma)$ and $P_{\mathrm{c}} := P_{\mathrm{c}}(R(\varsigma))$, as ς is fixed. Also let $R_A(z) := (z - A/L)^{-1}$, where $L \in \mathbb{R}^{+}$.

Part 2: Let $\theta, \eta, \chi \in C_c^{\infty}(\mathbb{R})$ be bump functions such that $f(\lambda) \in \mathrm{supp}(\theta) \subset \mathrm{supp}(\eta) \subset \mathrm{supp}(\chi) \subset f(\mathcal{I})$, $\eta\theta = \theta$ and $\chi\eta = \eta$. Let $s \in (1/2, 1)$ be given. Define

$$\varphi : \mathbb{R} \mapsto \mathbb{R}, \qquad \varphi : t \mapsto \int_{-\infty}^{t} \langle x\rangle^{-2s} dx.$$

Note that $\varphi \in \mathcal{S}^0(\mathbb{R})$. The definition of $\mathcal{S}^0(\mathbb{R})$ is given in (C.1). Consider the bounded operator

$$F := P_{\mathrm{c}}\theta(R)[R, \mathrm{i}\varphi(A/L)]_{\circ}\theta(R)P_{\mathrm{c}} = \frac{\mathrm{i}}{2\pi L}\int_{\mathbb{C}} \frac{\partial\tilde{\varphi}}{\partial\overline{z}}(z)P_{\mathrm{c}}\theta(R)R_A(z)[R, \mathrm{i}A]_{\circ}R_A(z)\theta(R)P_{\mathrm{c}}\; dz\wedge d\overline{z}.$$

By Lemma 6.1 with $T = R$, $P_{\mathrm{c}}\eta(R) \in C^1(A)$, so

$$[P_{\mathrm{c}}\eta(R), R_A(z)]_{\circ} = L^{-1}R_A(z)[P_{\mathrm{c}}\eta(R), A]_{\circ}R_A(z).$$

In the formula defining F, we introduce $P_{\mathrm{c}}\eta(R)$ next to $P_{\mathrm{c}}\theta(R)$ and commute it with $R_A(z)$:

$$\begin{aligned} F &= \frac{\mathrm{i}}{2\pi L}\int_{\mathbb{C}} \frac{\partial\tilde{\varphi}}{\partial\overline{z}}(z)P_{\mathrm{c}}\theta(R)\Big(R_A(z)P_{\mathrm{c}}\eta(R) + [P_{\mathrm{c}}\eta(R), R_A(z)]_{\circ}\Big)[R, \mathrm{i}A]_{\circ}\times \\ &\qquad \Big(\eta(R)P_{\mathrm{c}}R_A(z) + [R_A(z), P_{\mathrm{c}}\eta(R)]_{\circ}\Big)\theta(R)P_{\mathrm{c}}\; dz\wedge d\overline{z} \\ &= \frac{\mathrm{i}}{2\pi L}\int_{\mathbb{C}} \frac{\partial\tilde{\varphi}}{\partial\overline{z}}(z)P_{\mathrm{c}}\theta(R)R_A(z)P_{\mathrm{c}}\eta(R)[R, \mathrm{i}A]_{\circ}\eta(R)P_{\mathrm{c}}R_A(z)\theta(R)P_{\mathrm{c}}\; dz\wedge d\overline{z} \\ &\quad + L^{-1}P_{\mathrm{c}}\theta(R)\,(I_1 + I_2 + I_3)\,\theta(R)P_{\mathrm{c}}, \end{aligned}$$

where

$$I_1 = \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial\tilde{\varphi}}{\partial\bar{z}}(z)[P_{\mathrm{c}}\eta(R), R_A(z)]_\circ[R,\mathrm{i}A]_\circ\eta(R)P_{\mathrm{c}}R_A(z)\, dz\wedge d\bar{z},$$
$$I_2 = \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial\tilde{\varphi}}{\partial\bar{z}}(z)[P_{\mathrm{c}}\eta(R), R_A(z)]_\circ[R,\mathrm{i}A]_\circ\, dz\wedge d\bar{z},$$
$$I_3 = \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial\tilde{\varphi}}{\partial\bar{z}}(z)R_A(z)P_{\mathrm{c}}\eta(R)[R,\mathrm{i}A]_\circ[R_A(z), P_{\mathrm{c}}\eta(R)]_\circ\, dz\wedge d\bar{z}.$$

Applying (C.5) and Lemma C.4, and recalling that $s<1$, we have for some operators B_i uniformly bounded with respect to L that

$$I_i = \left\langle\frac{A}{L}\right\rangle^{-s}\frac{B_i}{L}\left\langle\frac{A}{L}\right\rangle^{-s}, \quad \text{for } i=1,2,3.$$

Using $\chi\eta=\eta$, we insert $\chi(R)$ next to $\eta(R)$. So far we get the following expression for F :

$$F = \frac{\mathrm{i}}{2\pi L}\int_{\mathbb{C}} \frac{\partial\tilde{\varphi}}{\partial\bar{z}}(z)P_c\theta(R)R_A(z)P_{\mathrm{c}}\chi(R)\underbrace{\eta(R)[R,\mathrm{i}A]_\circ\eta(R)}_{\text{to be developed}}\chi(R)P_{\mathrm{c}}R_A(z)\theta(R)P_{\mathrm{c}}\, dz\wedge d\bar{z}$$
$$+ P_{\mathrm{c}}\theta(R)\left\langle\frac{A}{L}\right\rangle^{-s}\left(\frac{B_1+B_2+B_3}{L^2}\right)\left\langle\frac{A}{L}\right\rangle^{-s}\theta(R)P_{\mathrm{c}}.$$

Now write

$$\eta(R)[R,\mathrm{i}A]_\circ\eta(R) = \eta(R)R[H,\mathrm{i}A]_\circ R\eta(R) = \eta(R)R[H_0,\mathrm{i}A]_\circ R\eta(R) + \eta(R)R[V,\mathrm{i}A]_\circ R\eta(R).$$

Let us start with the second term on the r.h.s. of this equation. It decomposes into

$$\eta(R)R[V,\mathrm{i}A]_\circ R\eta(R) = \eta(R)\underbrace{R\langle H\rangle}_{\in\mathcal{B}(\mathcal{H})}\langle H\rangle^{-1/2}\underbrace{\langle H\rangle^{-1/2}\langle H_0\rangle^{1/2}}_{\in\mathcal{B}(\mathcal{H})}\underbrace{\langle H_0\rangle^{-1/2}[V,\mathrm{i}A]_\circ\langle H_0\rangle^{-1/2}}_{\in\mathcal{K}(\mathcal{H})\text{ by A6}'}\times$$
$$\times\underbrace{\langle H_0\rangle^{1/2}\langle H\rangle^{-1/2}}_{\in\mathcal{B}(\mathcal{H})}\langle H\rangle^{-1/2}\underbrace{\langle H\rangle R}_{\in\mathcal{B}(\mathcal{H})}\eta(R).$$

It is therefore compact. As for the first term on the r.h.s., it decomposes as follows

$$\eta(R)R[H_0,\mathrm{i}A]_\circ R\eta(R) = \eta(R_0)R_0[H_0,\mathrm{i}A]_\circ R_0\eta(R_0) + \Xi_1 + \Xi_2,$$

where

$$\Xi_1 := (\eta(R)R-\eta(R_0)R_0)[H_0,\mathrm{i}A]_\circ R\eta(R) \quad\text{and}\quad \Xi_2 := \eta(R_0)R_0[H_0,\mathrm{i}A]_\circ(R\eta(R)-R_0\eta(R_0)).$$

We show tht Ξ_1 is compact, and similarly one shows that Ξ_2 is compact. We have

$$\Xi_1 = \underbrace{(\eta(R)R-\eta(R_0)R_0)\langle H_0\rangle^{1/2}}_{\in\mathcal{K}(\mathcal{H})}\underbrace{\langle H_0\rangle^{-1/2}[H_0,\mathrm{i}A]_\circ\langle H_0\rangle^{-1/2}}_{\in\mathcal{B}(\mathcal{H})\text{ by A5}}\underbrace{\langle H_0\rangle^{1/2}\langle H\rangle^{-1/2}}_{\in\mathcal{B}(H)}\langle H\rangle^{-1/2}\underbrace{\langle H\rangle R}_{\in\mathcal{B}(\mathcal{H})}\eta(R).$$

Let us justify that $(\eta(R)R - \eta(R_0)R_0)\langle H_0\rangle^{1/2}$ is compact. Let $\kappa : x \mapsto x\eta(x)$. By the Helffer-Sjöstrand formula,

$$\begin{aligned}(\eta(R)R - \eta(R_0)R_0)\langle H_0\rangle^{1/2} &= \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial\tilde{\kappa}}{\partial\overline{z}}(z)\left((z-R)^{-1} - (z-R_0)^{-1}\right)\langle H_0\rangle^{1/2}\, dz\wedge d\overline{z} \\ &= \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial\tilde{\kappa}}{\partial\overline{z}}(z)(z-R)^{-1}RVR_0(z-R_0)^{-1}\langle H_0\rangle^{1/2}\, dz\wedge d\overline{z} \\ &= \frac{\mathrm{i}}{2\pi}\int_{\mathbb{C}} \frac{\partial\tilde{\kappa}}{\partial\overline{z}}(z)(z-R)^{-1}\underbrace{R\langle H\rangle^{1/2}}_{\in\,\mathcal{B}(\mathcal{H})}\underbrace{\langle H\rangle^{-1/2}\langle H_0\rangle^{1/2}}_{\in\,\mathcal{B}(H)}\times \\ &\quad\times \underbrace{\langle H_0\rangle^{-1/2}V\langle H_0\rangle^{-1/2}}_{\in\,\mathcal{K}(\mathcal{H})\text{ by A3}}\underbrace{\langle H_0\rangle^{1/2}R_0\langle H_0\rangle^{1/2}}_{\in\,\mathcal{B}(\mathcal{H})}(z-R_0)^{-1}\, dz\wedge d\overline{z}.\end{aligned}$$

The integrand of this integral is compact for all $z\in\mathbb{C}\setminus\mathbb{R}$, and moreover the integral converges in norm since κ has compact support. It follows that $(\eta(R)R - \eta(R_0)R_0)\langle H_0\rangle^{1/2}$, and thus Ξ_1, is compact. Thus we have shown that

$$\eta(R)[R,\mathrm{i}A]_\circ\eta(R) = \eta(R_0)[R_0,\mathrm{i}A]_\circ\eta(R_0) + \text{compact}. \tag{6.5}$$

Therefore there is a compact operator K_1 uniformly bounded in L such that

$$\begin{aligned}F &= \frac{\mathrm{i}}{2\pi L}\int_{\mathbb{C}}\frac{\partial\tilde{\varphi}}{\partial\overline{z}}(z)P_{\mathrm{c}}\theta(R)R_A(z)MR_A(z)\theta(R)P_{\mathrm{c}}\, dz\wedge d\overline{z} \\ &\quad + P_{\mathrm{c}}\theta(R)\frac{K_1}{L}\theta(R)P_{\mathrm{c}} \;+\; P_{\mathrm{c}}\theta(R)\left\langle\frac{A}{L}\right\rangle^{-s}\left(\frac{B_1+B_2+B_3}{L^2}\right)\left\langle\frac{A}{L}\right\rangle^{-s}\theta(R)P_{\mathrm{c}}.\end{aligned}$$

Here $M := P_{\mathrm{c}}\chi(R)\eta(R_0)[R_0,\mathrm{i}A]_\circ\eta(R_0)\chi(R)P_{\mathrm{c}}$. Since $P_{\mathrm{c}}\chi(R),\eta(R_0)$ and $[R_0,\mathrm{i}A]_\circ$ belong to $\mathcal{C}^1(A)$, it follows by product that $M\in\mathcal{C}^1(A)$ and we may commute $R_A(z)$ with M:

$$\begin{aligned}F &= \frac{\mathrm{i}}{2\pi L}\int_{\mathbb{C}}\frac{\partial\tilde{\varphi}}{\partial\overline{z}}(z)P_{\mathrm{c}}\theta(R)R_A(z)^2M\theta(R)P_{\mathrm{c}}\, dz\wedge d\overline{z} \\ &\quad + \frac{\mathrm{i}}{2\pi L}\int_{\mathbb{C}}\frac{\partial\tilde{\varphi}}{\partial\overline{z}}(z)P_{\mathrm{c}}\theta(R)R_A(z)[M,R_A(z)]_\circ\theta(R)P_{\mathrm{c}}\, dz\wedge d\overline{z} \\ &\quad + P_{\mathrm{c}}\theta(R)\frac{K_1}{L}\theta(R)P_{\mathrm{c}} \;+\; P_{\mathrm{c}}\theta(R)\left\langle\frac{A}{L}\right\rangle^{-s}\left(\frac{B_1+B_2+B_3}{L^2}\right)\left\langle\frac{A}{L}\right\rangle^{-s}\theta(R)P_{\mathrm{c}}.\end{aligned}$$

We apply (C.8) to the first integral (which converges in norm), while for the second integral we use the fact that $M\in\mathcal{C}^1(A)$ to conclude that there exists an operator B_4 uniformly bounded in L such that

$$\begin{aligned}F &= L^{-1}P_{\mathrm{c}}\theta(R)\varphi'(A/L)M\theta(R)P_{\mathrm{c}} \\ &\quad + P_{\mathrm{c}}\theta(R)\frac{K_1}{L}\theta(R)P_{\mathrm{c}} \;+\; P_{\mathrm{c}}\theta(R)\left\langle\frac{A}{L}\right\rangle^{-s}\left(\frac{B_1+B_2+B_3+B_4}{L^2}\right)\left\langle\frac{A}{L}\right\rangle^{-s}\theta(R)P_{\mathrm{c}}.\end{aligned}$$

Now $\varphi'(A/L) = \langle A/L\rangle^{-2s}$. As a result of the Helffer-Sjöstrand formula, (C.5) and (C.10),

$$[\langle A/L\rangle^{-s}, M]_\circ\langle A/L\rangle^{s} = L^{-1}B_5$$

for some operator B_5 uniformly bounded in L. Thus commuting $\langle A/L\rangle^{-s}$ and M gives

$$\begin{aligned}F &= L^{-1}P_c\theta(R)\Big\langle\frac{A}{L}\Big\rangle^{-s}M\Big\langle\frac{A}{L}\Big\rangle^{-s}\theta(R)P_c\\ &\quad + P_c\theta(R)\frac{K_1}{L}\theta(R)P_c \;+\; P_c\theta(R)\Big\langle\frac{A}{L}\Big\rangle^{-s}\left(\frac{B_1+B_2+B_3+B_4+B_5}{L^2}\right)\Big\langle\frac{A}{L}\Big\rangle^{-s}\theta(R)P_c\\ &\geqslant cL^{-1}P_c\theta(R)\Big\langle\frac{A}{L}\Big\rangle^{-s}P_c\chi(R)\eta(R_0)^2\chi(R)P_c\Big\langle\frac{A}{L}\Big\rangle^{-s}\theta(R)P_c\\ &\quad + P_c\theta(R)\frac{K_1+K_2}{L}\theta(R)P_c \;+\; P_c\theta(R)\Big\langle\frac{A}{L}\Big\rangle^{-s}\left(\frac{B_1+B_2+B_3+B_4+B_5}{L^2}\right)\Big\langle\frac{A}{L}\Big\rangle^{-s}\theta(R)P_c,\end{aligned}$$

where $c>0$ and K_2 come from applying the Mourre estimate (3.1) to R_0 on $f(\mathcal{I})$. Exchanging $\eta(R_0)^2$ for $\eta(R)^2$, we have a compact operator K_3 uniformly bounded in L such that

$$\begin{aligned}F &\geqslant cL^{-1}P_c\theta(R)\Big\langle\frac{A}{L}\Big\rangle^{-s}P_c\chi(R)\eta(R)^2\chi(R)P_c\Big\langle\frac{A}{L}\Big\rangle^{-s}\theta(R)P_c \;+\; P_c\theta(R)\frac{K_1+K_2+K_3}{L}\theta(R)P_c\\ &\quad + P_c\theta(R)\Big\langle\frac{A}{L}\Big\rangle^{-s}\left(\frac{B_1+B_2+B_3+B_4+B_5}{L^2}\right)\Big\langle\frac{A}{L}\Big\rangle^{-s}\theta(R)P_c.\end{aligned}$$

We commute $P_c\chi(R)\eta(R)^2\chi(R)P_c = P_c\eta(R)^2P_c$ with $\langle A/L\rangle^{-s}$, and see that

$$[P_c\eta(R)^2P_c, \langle A/L\rangle^{-s}]_\circ\langle A/L\rangle^{s} = L^{-1}B_6$$

for some operator B_6 uniformly bounded in L. Thus

$$\begin{aligned}F &\geqslant cL^{-1}P_c\theta(R)\Big\langle\frac{A}{L}\Big\rangle^{-2s}\theta(R)P_c \;+\; P_c\theta(R)\frac{K_1+K_2+K_3}{L}\theta(R)P_c\\ &\quad + P_c\theta(R)\Big\langle\frac{A}{L}\Big\rangle^{-s}\left(\frac{B_1+B_2+B_3+B_4+B_5+B_6}{L^2}\right)\Big\langle\frac{A}{L}\Big\rangle^{-s}\theta(R)P_c.\end{aligned}$$

Taking L large enough gives $C>0$ such that $c+(B_1+B_2+B_3+B_4+B_5+B_6)/L \geqslant C$. Denoting $K := K_1+K_2+K_3$ yields formula (6.1).

Part 3: For all open intervals (e_1,e_2) located strictly above or below ς we have the identity

$$E_{(e_1,e_2)}(H) = E_{(f(e_1),f(e_2))}(R(\varsigma)), \tag{6.6}$$

where f is the function defined in (6.4). Now let $\mathcal{J} := \text{interior}(\theta^{-1}\{1\})$. This is an open interval and we have $E_{\mathcal{J}}(R)\theta(R) = E_{\mathcal{J}}(R)$. Thus applying $E_{\mathcal{J}}(R)$ to (6.1) gives

$$P_cE_{\mathcal{J}}(R)[R,\mathrm{i}\varphi(A/L)]_\circ E_{\mathcal{J}}(R)P_c \geqslant L^{-1}P_cE_{\mathcal{J}}(R)\left(C\langle A/L\rangle^{-2s}+K\right)E_{\mathcal{J}}(R)P_c.$$

We have that $P_cE_{\mathcal{J}}(R) := P_c(R)E_{\mathcal{J}}(R)$ is a spectral projector of R onto a finite disjoint union of open intervals. Let $\{\lambda_i\}$ be the (finite) collection of eigenvalues of R located in $\mathcal{J}$. Then $\{f^{-1}(\lambda_i)\}$ are the eigenvalues of H located in $f^{-1}(\mathcal{J})$, and by (6.6),

$$P_c(R)E_{\mathcal{J}}(R) = \sum_i E_{\mathcal{J}_i}(R) = \sum_i E_{f^{-1}(\mathcal{J}_i)}(H) = P_c(H)E_{f^{-1}(\mathcal{J})}(H),$$

where the $\mathcal{J}_i$ are the open intervals such that $\cup_i\mathcal{J}_i\cup\{\lambda_i\} = \mathcal{J}$. Denoting the open interval $J := f^{-1}(\mathcal{J})$ proves formula (6.2). Note that $\lambda\in J$.

Part 4: Let F' be the l.h.s. of (6.2), i.e.

$$F' := P_c(H)E_J(H)[R(\varsigma),\mathrm{i}\varphi(A/L)]_\circ E_J(H)P_c(H).$$

Formula (6.2) implies that for all $\psi \in \mathcal{H}$ and all $T > 0$:

$$\frac{L}{T}\int_0^T \langle e^{-\mathrm{i}tH}\psi, F' e^{-\mathrm{i}tH}\psi\rangle dt \geqslant \frac{C}{T}\int_0^T \left\| \langle A/L\rangle^{-s} E_J(H) P_{\mathrm{c}}(H) e^{-\mathrm{i}tH}\psi \right\|^2 dt + \\ + \frac{1}{T}\int_0^T \langle E_J(H)P_{\mathrm{c}}(H)e^{-\mathrm{i}tH}\psi, K E_J(H) P_{\mathrm{c}}(H) e^{-\mathrm{i}tH}\psi\rangle \, dt.$$

First, for all $L \geqslant 1$,

$$\frac{L}{T}\int_0^T e^{\mathrm{i}tH} F' e^{-\mathrm{i}tH} \, dt = \frac{L}{T}\left[e^{\mathrm{i}tH} P_{\mathrm{c}}(H) E_J(H) R(\varsigma)\varphi(A/L) R(\varsigma) E_J(H) P_{\mathrm{c}}(H) e^{-\mathrm{i}tH}\right]_0^T \xrightarrow[T\to\pm\infty]{} 0.$$

Second, by the RAGE Theorem (B.1),

$$\begin{aligned} &\sup_{\|\psi\|\leqslant 1} \frac{1}{T}\int_0^T \langle E_J(H)P_{\mathrm{c}}(H)e^{-\mathrm{i}tH}\psi, K E_J(H)P_{\mathrm{c}}(H)e^{-\mathrm{i}tH}\psi\rangle \, dt \\ &\qquad \leqslant \sup_{\|\psi\|\leqslant 1} \frac{1}{T}\int_0^T \|K E_J(H) e^{-\mathrm{i}tH} P_{\mathrm{c}}(H)\psi\| \, dt \\ &\qquad \leqslant \sup_{\|\psi\|\leqslant 1} \left(\frac{1}{T}\int_0^T \|K E_J(H) e^{-\mathrm{i}tH} P_{\mathrm{c}}(H)\psi\|^2 \, dt\right)^{1/2} \xrightarrow[T\to\pm\infty]{} 0. \end{aligned}$$

It follows that for L sufficiently large (but finite),

$$\lim_{T\to\pm\infty} \sup_{\|\psi\|\leqslant 1} \frac{1}{T}\int_0^T \left\| \left\langle \frac{A}{L}\right\rangle^{-s} e^{-\mathrm{i}tH} P_{\mathrm{c}}(H) E_J(H)\psi \right\|^2 dt = 0.$$

Finally (6.3) follows by noting that $\langle A\rangle^{-s}\langle A/L\rangle^{s}$ is a bounded operator. □

7. A discussion about the compactness of operators of the form $\langle A\rangle^{-s} E_{\mathcal{I}}(H)$

As pointed out in the Introduction, the novelty of formula (1.12) is conditional on the non-relative compactness of the operator $\langle A\rangle^{-s}E_{\mathcal{I}}(H)$. The non-compactness of $\langle A\rangle^{-s}E_{\mathcal{I}}(H)$ is also what sets (1.5) apart from (1.6). We start by noting that $\langle A\rangle^{-s}E_{\mathcal{I}}(H)$ is H-relatively compact if and only if it is compact, since $\mathcal{I} \subset \mathbb{R}$ is a bounded interval.

We will allow ourselves to consider operators of the form $\langle A\rangle^{-s}\chi(H)$, where χ is a smooth function, rather than $\langle A\rangle^{-s}E_{\mathcal{I}}(H)$. On the one hand, if $\langle A\rangle^{-s}E_{\mathcal{I}}(H)$ is compact, then so is $\langle A\rangle^{-s}\chi(H)$, where χ is any smooth function that has support contained in $\mathcal{I}$. On the other hand, if $\langle A\rangle^{-s}\chi(H)$ is compact, where χ is a smooth bump function that approximates the characteristic function of $\mathcal{I}$ and equals one above $\mathcal{I}$, then so is $\langle A\rangle^{-s}E_{\mathcal{I}}(H)$.

We will also suppose that $H = H_0 + V$, where V is some H_0-form compact operator, and H_0 is viewed as the "free" operator. In other words we will work under the assumption A3. The reason for doing so is that H_0 is much easier to work with than H in practice. In this case we note that $\langle A\rangle^{-s}\chi(H)$ is compact if and only if $\langle A\rangle^{-s}\chi(H_0)$. We therefore have the question: Is $\langle A\rangle^{-s}\chi(H_0)$ a compact operator? A first result is:

Proposition 7.1. *Let H_0, A be self-adjoint operators in $\mathcal{H}$. Suppose that H_0 has a spectral gap. Suppose that $H_0 \in \mathcal{C}^1(A)$ and that for some $\lambda \in \mathbb{R}$, $[(H_0-\lambda)^{-1}, \mathrm{i}A]_\circ := C \geqslant 0$ is an injective operator. Then A does not have any eigenvalues. In particular, $\langle A\rangle^{-s} \notin \mathcal{K}(\mathcal{H})$ for any $s > 0$.*

Remark 7.1. *The examples of Section 4 satisfy the hypotheses of Proposition 7.1. The positivity of C holds because $\sigma(H_0) \subset [0, +\infty)$. The injectivity holds because 0 is not an eigenvalue of H_0.*

Proof. Let ψ be an eigenvector of A. Since $A \in \mathcal{C}^1((H_0 - \lambda)^{-1})$, the Virial Theorem ([ABG, Proposition 7.2.10]) says that $0 = \langle \psi, [(H_0 - \lambda)^{-1}, \mathrm{i}A]_\circ \psi \rangle = \langle \psi, C\psi \rangle = \|\sqrt{C}\psi\|^2$. The injectivity of $\sqrt{C}$ forces $\psi = 0$, i.e. $\sigma_{\mathrm{p}}(A) = \emptyset$. Now, it is known that the spectrum of a self-adjoint operator with compact resolvent consists solely of isolated eigenvalues of finite multiplicity, see e.g. [K, Theorem 6.29]. So if A had compact resolvent, then we would have $\sigma(A) = \sigma_{\mathrm{p}}(A) = \emptyset$. However this is not possible because the spectrum of a self-adjoint operator is non-empty. We conclude that A does not have compact resolvent. Writing $(z - A)^{-1} = (z - A)^{-1}\langle A \rangle \langle A \rangle^{-1}$, we infer that $\langle A \rangle^{-1} \notin \mathcal{K}(\mathcal{H})$. Finally, consider the bounded self-adjoint operator $\langle A \rangle^{-s}$ for some $s > 0$. If this operator were compact, then by the spectral theorem for such operators we would have $\langle A \rangle^{-s} = \sum_i \lambda_i \langle \phi_i, \cdot \rangle \phi_i$ for some eigenvalues $\{\lambda_i\}$ and eigenvectors $\{\phi_i\}$ which form an orthonormal basis of $\mathcal{H}$. But then $\langle A \rangle^{-1} = \sum_i \lambda_i^{1/s} \langle \phi_i, \cdot \rangle \phi_i$, implying that the latter operator is compact. This contradiction proves $\langle A \rangle^{-s} \notin \mathcal{K}(\mathcal{H})$ for all $s > 0$. □

Unfortunately, this result does not settle the debate because it does not guarantee the non-compactness of $\langle A \rangle^{-s}\chi(H_0)$. In fact, we have examples where this operator is compact. For lack of a more robust result, we shall spend the rest of this section examining several examples. Our conclusion is that $\langle A \rangle^{-s}\chi(H_0)$ is sometimes compact, sometimes not. Specifically, in each of our examples, the compactness holds in dimension one but does not in higher dimensions. To start off, we cook up a simple example that will reinforce the viewpoint that non-compactness is possible, especially in higher dimensions.

Example 7.2. *Let $\mathcal{H} := L^2(\mathbb{R}^2)$, $H_0 := -\partial^2/\partial x_1^2$ and $A := -\mathrm{i}(x_1\partial/\partial x_1 + \partial/\partial x_1 x_1)$ be a conjugate operator to H_0. The spectrum of H_0 is purely absolutely continuous and $\sigma(H_0) = [0, +\infty)$. In particular, $\ker(H_0 - \lambda) = \emptyset$ for all $\lambda \in \mathbb{R}$. Also $[H_0, \mathrm{i}A]_\circ = 2H_0$ exists as a bounded operator from $\mathcal{D}(\langle H_0 \rangle^{1/2})$ to $\mathcal{D}(\langle H_0 \rangle^{1/2})^*$, implying that $H_0 \in \mathcal{C}^\infty(A)$ and that the Mourre estimate holds for all positive intervals supported away from zero. In addition, $\{e^{\mathrm{i}tA}\}_{t \in \mathbb{R}}$ stabilizes $\mathcal{D}(H_0)$. The assumptions of Theorems 1.2 and 1.3 are therefore thoroughly verified. Moreover $\langle A \rangle^{-s}\chi(H_0)$ is clearly not compact in $L^2(\mathbb{R}^2)$. This can be seen by applying $\langle A \rangle^{-s}\chi(H_0)$ to a sequence of functions $(f(x_1)g_n(x_2))_{n=1}^{+\infty}$ with g_n chosen so that $\int_{\mathbb{R}} |g_n(x_2)|^2 dx_2$ is constant.*

To continue with other examples, we set up notation. Let $\mathcal{C}_0(\mathbb{R})$ be the continuous functions vanishing at infinity and $\mathcal{C}_c^\infty(\mathbb{R})$ the compactly supported smooth functions.

Example 7.3. *Let $\mathcal{H} := L^2(\mathbb{R}^d)$, $H_0 := x_1 + ... + x_d$ and $A := \mathrm{i}(\partial/\partial x_1 + ... + \partial/\partial x_d)$. This system verifies the Mourre estimate at all energies thanks to commutator relation $[H_0, \mathrm{i}A]_\circ = dI$, and $H_0 \in \mathcal{C}^\infty(A)$ holds. Although this system does not quite fall within the framework of this article because H_0 is not semi-bounded ($\sigma(H_0) = \mathbb{R}$), it conveys the idea that compactness holds only in dimension one:*

Proposition 7.4. *Let H_0 and A be those from Example 7.3. Let $\chi \in \mathcal{C}_0(\mathbb{R})$ and $s \in \mathbb{R}$ be given. If $d = 1$, then $\langle A \rangle^{-s}\chi(H_0) \in \mathcal{K}(L^2(\mathbb{R}))$. If $d = 2$, then $\langle A \rangle^{-s}\chi(H_0) \notin \mathcal{K}(L^2(\mathbb{R}^2))$.*

Proof. The one-dimensional result is a classic, see Proposition 4.1. We prove the two-dimensional result. Let $\mathcal{I}(\lambda, r)$ denote the open interval centered at $\lambda \in \mathbb{R}$ and of radius $r > 0$. Fix λ and r such that $\mathcal{I}(\lambda, r) \subset \mathrm{supp}(\chi)$. Then the function of two variables $\chi(x_1 + x_2)$ has support containing the oblique strip $\cup_{t\in\mathcal{I}(\lambda,r)}\{(s,t-s):s\in\mathbb{R}\}\subset\mathbb{R}^2$. Let $\psi\in\mathcal{C}_c^\infty(\mathbb{R})$ be a bump function that equals one on $\mathcal{I}(\lambda,r)$ and zero on $\mathbb{R}\setminus\mathcal{I}(\lambda,2r)$. Let $\theta\in\mathcal{C}_c^\infty(\mathbb{R})$ be a bump function that equals one on $[-1,1]$ and zero on $\mathbb{R}\setminus[-2,2]$. Let $\Psi_n(x,y):=n^{-1/2}\psi(x+y)\theta(y/n)$. Then $\|\Psi_n\|\equiv\|\psi\|\|\theta\|$. Here $\|\cdot\|$ denotes the norm on $L^2(\mathbb{R}^2)$. Fix $\nu\in\mathbb{N}$, and let $\varphi_n^\nu:=(A+\mathrm{i})^\nu\Psi_n$. For $\nu=0$, clearly $\|\varphi_n^\nu\|=\|\Psi_n\|$ is uniformly bounded in n and an easy induction proves it for all fixed values of $\nu\in\mathbb{N}$. Consider now $\phi_n:=\chi(H_0)(A+\mathrm{i})^{-\nu}\varphi_n^\nu=\chi(H_0)\Psi_n$. Since $\chi\in\mathcal{C}_0(\mathbb{R})$ and $\Psi_n\stackrel{w}{\to}0$, $\phi_n\stackrel{w}{\to}0$. If $\chi(H_0)(A+\mathrm{i})^{-\nu}\in\mathcal{K}(L^2(\mathbb{R}^2))$ for some $\nu\in\mathbb{N}$, then the image of the ball $B(0,\sup_{n\geqslant1}\|\varphi_n^\nu\|)$ by this operator is pre-compact in $L^2(\mathbb{R}^2)$, and so there exists $\phi\in L^2(\mathbb{R}^2)$ and a subsequence $(n_k)_{k=1}^\infty$ such that $\lim\|\phi_{n_k}-\phi\|=0$ as $k\to+\infty$. Since $\phi_{n_k}\stackrel{w}{\to}0$, it must be that $\phi=0$ since the strong and weak limits coincide and are unique. But this contradicts the fact that $\|\phi_{n_k}\|\geqslant\|\chi\mathbf{1}_{\mathcal{I}(\lambda,r)}(\cdot)\|\|\theta\|$ for all $k\geqslant1$. So $\chi(H_0)(A+\mathrm{i})^{-\nu}\notin\mathcal{K}(L^2(\mathbb{R}^2))$, and this implies that $\chi(H_0)\langle A\rangle^{-s}\notin\mathcal{K}(L^2(\mathbb{R}^2))$ for all $s\leqslant\nu$. The result follows by taking adjoints. □

For what it is worth, we tweak Example 7.3 to create a system that fits all the assumptions of this article. We state a variation of it and leave the details of the proof to the reader.

Example 7.5. *Let $\mathcal{H}:=L^2(\mathbb{R}^d)$. Let H_0 be the operator of multiplication by $x_1h(x_1)+\ldots+x_dh(x_d)$, where $h\in\mathcal{C}^\infty(\mathbb{R})$ is a smooth version of the Heaviside function (which is zero below the origin, positive above the origin and strictly increasing). Then $\sigma(H_0)=[0,+\infty)$. In particular, H_0 is a positive operator. The conjugate operator is still $A:=\mathrm{i}(\partial/\partial x_1+\ldots+\partial/\partial x_d)$. We have $H_0\in\mathcal{C}^\infty(A)$ and the Mourre estimate holds on all positive bounded intervals. One also verifies that $\{e^{\mathrm{i}tA}\}_{t\in\mathbb{R}}$ stabilizes $\mathcal{D}(H_0)$ (note that $\{e^{\mathrm{i}tA}\}_{t\in\mathbb{R}}$ is the group of translations on $L^2(\mathbb{R}^d)$). Assumptions A1 - A5 are verified. With regard to the compactness issue, Proposition 7.4 holds, but for the two-dimensional result, one must also assume that χ has non empty support in $(0,+\infty)$.*

Our next model is the continuous Laplacian. We refer to Section 4.1 for a description of the model. The situation is the same as with the preceding example: compactness in dimension one, non-compactness in higher dimensions.

Example 7.6 (Continuous Laplacian with generator of dilations)**.** *Let $\mathcal{H}:=L^2(\mathbb{R}^d)$, $H_0:=-\Delta$ be the Laplacian and $A:=-\mathrm{i}(x\cdot\nabla+\nabla\cdot x)/2=-\mathrm{i}(2x\cdot\nabla+d)/2$ be the generator of dilations. We will be making use of the Fourier transform on $L^2(\mathbb{R}^d)$ given by*

$$(\mathcal{F}\psi)(\xi)=(2\pi)^{-d/2}\int_{\mathbb{R}^d}\psi(x)e^{-\mathrm{i}\xi\cdot x}dx. \tag{7.1}$$

Note that $\mathcal{F}A\mathcal{F}^{-1}=-A=\sum_{i=1}^d\mathrm{i}(\xi_i\partial/\partial\xi_i+\partial/\partial\xi_i\xi_i)/2$ and $\mathcal{F}H_0\mathcal{F}^{-1}=|\xi|^2:=\sum_{i=1}^d\xi_i^2$.

Proposition 7.7. *Let H_0 and A be those from Example 7.6. We have $\tau(A)\chi(H_0)\in\mathcal{K}(L^2(\mathbb{R}))$ for all $\tau,\chi\in\mathcal{C}_0(\mathbb{R})$, with χ supported away from zero.*

First proof: Let Q be the operator of multiplication by the variable x and $P:=-\mathrm{i}d/dx$. Let $\chi\in\mathcal{C}_c^\infty(\mathbb{R})$ be supported away from zero. Let $(A+\mathrm{i})^{-1}\chi(H_0)=(A+\mathrm{i})^{-1}\chi_1(P)$, where $\chi_1:=\chi\circ\sigma$ and $\sigma(\xi)=\xi^2$. We implement a binary relation $\approx$ on $\mathcal{B}(L^2(\mathbb{R}))$ whereby two operators are equivalent if their difference is a compact operator. We have:

$$\begin{aligned}(A+\mathrm{i})^{-1}\chi(H_0) &= (A+\mathrm{i})^{-1}\chi_1(P)(Q+\mathrm{i})(Q+\mathrm{i})^{-1}\\ &\approx (A+\mathrm{i})^{-1}\chi_1(P)Q(Q+\mathrm{i})^{-1}\\ &\approx (A+\mathrm{i})^{-1}Q\chi_1(P)(Q+\mathrm{i})^{-1}\\ &= (A+\mathrm{i})^{-1}(QP)\chi_2(P)(Q+\mathrm{i})^{-1}\\ &\approx (A+\mathrm{i})^{-1}(A+\mathrm{i})\chi_2(P)(Q+\mathrm{i})^{-1}\approx 0.\end{aligned}$$

Note the use of Proposition 7.4 each time a compact operator was removed. In the third step we used that $[\chi_1(P),Q]_\circ(Q+\mathrm{i})^{-1}=\chi_1'(P)(Q+\mathrm{i})^{-1}\approx 0$. In the fourth step we took advantage of the fact that χ_1 is supported away from zero to let $\chi_2(P):=P^{-1}\chi_1(P)$ and thereby allow to recreate $A:=(QP+PQ)/2=QP-\mathrm{i}/2$.

Thus we have shown that $(A+\mathrm{i})^{-1}\chi(H_0)\in\mathcal{K}(L^2(\mathbb{R}))$. It follows that $(A-z)^{-1}\chi(H_0)\in\mathcal{K}(L^2(\mathbb{R}))$ for all $z\in\mathbb{C}\setminus\mathbb{R}$. Note that the functions $\{(x-z)^{-1}:z\in\mathbb{C}\setminus\mathbb{R}\}$ and $\mathcal{C}_c^\infty(\mathbb{R})$ are dense in $\mathcal{C}_0(\mathbb{R})$ with respect to the uniform norm. Since H_0 and A are self-adjoint operators, they are unitarily equivalent to a multiplication operator by a real-valued function in some appropriate $L^2(M)$ space. The norm of a multiplication operator from $L^2(M)$ to $L^2(M)$ is equal to the uniform norm of the multiplication function. Two limiting arguments, one for the H_0 first and then one for A_0, or vice-versa, extends the compactness to $\tau(A)\chi(H_0)$ as in the statement of the Proposition. □

Second proof: We see that $\mathcal{F}(A-\mathrm{i}/2)^{-1}\chi(H_0)\mathcal{F}^{-1}$ is an integral transform acting in the momentum space as follows:

$$L^2(\mathbb{R})\ni\varphi\mapsto(\mathcal{F}(A-\mathrm{i}/2)^{-1}\chi(H_0)\mathcal{F}^{-1}\varphi)(\xi)=\frac{\mathrm{i}}{\xi}\int_0^\xi\chi(t^2)\varphi(t)dt\in L^2(\mathbb{R}).$$

The fact that χ is supported away from zero is crucial here. Moreover, if $\chi\in\mathcal{C}_c^\infty(\mathbb{R})$, then this integral transform is Hilbert-Schmidt and there is $c>0$ such that

$$\|(A-\mathrm{i}/2)^{-1}\chi(H_0)\|_{HS}^2=\int_{\mathbb{R}}\int_{\mathbb{R}}\mathbf{1}_{(0,\xi)}(t)\xi^{-2}|\chi(t^2)|^2dtd\xi\leqslant c\|\chi\|_2^2.$$

In particular, $(A-\mathrm{i}/2)^{-1}\chi(H_0)$ is compact. One extends the compactness to operators of the form $\tau(A)\chi(H_0)$ as in the statement of the Proposition using the same limiting argument explained in the first proof. □

To complete the one-dimensional picture, we mention for what it is worth that it is possible to show that $(A+\mathrm{i})^{-1}\chi(H_0)\notin\mathcal{K}(L^2(\mathbb{R}))$ for any $\chi\in\mathcal{C}_c^\infty(\mathbb{R})$ with $\chi(0)\neq 0$. We now turn to the multi-dimensional case.

Proposition 7.8. *Let H_0 and A be those from Example 7.6. If $d\geqslant 2$, then $\langle A\rangle^{-s}\chi(H_0)\notin\mathcal{K}(L^2(\mathbb{R}^d))$ for any $\chi\in\mathcal{C}_c^\infty(\mathbb{R})$ whose support is non-empty in $(0,+\infty)$ and for any $s\in\mathbb{R}$.*

Proof. Let $\mathcal{I}(\lambda,r)$ denote the interval of radius $r>0$ centered at λ. There are $\lambda\in(0,+\infty)$ and $r>0$ such that $\mathcal{I}(\lambda,r)\subset(0,+\infty)$ and $m:=\inf_{x\in\mathcal{I}(\lambda,r)}|\chi(x)|>0$. Consider the constant energy curves

$$\{(\xi_1,...,\xi_d)\in\mathbb{R}^d:E=\xi_1^2+...+\xi_d^2\}.$$

For $d=2$, these are just circles centered at the origin. Forth we work in dimension two to keep the notation clean, but the necessary adjustments are obvious for $d\geqslant 2$. The support of the function of two variables $\chi(\xi_1^2+\xi_2^2)$ contains the annulus obtained by rotating $\mathcal{I}(\lambda',r')$ about the origin, where

$$\lambda' := (\sqrt{\lambda+r}+\sqrt{\lambda-r})/2, \quad r' := (\sqrt{\lambda+r}-\sqrt{\lambda-r})/2.$$

Let $\psi_1,\psi_2 \in \mathcal{C}_c^\infty(\mathbb{R})$ be any bump functions verifying : a) $\psi_1(0)\neq 0$, b) $\text{supp}(\psi_1)=[-1,1]$, c) $\text{supp}(\psi_2)\subset \mathcal{I}(\lambda',r'/2)$, and d) $\|\psi_i\|=1$, where $\|\cdot\|$ denotes the L^2 norm. Now let $\Psi_n(\xi_1,\xi_2) := \sqrt{n}\psi_1(\xi_1 n)\psi_2(\xi_2)$. Then $\|\Psi_n\|=1$ for all $n\geqslant 1$, and $\Psi_n \xrightarrow{w} 0$. Also, for n sufficiently large, Ψ_n is supported in the aforementioned annulus. Now fix $\nu\in\mathbb{N}$ and let $\varphi_n^\nu := \mathcal{F}(A+\mathrm{i})^\nu\mathcal{F}^{-1}\Psi_n$. Then for $\nu=0$, $\|\varphi_n^\nu\|=\|\Psi_n\|\equiv 1$, while for $\nu=1$,

$$\varphi_n^\nu(\xi_1,\xi_2) = -2n^{3/2}\mathrm{i}\xi_1\psi_1'(\xi_1 n)\psi_2(\xi_2) - 2n^{1/2}\mathrm{i}\psi_1(\xi_1 n)\xi_2\psi_2'(\xi_2) - \mathrm{i}\Psi_n(x),$$

and we see that $\|\varphi_n^\nu\|$ is uniformly bounded in n. A simple induction on ν shows that for every fixed value of $\nu\in\mathbb{N}$, $\|\varphi_n^\nu\|$ is uniformly bounded in n. Consider $\phi_n := \mathcal{F}\chi(H_0)(A+\mathrm{i})^{-\nu}\mathcal{F}^{-1}\varphi_n^\nu = \mathcal{F}\chi(H_0)\mathcal{F}^{-1}\Psi_n$. If $\mathcal{F}\chi(H_0)(A+\mathrm{i})^{-\nu}\mathcal{F}^{-1}\in\mathcal{K}(L^2(\mathbb{R}^2))$ for some value of ν, the image of the ball $B(0,\sup_{n\geqslant 1}\|\varphi_n^\nu\|)$ by this operator is pre-compact in $L^2(\mathbb{R}^2)$, and so there exists $\phi\in L^2(\mathbb{R}^2)$ and a subsequence $(n_k)_{k=1}^\infty$ such that $\lim_{k\to+\infty}\|\phi_{n_k}-\phi\|=0$. Since $\phi_{n_k}\xrightarrow{w} 0$, it must be that $\phi=0$ since the strong and weak limits coincide and are unique. But this contradicts the fact that $\|\phi_{n_k}\|\geqslant m\|\Psi_{n_k}\| = m>0$ for all $k\geqslant 1$. So $\chi(H_0)(A+\mathrm{i})^{-\nu}\notin\mathcal{K}(L^2(\mathbb{R}^2))$ and this implies that $\chi(H_0)\langle A\rangle^{-s}\notin\mathcal{K}(L^2(\mathbb{R}^2))$ for all $s\leqslant\nu$. The result follows by taking adjoints. □

A nice corollary of Proposition 7.8 that deserves a mention is the following. It uses Proposition 4.1. The result can also be proven to hold in dimension one.

Corollary 7.9. *Let A be that from Example 7.6. Let $d\geqslant 2$. Then for all $(s,\varepsilon)\in\mathbb{R}\times(0,+\infty)$, $\langle A\rangle^{-s}\langle Q\rangle^{\varepsilon}\notin\mathcal{B}(L^2(\mathbb{R}^d))$.*

Example 7.10 (Continuous Laplacian with Nakamura's conjugate operator)**.** *In* [N]*, Nakamura presents an alternate conjugate operator to the continuous Laplacian H_0. Let $\beta>0$. In momentum space it reads*

$$\mathcal{F}A\mathcal{F}^{-1} := \frac{\mathrm{i}}{2\beta}\sum_{i=1}^{d}\left(\sin(\beta\xi_i)\frac{\partial}{\partial\xi_i}+\frac{\partial}{\partial\xi_i}\sin(\beta\xi_i)\right).$$

Under some conditions on the potential V, it is shown that the Mourre theory holds for $H := H_0+V$ with respect to A on the interval $(0,(\pi/\beta)^2/2)$. We refer also to [Ma] *for a generalization of this conjugate operator and a more in-depth discussion. An argument as in Propositions 7.8 and 7.13 shows that, for $d\geqslant 2$, $\langle A\rangle^{-s}\chi(H_0)\notin\mathcal{K}(L^2(\mathbb{R}^d))$ for all $\chi\in\mathcal{C}_0(\mathbb{R})$ and $s\in\mathbb{R}$.*

Our last example is the discrete Laplacian on $\mathbb{Z}^d$. We refer to Section 4.2 for the details on the model.

Example 7.11 (Discrete Schrödinger operators)**.** *Let $\mathcal{H} := \ell^2(\mathbb{Z}^d)$, $H_0 := \Delta$ be the discrete Laplacian and A be its conjugate operator as in Example 4.2. Let*

$$\ell^2(\mathbb{Z}^d)\ni u\mapsto(\mathcal{F}u)(\theta) = (2\pi)^{-d/2}\sum_{n\in\mathbb{Z}^d}u(n)e^{\mathrm{i}\theta\cdot n}\in L^2([-\pi,\pi]^d)$$

be the Fourier transform. We recall that H_0 is unitarily equivalent to the operator of multiplication by $\sum_{i=1}^d(2-2\cos(\theta_i))$ and that A is unitarily equivalent to the self-adjoint realization of the operator $\mathrm{i}\sum_{i=1}^d(\sin(\theta_i)\partial/\partial\theta_i+\partial/\partial\theta_i\sin(\theta_i))$, which we denote by $A_{\mathcal{F}}$.

Proposition 7.12. *Let H_0 and A be those from Example 7.11. If $d = 1$, then $\tau(A)\chi(H_0) \in \mathcal{K}(\ell^2(\mathbb{Z}))$ for all $\tau \in \mathcal{C}_0(\mathbb{R})$ and $\chi \in \mathcal{C}([0, 4])$ supported away from zero and four.*

Proof. Using simple techniques from the theory of first order differential equations, we see that $\chi(H_0)(A + \mathrm{i})^{-1}$ is a Hilbert-Schmidt integral transform acting as follows:

$$L^2([-\pi, \pi]) \ni \psi \mapsto (\mathcal{F}\chi(H)(A+\mathrm{i})^{-1}\mathcal{F}^{-1}\psi)(\theta) = \frac{1}{2\mathrm{i}\sin(\theta/2)} \int_0^\theta \frac{\sin(t/2)}{\sin(t)} \chi\left(2 - 2\cos(t)\right)\psi(t)dt.$$

Note that it is crucial that $\chi(2 - 2\cos(t))$ be supported away from zero and $\pm\pi$. □

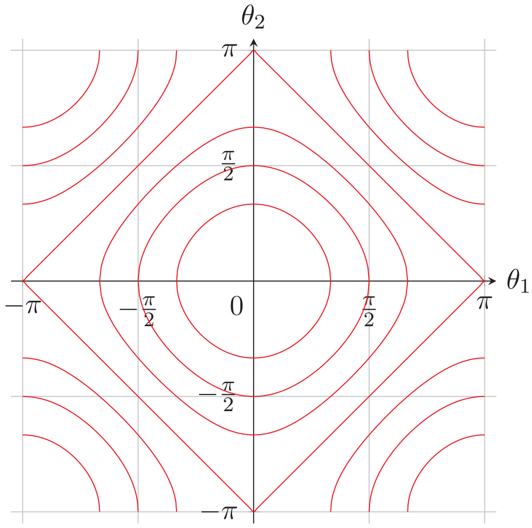

FIGURE 1. Level curves $\{(\theta_1, \theta_2) \in [-\pi, \pi]^2 : E = 2 - 2\cos(\theta_1) + 2 - 2\cos(\theta_2)\}$ of constant energy for $d = 2$

Proposition 7.13. *Let H_0 and A be those from Example 7.11. If $d \geqslant 2$, then $\langle A\rangle^{-s}\chi(H_0) \notin \mathcal{K}(\ell^2(\mathbb{Z}^d))$ for all $\chi \in \mathcal{C}([0, 4d])$ with non-empty support in $(0, 4d)$, and for all $s \in \mathbb{R}$.*

Proof. Let $\lambda \in (0, 4d)$ and $r > 0$ be such that $\mathcal{I}(\lambda, r) \subset (0, 4d)$ and $m := \inf_{x\in\mathcal{I}(\lambda,r)} |\chi(x)| > 0$. Fix an energy $E \in \mathcal{I}(\lambda, r)$. Consider the constant energy curves

$$\{(\theta_1, ..., \theta_d) \in [-\pi, \pi]^d : E = 2 - 2\cos(\theta_1) + ... + 2 - 2\cos(\theta_d)\}.$$

For $d = 2$, these level curves are drawn in Figure 1 for various energies in $[0, 8]$. Let us proceed in dimension two to keep things simple. The aim is to show that $\mathcal{F}\chi(H_0)\mathcal{F}^{-1}(A_\mathcal{F} + \mathrm{i})^{-\nu}$ is not compact for every fixed value of $\nu \in \mathbb{N}$. Now $\mathcal{F}\chi(H_0)\mathcal{F}^{-1}$ is equal to the operator of multiplication by $\chi(2-2\cos(\theta_1)+2-2\cos(\theta_2))$. The support of this function of two variables contains a neighborhood of a portion of the following vertical axes : $\theta_1 = -\pi, 0$ or π. Let $\mathcal{N}$ be such a neighborhood. Let T be one of these three values depending on the situation. We can then create a sequence $\Psi_n(\theta_1, \theta_2) = \sqrt{n}\psi_1((\theta_1 - T)n)\psi_2(\theta_2)$ that is supported in $\mathcal{N}$, converges weakly to zero and $\|\Psi_n\| \equiv 1$. Now let $\varphi_n^\nu := (A_\mathcal{F} + \mathrm{i})^\nu\Psi_n$. Then for every fixed value of ν, $\|\varphi_n^\nu\|$ is uniformly bounded in n. The rest of the proof follows the guidelines as that of Proposition 7.8. □

Finally, as in the continuous case, we have:

Corollary 7.14. *Let A be that from Example 7.11. Let $d \geqslant 2$. Then for all $(s, \varepsilon) \in \mathbb{R} \times (0, +\infty)$, $\langle A\rangle^{-s}\langle N\rangle^{\varepsilon} \notin \mathcal{B}(\ell^2(\mathbb{Z}^d))$.*

Appendix A. Why scattering states evolve where A is prevalent

This appendix is based on [Go, Section 3.2]. We give an idea why it is not unreasonable to expect both purely absolutely continuous spectrum and a propagation estimate under the only assumptions $H \in \mathcal{C}^1(A)$ and the Mourre estimate (1.2) on $\mathcal{I}$, when $\mathcal{I}$ is void of eigenvalues. Without loss of generality, we may assume that the Mourre estimate for H is strict over the interval $\mathcal{I}$. Given a state f and $f_t := e^{-\mathrm{i}tH}f$ its evolution at time $t \in \mathbb{R}$ under the dynamics generated by the operator H, one looks at the Heisenberg picture:

$$\mathcal{A}_f(t) := \langle f_t, Af_t\rangle. \tag{A.1}$$

This is the time-evolution of the expectation value of the observable A. Since we are localized in energy in $\mathcal{I}$, and A is generally an unbounded operator, we take $f := \varphi(H)g$, with $g \in \mathcal{D}(A)$ and $\varphi \in C_c^{\infty}(\mathcal{I})$, the smooth functions compactly supported on the interval $\mathcal{I}$. In addition to imply that $[H, \mathrm{i}A]_\circ \in \mathcal{B}(\mathcal{D}(H), \mathcal{D}(H)^*)$, the assumption $H \in \mathcal{C}^1(A)$ implies that $e^{-\mathrm{i}tH}\varphi(H)$ stabilizes the domain of A, ensuring that $\mathcal{A}_f(t)$ is well defined. Differentiating (A.1) gives

$$\mathcal{A}_f'(t) := \langle f_t, [H, \mathrm{i}A]_\circ f_t\rangle = \langle f_t, E_{\mathcal{I}}(H)[H, \mathrm{i}A]_\circ E_{\mathcal{I}}(H)f_t\rangle. \tag{A.2}$$

By using the strict Mourre estimate and the boundedness of $[H, \mathrm{i}A]_\circ$ we get

$$c\|f\|^2 \leqslant \mathcal{A}_f'(t) \leqslant k\|f\|^2,$$

where $k := \|[H, \mathrm{i}A]_\circ\|_{\mathcal{B}(\mathcal{D}(H),\mathcal{D}(H)^*)}$. Integrating this equation yields

$$ct\|f\|^2 \leqslant \mathcal{A}_f(t) - \mathcal{A}_f(0) \leqslant kt\|f\|^2, \text{ for all } t \geqslant 0.$$

The transport of the particle is therefore ballistic with respect to A. This is characteristic of purely absolutely continuous states and propagation estimates are usually obtained in these circumstances.

Appendix B. A uniform RAGE Theorem

We would like to make a relevant observation about the RAGE Theorem that appears to be absent from the literature. A small modification of the proof of [CFKS, Theorem 5.8] leads to:

Theorem B.1 (RAGE)**.** *Let H be a self-adjoint operator on $\mathcal{H}$. Let $\mathcal{I}$ be a bounded interval.*
(1) *If $W \in \mathcal{K}(\mathcal{H})$,*

$$\sup_{\psi\in\mathcal{H},\|\psi\|=1} \frac{1}{T}\int_0^T \|We^{-\mathrm{i}tH}P_{\mathrm{c}}(H)\psi\|^2\, dt \to 0 \quad \textit{as } T \to \infty. \tag{B.1}$$

(2) *If $W \in \mathcal{B}(\mathcal{H})$ and is H-relatively compact, then for all $\psi \in \mathcal{H}$,*

$$\frac{1}{T}\int_0^T \|We^{-\mathrm{i}tH}P_{\mathrm{c}}(H)\psi\|^2\, dt \to 0 \quad \textit{as } T \to \infty.$$

and

$$\sup_{\psi\in\mathcal{H},\|\psi\|=1} \frac{1}{T}\int_0^T \|We^{-\mathrm{i}tH}P_{\mathrm{c}}(H)E_{\mathcal{I}}(H)\psi\|^2\, dt \to 0 \quad \textit{as } T \to \infty.$$

(3) *If* $W \in \mathcal{K}(\mathcal{H})$, *then*

$$\left\| \frac{1}{T} \int_0^T e^{\mathrm{i}tH} W e^{-\mathrm{i}tH} P_{\mathrm{c}}(H)\, dt \right\| \to 0 \quad \text{as } T \to \infty.$$

The improvement consists in the supremum which is absent in the standard version of the Theorem. In [CFKS], they prove (3). They state a weaker version of (1), although their proof gives in fact (1). The first part of (2) is proven in [CFKS]. For the second part, apply (1) with $\tilde{\psi} := (H + \mathrm{i})E_{\mathcal{I}}(H)\psi$ and conclude by noticing that $(H + \mathrm{i})E_{\mathcal{I}}(H)$ is a bounded operator.

Appendix C. Overview of almost analytic extension of smooth functions

We refer to [D], [DG], [GJ1], [GJ2], [HS2] and [M] for more details. We review basic results that are spread out in the mentioned literature. Let $\rho \in \mathbb{R}$ and denote by $\mathcal{S}^\rho(\mathbb{R})$ the class of functions φ in $\mathcal{C}^\infty(\mathbb{R})$ such that

$$|\varphi^{(k)}(x)| \leqslant C_k \langle x \rangle^{\rho - k}, \quad \text{for all } k \in \mathbb{N}. \tag{C.1}$$

For the purpose of this article we only need the class $\mathcal{S}^0(\mathbb{R})$. This class consists of the smooth bounded functions having derivatives with suitable decay.

Lemma C.1. [D] *and* [DG] *Let* $\varphi \in \mathcal{S}^\rho(\mathbb{R})$, $\rho \in \mathbb{R}$. *Then for every* $N \in \mathbb{Z}^+$ *there exists a smooth function* $\tilde{\varphi}_N : \mathbb{C} \to \mathbb{C}$, *called an almost analytic extension of* φ, *satisfying:*

$$\tilde{\varphi}_N(x + \mathrm{i}0) = \varphi(x)\ \forall x \in \mathbb{R}; \tag{C.2}$$

$$\text{supp}\ (\tilde{\varphi}_N) \subset \{x + \mathrm{i}y : |y| \leqslant \langle x \rangle\}; \tag{C.3}$$

$$\tilde{\varphi}_N(x + \mathrm{i}y) = 0\ \forall y \in \mathbb{R} \text{ whenever } \varphi(x) = 0; \tag{C.4}$$

$$\forall \ell \in \mathbb{N} \cap [0, N], \left| \frac{\partial \tilde{\varphi}_N}{\partial \overline{z}}(x + \mathrm{i}y) \right| \leqslant c_\ell \langle x \rangle^{\rho - 1 - \ell} |y|^\ell \text{ for some constants } c_\ell > 0. \tag{C.5}$$

Lemma C.2. [GJ1] *Let* $\rho \geqslant 0$ *and* $\varphi \in \mathcal{S}^\rho(\mathbb{R})$. *Let* $\varphi(A)$ *with domain* $\mathcal{D}(\varphi(A)) \supset \mathcal{D}(\langle A \rangle^\rho)$ *be the operator whose existence is assured by the spectral theorem. Then for* $f \in \mathcal{D}(\langle A \rangle^\rho)$,

$$\varphi(A) f = \lim_{R \to \infty} \frac{\mathrm{i}}{2\pi} \int_{\mathbb{C}} \frac{\partial (\varphi \tilde{\theta}_R)_N}{\partial \overline{z}}(z)(z - A)^{-1} f\, dz \wedge d\overline{z}, \tag{C.6}$$

where $\theta_R(x) := \theta(x/R)$ *and* $\theta \in \mathcal{C}_c^\infty(\mathbb{R})$ *is a bump function such that* $\theta(x) = 1$ *for* $x \in [-1/2, 1/2]$ *and* $\theta(x) = 0$ *for* $x \in \mathbb{R} \setminus [-1, 1]$.

Lemma C.3. *For* $\rho \geqslant 0$ *and* $\varphi \in \mathcal{S}^\rho(\mathbb{R})$, *the following limit exists:*

$$\varphi^{(k)}(A) f = \lim_{R \to \infty} \frac{\mathrm{i}(k!)}{2\pi} \int_{\mathbb{C}} \frac{\partial (\varphi \tilde{\theta}_R)_N}{\partial \overline{z}}(z)(z - A)^{-1-k} f\, dz \wedge d\overline{z}, \quad \textit{for all } f \in \mathcal{D}(\langle A \rangle^\rho), \tag{C.7}$$

where θ *is the same as in Lemma C.2. Moreover, if* $0 \leqslant \rho < k$ *and* $\varphi^{(k)}$ *is a bounded function, then* $\varphi^{(k)}(A)$ *is a bounded operator and*

$$\varphi^{(k)}(A) = \frac{\mathrm{i}(k!)}{2\pi} \int_{\mathbb{C}} \frac{\partial \tilde{\varphi}_N}{\partial \overline{z}}(z)(z - A)^{-1-k}\, dz \wedge d\overline{z} \tag{C.8}$$

holds with the integral converging in norm.

Lemma C.4. [GJ2] *Let $s \in [0,1]$ and $\mathbb{D} := \{(x,y) \in \mathbb{R}^2 : 0 < |y| \leqslant \langle x \rangle\}$. Then there exists $c > 0$ independent of A such that for all $z = x + \mathrm{i}y \in \mathbb{D}$:*

$$\|\langle A \rangle^s (A - z)^{-1}\| \leqslant c \cdot \langle x \rangle^s \cdot |y|^{-1}. \tag{C.9}$$

Proposition C.5. [GJ1] *Let T be a bounded self-adjoint operator satisfying $T \in \mathcal{C}^1(A)$. Then for any $\varphi \in \mathcal{S}^\rho(\mathbb{R})$ with $\rho < 1$, $T \in \mathcal{C}^1(\varphi(A))$ and*

$$[T, \varphi(A)]_\circ = \frac{\mathrm{i}}{2\pi} \int_{\mathbb{C}} \frac{\partial \tilde{\varphi}_N}{\partial \overline{z}} (z - A)^{-1} [T, A]_\circ (z - A)^{-1} \, dz \wedge d\overline{z}. \tag{C.10}$$

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