Diplomarbeit

Spectral theory of anisotropic discrete Schrödinger operators in dimension one

Spektraltheorie anisotroper diskreter Schrödinger Operatoren in der Dimension eins.

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1 Introduction

Nonrelativistic quantum mechanics is the study of selfadjoint operators, which are taking the place of ordinary observables or even describing the time evolution and, by that, the whole dynamics of an experiment. Interest is focused onto the time-independent Schrödinger Equation, 1926 described by Erwin Schrödinger in his famous series of articles in the journal "Annalen der Physik" (see [Sch26a] and [Sch26b]). For a quantum mechanical state $f(t)$ at time t he heuristically deduced the time development

$$i\hbar\frac{df}{dt} = Hf.$$

The operator H is called Hamilton Operator and is itself an observable describing the total energy of the system. Considering one particle systems, H takes the form $H = H_0 + V$, where the positive Laplacian $H_0 = -\Delta$ is the observable for the kinetic energy and the multiplication operator V for the potential energy. When in 1906 Hilbert shaped the concept of the spectrum of an operator he was unaware of the coincidence with the physical spectrum that became obvious through the research of Schrödinger. It is still subject to prolific scientific research, so the spectrum of H describes the possible bounded and unbounded energy levels of the system and hence we will take a deep look into the spectrum of H. In scattering theory, bounded states corresponding to isolated points in the spectrum, because of lacking scattering capabilities, are of no interest; instead we will centre on the continuous spectrum. Many potentials are periodic, as encountered in crystals. The idea is to approximate the system at the lattice points of atoms of the crystal where the potential V "attracts" the particle. The eigenfunctions of H are thus assumed to be small at a given distance to these lattice points. Therefore in the application of the theory we simplify our life by restricting the phase space to these points — also known as the tight binding method — and main topics to be answered are the absence of singularly continuous spectrum and asymptotic completeness.

Fast decaying potentials V have been thoroughly investigated; instead this work mines anisotropic, non decaying potentials in one dimension.

We now give a short sketch of the main ideas and some well known facts. In Chapter 2 on the essential spectrum we introduce the needed vocabulary and general properties of the essential spectrum σ_{ess}, which is defined for a bounded operator $B : \mathcal{H} \to \mathcal{H}$, on a complex Hilbert Space $\mathcal{H}$, as the spectrum $\sigma(B)$ excluding isolated eigenvalues of finite multiplicity. Assume that B is also selfadjoint. For $f \in \mathcal{H}$ we notice that $\mu_f(\cdot) := \langle f, E_B(\cdot)f\rangle$ on the Borel sigma algebra $\mathcal{B}(\mathbb{R})$ is a measure. With the Lebesgue Measure Decomposition Theorem we can disassemble μ_f into a *pure point* measure, a measure which is *absolutely continuous* with respect to the Lebesgue measure and a *singularly continuous* measure, singular to the other two. In return we divide the spectrum $\sigma(B)$ into the the pure point spectrum $\sigma_{pp}(B)$, covering the eigenvalues of B and relating to the bounded states of the quantum mechanical system, and the continuous spectra $\sigma_{ac}(B)$ and $\sigma_{sc}(B)$, relating to scattering states. For details see Section 2.4.

This thesis examines the absence of singularly continuous spectrum for the discrete Laplace operator Δ on $\mathcal{H} = \ell^2(\mathbb{Z})$ under certain perturbations. It is introduced in Chapter 3. Let U, U^* denote the composition with right and left shift on $\mathcal{H}$, then

$$\Delta := 1 - \frac{1}{2}(U + U^*) \qquad \text{on } \ell^2(\mathbb{Z}).$$

So Δ is a bounded and selfadjoint convolution operator. Using the unitary Fourier Transformation $\mathcal{F}$ we obtain

$$\mathcal{F}\Delta\mathcal{F}^{-1} = 1 - \cos(Q) \qquad \text{on } L^2(\mathcal{S}^1).$$

The operator Q in this expression is defined by $(Qf)(k) = kf(k)$, such that $\cos(Q)$ gets its sense from the Spectral Theorem, i.e. $\cos(Q)$ means multiplication with cosine. As in Corollary 3.6, the above equation implies that $\sigma(\Delta) = \sigma_{ess}(\Delta) = \sigma_{ac}(\Delta) = [0, 2]$.

Our aim is to perturb Δ with different potentials such that no singularly continuous spectrum occurs. Take a potential $V_0 : \mathbb{Z} \to \mathbb{R}$ such that $V_0(n) \to 0$ with $|n| \to \infty$. As the difference of Δ and $\Delta + V_0(Q)$ is a compact operator, the Weyl Theorem 2.13 ensures

$$\sigma_{ess}(\Delta + V_0(Q)) = \sigma_{ess}(\Delta) = [0, 2].$$

This behaviour changes with the limit at infinity of the potential. Also this stability is not true for σ_{ac}, σ_{sc} and σ_{pp}.

Now add a Barrier potential $L : \mathbb{Z} \mapsto \mathbb{R}$ to Δ such that $L|_{\mathbb{Z}_\pm} = l_\pm$ on the sets $\mathbb{Z}_+ := \mathbb{N}_0$ and $\mathbb{Z}_- := \mathbb{Z}\backslash\mathbb{Z}_+$. In case of $l_+ = l_-$, i.e. in case of constant L, the spectra are shifted by $l_\pm$, which is easily verified using the definitions. In case of $l_+ \neq l_-$, using Weyl and Zhislin sequences, we see that the essential spectrum is shifted in two directions simultaneously, i.e.

$$\sigma_{ess}(\Delta + L(Q) + V_0(Q)) = \sigma_{ess}(\Delta + L(Q)) = [0, 2] + \{l_\pm\}.$$

To examine the singularly continuous spectrum we return to the more general selfadjoint and bounded operator B. By way of Proposition 4.1, taking a dense set $G \subset \mathcal{H}$ and an interval I, and having for every $f \in G$ a finite constant $c(f)$ such that $\sup_{\epsilon>0,\lambda\in I} |\mathrm{Im}\,\langle f, (B - \lambda - i\epsilon)^{-1} f\rangle| \leqslant c(f)$, implies that B has purely absolutely continuous spectrum in I. The possible dependence of $c(f)$ on f makes perturbation theory hard. For the Laplace operator, we find $\sup_{\varepsilon>0,\lambda\in I} |\langle f, (\Delta - \lambda - i\epsilon)^{-1} f\rangle| \leqslant \|\langle Q\rangle^{\alpha} f\|^2$ for an interval $I \subset\subset (0, 2)$ and for $\alpha > 1/2$. Here $\langle Q\rangle := \sqrt{1 + Q^2}$. To bring back L, we split $\ell^2(\mathbb{Z})$ into the direct sum of $\ell^2(\mathbb{Z}_-)$ and $\ell^2(\mathbb{Z}_+)$, on which L is constant, so after investigating $\ell^2(\mathbb{Z}_\pm)$ separately, we will glue them together. We obtain for $\alpha > 1/2$ and for an interval $I \subset\subset \sigma_{ess}(\Delta + L)\backslash\{l_\pm, l_\pm + 2\}$

$$\sup_{\epsilon>0,\lambda\in I} \left\|\langle Q\rangle^{-\alpha} (\Delta + L(Q) - \lambda - i\epsilon)^{-1} \langle Q\rangle^{-\alpha}\right\| < \infty, \tag{1.1}$$

which we call the Limiting Absorption Principle. This particular result takes place in Theorem 5.21 and in Proposition 6.4, which rely on commutator methods called the Mourre Theory, see Chapter 4. Again this estimate covers the claim that the spectrum of $\Delta + L(Q)$ in I is purely absolutely continuous.

Why is this estimate better suited for perturbation theory? Fix the operators $H_L := \Delta + L(Q)$ and $H_\kappa := H_L + \kappa V(Q)$ for $\kappa \in \mathbb{R}$, taking $V \in O(1/|n|^{1+\varepsilon})$ for a fixed $\varepsilon > 0$. For $z \in \mathbb{C}$ with $\mathrm{Re}(z) \in I$ and $\mathrm{Im}(z) > 0$ the equation

$$\begin{aligned}&\langle Q\rangle^{-\alpha} (H_\kappa - z)^{-1} \langle Q\rangle^{-\alpha} \left(1 + \langle Q\rangle^{\alpha} \kappa V \langle Q\rangle^{\alpha} \langle Q\rangle^{-\alpha} (H_L - z)^{-1} \langle Q\rangle^{-\alpha}\right)\\ &\qquad = \langle Q\rangle^{-\alpha} (H_L - z)^{-1} \langle Q\rangle^{-\alpha}.\end{aligned}$$

holds. Taking $\alpha \in (1/2, (1 + \varepsilon)/2)$ makes $\langle Q\rangle^{\alpha} V \langle Q\rangle^{\alpha}$ bounded. Due to equation (1.1), the resolvent of H_L in the corresponding weights is uniformly bounded in z. So for small κ the $(1+\ldots)$ expression has a bounded inverse, which is uniformly bounded in z. This provides

$$\sup_{\epsilon>0,\lambda\in I} \left\|\langle Q\rangle^{-\alpha} (\Delta + L(Q) + \kappa V(Q) - \lambda - i\epsilon)^{-1} \langle Q\rangle^{-\alpha}\right\| < \infty,$$

implying H_κ has purely absolutely continuous spectrum in I. Theorem 6.5 states this result. For large κ we also have Proposition 6.7.

At last we open Chapter 7 on Scattering Theory, where we introduce the generalized wave operators

$$\Omega^\pm(A,B) := \text{s-}\lim_{t\to\mp\infty} e^{iAt}e^{-iBt}P_{ac}(B),$$

where P_{ac} is the projection onto the absolutely continuous subspace of B. We discuss the existence and completeness. Calling $\mathcal{H}_\pm := \Omega^\pm(A,B)\mathcal{H}$ the incoming respectively outgoing states, completeness means that every outgoing state has exactly one corresponding incoming state and vice versa. In the Application of the Scattering Theory we explore the existence and completeness of $\Omega^\pm(H_\kappa, H_V)$.

Note that introducing the Barrier potential L has not been explained before. The central pivot and result of this thesis is the following theorem.

Theorem 1.1 Take $\mathcal{H} = \ell^2(\mathbb{Z})$. Let $\varepsilon > 0$ and potentials $V, V_s : \mathbb{Z} \to \mathbb{R}$ with $V \in O(1/|n|^{1+\varepsilon})$ and $V_s \in O(1/n^2)$; let $l_\pm \in \mathbb{R}$ and $L : \mathbb{Z} \to \mathbb{R}$ such that $L|_{\mathbb{Z}_\pm} = l_\pm$. Then for $H_s := \Delta + L(Q) + V_s(Q)$ and $H_\kappa := H_s + \kappa V(Q)$ where $\kappa \in \mathbb{R}$ and for the set D, consisting of the eigenvalues of H_s and of the points $\{l_\pm, l_\pm + 2\}$, we have

i) $\sigma_{ess}(H_\kappa) = \sigma_{ess}(H_s) = \sigma_{ess}(\Delta) + \{l_\pm\} = [0,2] + \{l_\pm\}$,

ii) the eigenvalues of H_s excluding $\{l_\pm, l_\pm + 2\}$ have finite multiplicity,

iii) the eigenvalues of H_s can accumulate only at $\{l_\pm, l_\pm + 2\}$,

iv) $\sigma_{ess}(H_s)\backslash D$ is purely absolutely continuous,

v) for any given interval $I \subset\subset ([0,2] + \{l_\pm\})\backslash D$ we find a bound for κ such that H_κ has purely absolutely continuous spectrum in I,

vi) the generalized wave operators $\Omega^\pm(H_\kappa, H_s)$ exist and are complete.

In fact, iv) and v) follow from the stronger Limiting Absorption Principle for H_s and H_κ, see Theorems 5.21 and 6.5. Moreover ii) holds true for $V_s \in O(1/|n|)$, due to the Virial Theorem 4.11.

2 Essential Spectrum

The essential spectrum is the elementary hinge in the theory to prove Theorem 1.1, i.e. being a close friend with it is necessary. Of course we commence with its introduction; then Proposition 2.11 and Corollary 2.13 scrutinize basic properties of its detection and of perturbation. The perfect examination tool are Weyl sequences and their relatives, the Zhislin sequences (see Definitions 2.10 and 2.19). Because selfadjoint operators are unitarily equivalent to multiplication operators, we will put deep emphasis on exploring their spectrum. For the spectrum does not look all the same on the whole range, we clean up this chapter by separating it into the pure point, absolutely continuous and singularly continuous spectrum. Except for Proposition 2.20, proofs are standard and can be found in every work about functional analysis, e.g. [RS] and [Wer].

2.1 Generalities on the Essential Spectrum

For use in spectral theory, we begin with the discussion of basic properties of sequences in a complex Hilbert Space $(\mathcal{H}, \langle\cdot,\cdot\rangle)$.

Definition 2.1 A sequence $(f_n)_{n\in\mathbb{N}}$ in $\mathcal{H}$ is said to

- *converge weakly* to f, if

$$\langle f_n, w\rangle \to \langle f, w\rangle \qquad \text{for all } w \in \mathcal{H}$$

and we write $f_n \rightharpoonup f$ or $\text{w-lim}_{n\to\infty} f_n = f$.

- *converge strongly* to f, if

$$\|f_n - f\| \to 0$$

and we write $f_n \to f$ or $\text{s-lim}_{n\to\infty} f_n = f$.

Fix a strongly convergent sequence $(f_n)_{n\in\mathbb{N}}$ with limit f and say there is another strong limit f'. Then, with the help of the triangle inequality, we have $\|f - f'\| \leqslant \|f - f_n\| + \|f_n - f'\|$. Both addends on the right converge to 0, so f and f' are equal. Replacing the sequence $(f_n)_{n\in\mathbb{N}}$ with a weakly convergent one and expressing $\|f - f'\|^2$ through $\langle f, f - f'\rangle - \langle f', f - f'\rangle$ which is the limit of $\langle f_n - f_n, f - f'\rangle = 0$, shows that weak limits are unique.

The name "strong convergence" suggests implication of weak convergence and, on the other hand, weak convergence is not sufficient for strong convergence:

Example 2.2 Set $\mathcal{H} = \ell^2(\mathbb{Z})$ and define $f_n := e_1 + e_{n+1}$, where $(e_i)_{i\in\mathbb{N}}$ is an orthonormal system for $\mathcal{H}$. Parseval's inequality $\sum_{n\in\mathbb{N}} |\langle g, e_n\rangle|^2 \leqslant \|g\|^2$ implies for all $g \in \mathcal{H}$ that the product $\langle g, e_n\rangle$ converges to 0 providing that $f_n \rightharpoonup e_1$. Then $\|f_n\|^2 = 2 \neq 1 = \|e_1\|^2$, so the limit of the norms of the sequence and the norm of the weak limit disagree. Since $\|f_{n+1} - f_n\|^2 = 2$ the sequence is no Cauchy Sequence and has therefore no strong limit.

But if the norm-limit of a weakly convergent sequence exists, and agrees with the norm of the weak limit, the sequence is strongly convergent. We put these findings in the next couple of propositions.

Proposition 2.3 Strong implies weak convergence to the same limit.

Proof: Take a strongly convergent sequence $(f_n)_{n\in\mathbb{N}}$ with limit f; then from Cauchy-Schwarz we get

$$|\langle f_n - f, w\rangle| \leqslant \|f_n - f\| \cdot \|w\|.$$

Hence $\langle f_n - f, w\rangle$ tends to 0 for all w and the sesquilinearity of the inner product supplies $\langle f_n, w\rangle \to \langle f, w\rangle$. □

Proposition 2.4 Weak convergence and $\|f_n\| \to \|f\|$ implies strong convergence.

Proof: Fixing $w := f$ in the weak property gains $\langle f_n, f\rangle \to \langle f, f\rangle$, i.e.

$$\langle f_n, f\rangle - \langle f, f\rangle \to 0. \tag{2.1}$$

Additionally from $\|f_n\| \to \|f\|$ we have

$$\langle f_n, f_n\rangle - \langle f, f\rangle \to 0.$$

The first argument allows us to replace $\langle f, f\rangle$ with $\langle f, f_n\rangle$, so

$$\langle f_n, f_n\rangle - \langle f, f_n\rangle \to 0.$$

We subtract expression (2.1)

$$\begin{aligned} 0 \leftarrow &\langle f_n, f_n\rangle - \langle f, f_n\rangle - \langle f_n, f\rangle + \langle f, f\rangle \\ &= \langle f_n, f_n - f\rangle - \langle f, f_n - f\rangle = \|f_n - f\|^2, \end{aligned}$$

which proves the proposition. □

There are also some weakly convergent sequences that we can not repair in the sense that there is a strongly convergent subsequence; the sequence of Example 2.2 is one of such:

Lemma 2.5 A sequence $(f_n)_{n\in\mathbb{N}}$ in $\mathcal{H}$ with $f_n \rightharpoonup f'$, but $\|f_n\| \to r \neq \|f'\|$ has no strongly convergent subsequence.

Proof: Without loss of generality we assume $f_n \rightharpoonup 0$ and $\|f_n\| \to 1$. A subsequence $(f_{n_k})_{k\in\mathbb{N}}$ with limit f would converge weakly to 0, in particular $\langle f_{n_k}, f\rangle \to 0$. Since $1 = \|f\| = \langle f, f\rangle = \lim_{k\to\infty} \langle f_{n_k}, f\rangle$ there is no such subsequence. □

We aim to uncover general properties of the essential spectrum; fix a bounded operator H on $\mathcal{H}$ and remember that the spectrum $\sigma(H)$ is the set $\mathbb{C}\backslash\{\lambda \in \mathbb{C} \mid (H-\lambda)^{-1}$ is bounded$\}$, consisting of the disjoint discrete and essential spectrum:

Definition 2.6 Let H be a bounded operator. We define the
• *discrete spectrum* $\sigma_{\text{disc}}(H)$ as the set of those $\lambda \in \sigma(H)$ that are isolated eigenvalues of finite multiplicity,
• *essential spectrum* $\sigma_{\text{ess}}(H) := \sigma(H)\backslash\sigma_{\text{disc}}(H)$.

Note that the essential spectrum may still contain isolated points. For example the essential spectrum of the identity on any infinite dimensional Hilbert Space consists solely of the point 1. Instead on finite dimensional spaces, the essential spectrum is always empty.

To discern between both kinds of spectrum, we need to look into compact operators.

Definition 2.7 We call a bounded operator $C : \mathcal{H} \to \mathcal{H}$ compact if the closure of C′s image of the closed unit ball is compact, i.e. by defining the closed unit ball $S := \{x \in \mathcal{H} \mid \|x\| \leqslant 1\}$, we require $\overline{C(S)}$ to be compact.

These operators form a closed subspace within the space of bounded operators on $\mathcal{H}$. Finite rank operators form a dense subspace. This and more information can be taken from [RS] and [Wer]. You may also find Lemma 2.8, showing a relationship between compact operators and weak and strong convergence, useful.

Lemma 2.8 Let $K : \mathcal{H} \to \mathcal{H}$ be compact. K maps

i) weakly convergent sequences $(f_n)_{n\in\mathbb{N}}$ with $f_n \in \mathcal{H}$ to strongly convergent sequences,

ii) weakly convergent sequences $(W_n)_{n\in\mathbb{N}}$ of continuous operators that are multiplied to K on the right to strongly convergent sequences,

iii) strongly convergent sequences $(S_n)_{n\in\mathbb{N}}$ of continuous operators to uniformly convergent sequences.

Proof: i) Take $f \in \mathcal{H}$ the weak limit of $(f_n)_{n\in\mathbb{N}}$. Weakly convergent sequences are bounded, which we can easily derive from the Principle of Uniform Boundedness (see [Wer] Korollar IV.2.3). Then for all $g \in \mathcal{H}$

$$\langle g, Kf_n\rangle - \langle g, Kf\rangle = \langle g, K(f_n - f)\rangle = \langle K^* g, f_n - f\rangle \to_{n\to\infty} 0.$$

In other words $(Kf_n)_{n\in\mathbb{N}}$ converges weakly to Kf. Suppose that $(Kf_n)_{n\in\mathbb{N}}$ does not converge strongly, i.e. there is some constant $\varepsilon > 0$ and a subsequence $(Kf_{n_k})_{k\in\mathbb{N}}$ with $\|Kf_{n_k} - Kf\| \geqslant \varepsilon$. For $(f_{n_k})_{k\in\mathbb{N}}$ is bounded and K compact, $(Kf_{n_k})_{k\in\mathbb{N}}$ has got itself a subsequence converging to $g \neq Kf$ and, as strong convergence implies weak convergence and weak limits are unique, the supposition is false.

ii) We fix W the weak limit of $(W_n)_{n\in\mathbb{N}}$. Then with i) we have for every $f \in \mathcal{H}$ that $KW_n f$ converges strongly to KWf.

iii) We fix S the strong limit and, as, by the Principle of Uniform Boundedness, strongly convergent sequences are bounded, fix $c > 0$ a bound of $(S_n)_{n\in\mathbb{N}}$ and then, from the definition of the operator norm, clearly $\|S\| \leqslant c$. We suppose that $S_n K$ does not converge to SK in norm or, to state it more tangible, there is $\varepsilon > 0$ and a sequence $(f_n)_{n\in\mathbb{N}}$ in $\mathcal{H}$ with $\|f_n\| = 1$ such that

$$\|S_n K f_n - SKf_n\| \geqslant \varepsilon \qquad \text{for all } n.$$

Since K is compact and $(f_n)_{n\in\mathbb{N}}$ bounded there is a strongly converging subsequence $(Kf_{n_j})_{j\in\mathbb{N}}$ of $(Kf_n)_{n\in\mathbb{N}}$ with limit $g \in \mathcal{H}$. For all j

$$\begin{aligned}\varepsilon &\leqslant \left\|S_{n_j} - SKf_{n_j}\right\| = \left\|(S_{n_j} - S)(Kf_{n_j} - g + g)\right\| \\ &\leqslant \left\|(S_{n_j} - S)(Kf_{n_j} - g)\right\| + \left\|(S_{n_j} - S)g\right\|.\end{aligned}$$

As Kf_{n_j} tends strongly to g we have J_1 such that for all $j > J_1$ the estimate $\left\|Kf_{n_j} - g\right\| \leqslant \varepsilon/(8c)$ holds and similarly, as S_{n_j} converges strongly, there is J_2 with $\left\|(S_{n_j} - S)g\right\| \leqslant \varepsilon/4$ for $j > J_2$. This means for $j > max\{J_1, J_2\}$

$$\begin{aligned}\varepsilon &\leqslant \left\|(S_{n_j} - S)(Kf_{n_j} - g)\right\| + \left\|(S_{n_j} - S)g\right\| \\ &\leqslant \left\|S_{n_j}(Kf_{n_j} - g)\right\| + \left\|S(Kf_{n_j} - g)\right\| + \left\|(S_{n_j} - S)g\right\| \\ &\leqslant \frac{\varepsilon c}{8c} + \frac{\varepsilon c}{8c} + \frac{\varepsilon}{4} = \frac{\varepsilon}{2}.\end{aligned}$$

This contradiction shows that the initial assumption is wrong and hence $\|S_n K - SK\| \to 0$. By considering the adjoint of K, we can switch K and S_n and thence see $\|KS_n - KS\| \to 0$. □

Compactly supported functions $\varphi : \mathbb{R} \to \mathbb{R}$ characterize both the discrete and the essential spectrum. Taking a small neighbourhood around a given point λ of the spectrum for support, will produce $\varphi(H)$ that are either compact or not.

Lemma 2.9 Let H be a bounded, selfadjoint operator. $\lambda \in \mathbb{R}$ lies in $\sigma_{\text{disc}}(H)$ if and only if there is a $\zeta > 0$ such that all $\varphi \in C_0^\infty(B(\lambda, \zeta))$ with $\varphi(\lambda) \neq 0$ applied on H produce compact operators $\varphi(H) \neq 0$.

Proof: For multiples of the identity the proof is clear, so we can exclude them from consideration. If $\lambda \in \sigma(H)$ lies in the discrete spectrum, it is isolated, so picking $\zeta := d(\sigma(H)\setminus\{\lambda\}, \lambda)$ gives $\zeta > 0$. So $\varphi(H)$ is a multiple of an orthogonal projection on the finite dimensional subspace $\ker(H - \lambda)$ and hence compact.

On the other hand we have a φ such that $\varphi'(\lambda) \neq 0$. Then, by the spectral theorem applied to compact operators, we write

$$\varphi(H) = \varphi(\lambda) E_{\{\varphi(\lambda)\}}(\varphi(H)) + \sum_{k \in N} \varphi(\lambda_k) E_{\{\varphi(\lambda_k)\}}(\varphi(H)) \text{ for some } N \subset \mathbb{N}.$$

As the $\varphi(\lambda_k)$ tend to 0, when $k \to \infty$, $\varphi(\lambda)$ is an isolated eigenvalue of $\varphi(H)$. As $E_{\{\varphi(\lambda_k)\}}(\varphi(H)) = E_{\varphi^{-1}(\{\lambda_k\})}(H)$ this property passes on to H. □

A related way to separate these spectra are Weyl sequences for (H, λ), $\lambda \in \mathbb{R}$. If such a sequence exists, λ belongs to the essential spectrum.

Definition 2.10 Let H be a bounded and selfadjoint operator and $\lambda \in \mathbb{R}$. A sequence $(f_n)_{n \in \mathbb{N}}$ in $\mathcal{H}$ is called a *Weyl sequence* for (H, λ), if $\|f_n\| = 1$, $f_n \rightharpoonup 0$ and $(H - \lambda) f_n \to 0$.

For the sake of completeness we mention Zhislin sequences being some special sort of Weyl sequences on $\mathcal{H} = L^2(X)$, where X is some topological measure space, and are introduced in Definition 2.19. Yet we have not prepared the required tools; instead we support the above claim for Weyl sequences, which is also in [RS] Volume I, Theorems VII.9 to VII.12.

Proposition 2.11 Let H be a bounded, selfadjoint operator on $\mathcal{H}$. The following statements are equivalent.

i) $\lambda \in \sigma_{\text{ess}}(H)$,

ii) For all $\varepsilon > 0$ the projection $E_{(-\varepsilon+\lambda,\lambda+\varepsilon)}(H)$ is not compact,

iii) For all $\varphi \in C_c^\infty(\mathbb{R})$ with $\varphi(\lambda) = 1$ the operator $\varphi(H)$ is not compact,

iv) There is a Weyl sequence $(f_n)_{n\in\mathbb{N}}$ for (H, λ).

Furthermore, the essential spectrum is closed.

Proof: i $\Leftrightarrow$ iii) For $\lambda \notin \sigma(H)$ and small support of φ, the operators $\varphi(H)$ are always 0. If λ is part of $\sigma(H)$ we use the negation of Lemma 2.9.

iii $\Rightarrow$ ii) We prove the contrapositive: Assume there is $\varepsilon > 0$ such that for $I_\lambda := (-\varepsilon + \lambda, \lambda + \varepsilon)$ the operator $E_{I_\lambda} := E_{I_\lambda}(H)$ is compact. Then by the spectral theorem applied to compact operators, the image of E_{I_λ} is of finite dimension. If the support of φ is contained in I_λ then the image of $\varphi(H)$ is of finite dimension, so $\varphi(H)$ is compact.

ii $\Rightarrow$ iv) We define a sequence $\varepsilon_n := 2^{-n}$ with a corresponding sequence of intervals $I_n := (-\varepsilon_n + \lambda, \lambda + \varepsilon_n)$ and note that $\dim(\mathrm{Im}(E_{I_n}(H))) = \infty$. Through orthogonalization choose $f_n \in \mathrm{Im}(E_{I_n}(H))$ such that $\|f_n\| = 1$ and $\langle f_n, f_m\rangle = \delta_{m,n}$, leading to $(f_n)_{n\in\mathbb{N}} \rightharpoonup 0$. Now, write $H - \lambda$ in its integral form and apply it to f_n

$$(H - \lambda)f_n = \int_{\mathbb{R}} (x - \lambda) dE(x) f_n = \int_{I_n} (x - \lambda) dE(x) f_n.$$

The absolute value of $x - \lambda$ is bounded by ε_n, so $(H - \lambda)f_n \to 0$.

iv $\Rightarrow$ iii) For every $f \in \mathcal{H}$ we know there is a measure μ_f with

$$\langle \varphi(H)f, \varphi(H)f\rangle = \int_{\sigma(H)} \varphi(x)^2 d\mu_f(x).$$

From continuity of φ we get for all $\varepsilon > 0$ a $\delta = \delta(\varepsilon) > 0$ such that $\sup_{x\in I_\delta} |\varphi(x) - 1| < \varepsilon$, where $I_\delta := [-\delta + \lambda, \lambda + \delta]$, $I_\delta^c = \mathbb{R}\backslash I_\delta$. Note that

$$\|(\varphi(H) - 1)f_n\|^2 = \underbrace{\int_{I_\delta} (\varphi(x) - 1)^2 d\mu_{f_n}(x)}_{\leqslant \varepsilon^2} + \int_{I_\delta^c} (\varphi(x) - 1)^2 d\mu_{f_n}(x)$$

Using $\int_{I_\delta^c}(x-\lambda)^2 d\mu_{f_n}(x) \leqslant \|(H-\lambda)f_n\|^2 \to 0$, whereas the integrand is positive and larger than ε^2 on I_δ^c, and the boundedness of φ we get

$$\text{s-}\lim_{n\to\infty}(\varphi(H)-1)f_n = 0.$$

Therefore for every $w \in \mathcal{H}$ the product $\langle \varphi(H)f_n - f_n, w\rangle \to 0$ and hence $\varphi(H)f_n$ converges weakly to zero, as

$$\begin{aligned} 0 &= \lim_{n\to\infty}\langle \varphi(H)f_n - f_n, w\rangle \\ &= \lim_{n\to\infty}\langle \varphi(H)f_n, w\rangle - \langle f_n, w\rangle = \lim_{n\to\infty}\langle \varphi(H)f_n, w\rangle\,. \end{aligned}$$

The triangle-inequality gives $\|\varphi(H)f_n\| \to 1$, which we use in combination with Lemma 2.5 to conclude that $(\varphi(H)f_n)_{n\in\mathbb{N}}$ has no strongly convergent subsequence, implying $\varphi(H)$ is not compact.

With these equivalences it is evident that essential spectra are closed; take a sequence $(\lambda_n)_{n\in\mathbb{N}}$ in $\sigma_{\text{ess}}(H)$ converging to λ. Any open interval $I \ni \lambda$ contains an interval I' embracing some λ_n, i.e. with $E_{I'}(H)$ is $E_I(H)$ not compact and therefore $\lambda \in \sigma_{\text{ess}}(H)$. □

Proposition 2.11 is a major tool to detect and examine the essential spectrum. Perturbations that do or do not affect the essential spectrum of an operator H_0 are also of interest. For example consider $c \in \mathbb{R}$, $H_1 := c\mathbb{1}$ and $H := H_0 + H_1$, then for Weyl sequences we have to shift λ in $(H-\lambda)f \to 0$ by c and hence the whole essential spectrum is moved. In Proposition 3.12 we will, by a similar argument, shift the spectrum of the Laplace operator simultaneously in two directions. Notice that this works for $\{c\}$ is the essential spectrum of c. Instead for a finite rank operator H_1, having only discrete spectrum, we will see $\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(H_0)$. This stays true for the uniform limits of finite rank operators, i.e. for compact operators. We place this result into Corollary 2.13 ii), but to open the door to compact operators we have to step into compactly supported functions $\varphi \in C_c^\infty(I)$ on a closed interval I, which are the uniform limit of polynomials, and with functional calculus, back to compact operators. To polynomials:

Lemma 2.12 Let R be a ring and $A, B \in R$. Then for $n \in \mathbb{N}$ holds

$$A^n - B^n = \sum_{i=0}^{n-1} A^i(A-B)B^{n-i-1} \tag{2.2}$$

Proof: Clearly (2.2) is true for $n = 1$. Assume the equation holds for n.

$$\sum_{i=0}^{n} A^k(A-B)B^{n-i} = \sum_{i=0}^{n-1} A^i(A-B)B^{n-i-1}B + A^n(A-B)$$
$$= (A^n - B^n)B + A^n(A-B) = A^{n+1} - B^{n+1}.$$

This little induction shows the validity of the lemma. □

Corollary 2.13 (Weyl Theorem) Suppose H_1, H_2 are bounded, selfadjoint operators and $H_1 - H_2$ is compact. Then

i) $\varphi(H_1) - \varphi(H_2)$ is compact for all $\varphi \in C_c^\infty(\mathbb{R})$.

ii) H_1, H_2 have identical essential spectra.

Proof: i) We can assume $\varphi \in C^\infty(I)$ with some compact interval I containing $\sigma(H_1) \cup \sigma(H_2)$. From the Stone-Weierstrass Theorem we know that restricted polynomials are, with respect to the maximum norm, dense in $C^\infty(I)$ and we can choose a sequence $(p_n)_{n\in\mathbb{N}}$ uniformly converging to φ and hence $\|(p_n(H_1) - p_n(H_2)) - (\varphi(H_1) - \varphi(H_2))\| \to 0$. From Lemma 2.12 and since the sum and products of finitely many compact operators are compact and as the constant parts cancel, we get that $p_n(H_1) - p_n(H_2)$ is compact, implying $\varphi(H_1) - \varphi(H_2)$ is compact.

ii) Assuming $\sigma_{ess}(H_1) \neq \sigma_{ess}(H_2)$, there exists a $\lambda \in \sigma_{ess}(H_i)$ not contained in the other essential spectrum. Without loss of generality set $i = 1$. As essential spectra are closed, we chose $\varepsilon > 0$ smaller than the distance of λ to $\sigma_{ess}(H_2)$ and we fix $\varphi \in C_c^\infty(\mathbb{R})$ such that $\varphi(\lambda) = 1$ and $(-\varepsilon + \lambda, \lambda + \varepsilon)$ contains $\text{supp}(\varphi)$. Then $\varphi(H_2)$ is compact. By Proposition 2.11, $\varphi(H_1)$ is not, so, through handing this property down to $\varphi(H_1) - \varphi(H_2)$, we would contradict i). □

2.2 Essential Range

The spectrum of multiplication operators is easier to compute than of general operators, which can be helpful, since selfadjoint operators are unitarily equivalent to multiplication operators. On $\mathcal{H} = L^2(\mathbb{R})$ the prototype of a multiplication operator is the operator Q that, applied on $f \in \mathcal{H}$, returns the pointwise product of f with the identity on $\mathbb{R}$.

Definition 2.14 Let $\mathcal{H} = L^2(X, \mu)$. We define the *Multiplication Operator* $\varphi(Q)$ for measurable functions $\varphi : X \to \mathbb{C}$ by

$$(\varphi(Q)f)(x) := \varphi(x)f(x) \qquad \text{for } x \in X.$$

For the spaces $\mathcal{H} = L^2(X)$, where $X \in \{\mathbb{Z}, \mathbb{R}\}$, we define the operator Q

$$(Qf)(x) := xf(x) \qquad \text{for } x \in X.$$

The *Multiplication operator* corresponding to $\varphi : X \to \mathbb{C}$ is then $\varphi(Q)$, given through the Spectral Theorem. We will often skip the Q, i.e. we write φ instead of $\varphi(Q)$.

Of course, both definitions of $\varphi(Q)$ coincide on the given set of Hilbert spaces $\mathcal{H} \in \{L^2(\mathbb{R}), \ell^2(\mathbb{Z})\}$. Taken an arbitrary X, then equivalence classes $\varphi \in L^\infty(X)$ are, as functions on X, with respect to the measure μ only defined nearly everywhere. Talking about the image of φ is not appropriate for we might change the "values" of any representative φ on measure zero sets to any value we like to, not even excluding dense sets, e.g. $\mathbb{Q}$ in $X = \mathbb{R}$ with the Lebesgue measure. This problem can be circumvented by the introduction of the essential range (see below), since it does not depend on the choice of representative of an equivalence class $\varphi \in L^2(X, \mu)$.

Remark 2.15 The coincidence that we can decorate both the spectrum and the range with the adjective "essential" is not intuitive, as the sets may be different. Instead the spectrum of $\varphi(Q)$ and the essential range of φ are concurrent.

Definition 2.16 Let $\mathcal{H}$ be the space $L^2(X, \mu)$, where X is a set and μ a measure. Let $\varphi : X \to \mathbb{C}$ be a μ-measurable function. The *essential range* is the set

$$\text{range}_{\text{ess}}(\varphi) := \{\lambda \in \mathbb{C} \mid \forall \zeta > 0 : \mu(\{x \in X \mid |\varphi(x) - \lambda| < \zeta\}) > 0\}.$$

Proposition 2.17 Take a σ-finite, complete measure μ and $\varphi \in L^\infty(X, \mu)$. The spectrum of the multiplication operator $\varphi(Q)$ equals $\text{range}_{\text{ess}}(\varphi)$.

Proof: Let $\lambda \notin \text{range}_{\text{ess}}(\varphi)$, then there is a $\zeta > 0$ such that the set $\{x \mid |\varphi(x) - \lambda| < \zeta\}$ is a set of measure 0. Fix the operators $A := (\varphi(Q) - \lambda)$ and B, defined by

$$(Bg)(x) := \begin{cases} 0 & \text{if } |(\varphi(x) - \lambda)| < \zeta, \\ \frac{g(x)}{\varphi(x) - \lambda} & \text{otherwise,} \end{cases} \qquad \text{for } g \in \mathcal{H}.$$

For a given $g \in \mathcal{H}$, the sets $\{x \mid (BAg)(x) \neq g(x)\}$ and $\{x \mid (ABg(x) \neq g(x)\}$ are of measure 0, as μ is complete and $\{x \mid |\varphi(x) - \lambda| < \zeta\})$ contains both. This means ABg, BAg and g lie in the same L^2 equivalence class, i.e. B is a bounded inverse of A and hence $\lambda \notin \sigma(\varphi(Q))$.

For $\lambda \in \text{range}_{\text{ess}}(\varphi)$ we suppose that $(\varphi(Q)-\lambda)^{-1}$ exists. We fix the sets $G_n := \left\{x \mid |\varphi(x) - \lambda| < \frac{1}{n}\right\}$ for $n \in \mathbb{N}$. In case of $\mu(G_n) = \infty$ we can replace G_n with an arbitrary subset of G_n that has finite but positive measure, since μ is σ-finite. We also fix the corresponding functions $g_n := \chi_{G_n}$ and vectors $y_n := (\varphi(Q) - \lambda)g_n$. Clearly,

$$\|y_n\| = \|(\varphi(Q) - \lambda)g_n\| \leqslant \frac{1}{n}\|g_n\|$$

This means for the norm of the inverse of $(\varphi(Q) - \lambda)$ that

$$\left\|(\varphi(Q) - \lambda)^{-1}\right\| \geqslant \frac{\|(\varphi(Q) - \lambda)^{-1}y_n\|}{\|y_n\|} = \frac{\|g_n\|}{\|(\varphi - \lambda)g_n\|} \geqslant \frac{\|g_n\|}{\frac{1}{n}\|g_n\|} = n,$$

i.e. the inverse would be unbounded and therefore $\lambda \in \sigma(\varphi(Q))$. □

Example 2.18 We take $\varphi \in C_c^\infty(\mathbb{R}, \mathbb{R})$ and immediately notice that the image of φ and thus the essential range of φ form the same closed interval. From Proposition 2.17 we know that $\lambda \in \sigma(\varphi(Q))$ resides in the essential range of φ. Intervals clearly have no isolated points, so λ can't be element of the discrete spectrum and is accordingly element of the essential spectrum of $\varphi(Q)$.

We are now going to build up a suitable Weyl sequence. We assume λ to be an element of the image of φ and therefore of the essential spectrum of $\varphi(Q)$ — a construction of the sequence for λ not in the image is similar. First we fix a $p \in \varphi^{-1}(\lambda)$ and choose a strictly monotonous, real sequence $(\varepsilon_n)_{n\in\mathbb{N}}$ that tends to zero and from the ε-δ-definition of continuity we gain corresponding δ_n, which we can also take to converge strictly monotonously to zero. We define the Weyl sequence $f_n : \mathbb{R} \to \mathbb{R}$ through

$$f_n(x) := \begin{cases} c_n & \text{if } x \in B_n, \\ 0 & \text{otherwise,} \end{cases}$$
$$c_n := \sqrt{\frac{1}{2(\delta_n - \delta_{n+1})}},$$
$$B_n := B_{\delta_n}(p) \backslash B_{\delta_{n+1}}(p).$$

Accordingly the $(f_n)_{n\in\mathbb{N}}$ form an orthonormal system and we are left to check that

$$\|(\varphi(Q)-\lambda)f_n\|^2 = \int_{B_n} (\varphi(x)c_n - \lambda c_n)^2 dx \leqslant \int_{B_n} c_n^2 \varepsilon_n^2 dx$$

tends to zero, but that is old news.

2.3 Zhislin Sequences

The Weyl sequences of Definition 2.10 are sometimes too general. For a Borel space X and $\mathcal{H} := L^2(X)$ there is more structure that we can take advantage of to identify the essential spectrum in more detail.

Definition 2.19 Let $\mathcal{H} = L^2(X)$ and $(f_n)_{n\in\mathbb{N}}$ be a Weyl sequence for (H,λ). We call that sequence a *Zhislin sequence* for (H,λ), if for all compact $K \subset X$ and for large n we have $K \cap \operatorname{supp} f_n = \emptyset$.

Zhislin sequences are some specialized sort of Weyl sequences on $L^2(X)$ and are, for being Weyl sequences, a tool to detect the essential spectrum. The assumption $K \cap \operatorname{supp} f_n = \emptyset$ is in some way an orthogonality feature. More importantly, there is a nifty proposition that, without directly addressing the spectrum of the operator nor functions applied on it, shows the existence of a Zhislin sequence through a sequence of compactly supported, with respect to the infinity norm uniformly bounded functions $(\theta_n)_{n\in\mathbb{N}}$. These properties make the θ_n easy to find. A proposition for $X = \mathbb{R}^d$, similar to the following, can be found in [HS]. $X = \mathbb{Z}^d$ suits our needs.

Proposition 2.20 Let $(\theta_n)_{n\in\mathbb{N}}$ be a sequence in $L^\infty(\mathbb{Z}^d)$ such that

i) there is $c > 0$ complying to $\|\theta_n\|_\infty < c$ for all n,

ii) θ_n is compactly supported,

iii) for all bounded $K \subset \mathbb{Z}^d$ there is $N \in \mathbb{N}$ with $\theta_n|_K = 1$ for $n > N$,

iv) $\|[H, \theta_n(Q)]\| \to 0$.

Then for $\lambda \in \sigma_{\text{ess}}(H)$ there exists a Zhislin sequence for (H,λ).

Proof: Let $(\varphi_n)_{n\in\mathbb{N}}$ be a Weyl sequence for $\lambda \in \sigma_{\text{ess}}(H)$ and choose a sequence $(m_n)_{n\in\mathbb{N}}$ of natural numbers growing monotonously to infinity such that $\|(1-\theta_n)\varphi_{m_n}\| \geqslant \frac{1}{2}$, being possible as θ_n is compactly supported and $\varphi_n \rightharpoonup 0$. Then we have

$$(H-\lambda)(1-\theta_n(Q))\varphi_{m_n} = (H-\lambda)\varphi_{m_n} \\ - [H, \theta_n(Q)]\,\varphi_{m_n} + \theta_n(Q)(H-\lambda)\varphi_{m_n}.$$

Using our presuppositions i), iv) on θ_n, we note that the above equation converges termwise to 0. Considering the construction of $(m_n)_{n\in\mathbb{N}}$ lets us normalize the sequence $((1-\theta_n(Q))\varphi_{m_n})_{n\in\mathbb{N}}$ without losing its Weyl property. Features ii) and iii) of $(\theta_n)_{n\in\mathbb{N}}$ provide the missing requirements for a Zhislin sequence. □

2.4 Spectral decomposition

Definition 2.6 divides the spectrum into an essential and a discrete part, and we have some tools at hand to discern between both. Definition 2.25 disassembles the spectrum somewhat further, using measure theoretic instruments. In case you need additional information on these topics, you may consult [RS] Section VII.2 and for generalities on measures [Bau].

Definition 2.21 Let $f \in \mathcal{H}$ and H be a selfadjoint operator on $\mathcal{H}$. We define the measure μ_f on the Borel sigma algebra $\mathcal{B}(\mathbb{R})$

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

where E_H is the spectral measure of H.

It is obvious to perceive that Definition 2.21 actually defines measures; the scalar product on the right side is greater equal to 0, since E_H is an orthogonal projection which we can square without changing anything and then (self-)adjoining it. Moreover $E_H(\emptyset) = 0$ and hence $\mu_f(\emptyset) = 0$. Write $E_H(\cup_n A_n) = \sum_n E_H(A_n)$ on a pairwise disjoint sequence of Borel sets $(A_n)_{n\in\mathbb{N}}$, to gain $\sigma-$additivity.

We apply the Lebesgue Measure Decomposition Theorem to compare these μ_f with the Lebesgue measure, pure point measures and measures singular to both. Restriction to pure measures of these kinds opens a interesting door to divide $\mathcal{H}$.

Definition 2.22 Every μ_f of Definition 2.21, can be uniquely disassembled into the sum of the *pure point measure* $\mu_{f_{pp}}$, i.e. the support of the measure is a countable union of single points, and the corresponding *continuous measure* $\mu_{f_{cont}}$, defined through the Lebesgue Measure Decomposition Theorem. Thus

$$\mu_f =: \mu_{f_{pp}} + \mu_{f_{cont}}.$$

In the same sense we disassemble $\mu_{f_{cont}}$ into a measure $\mu_{f_{ac}}$ which is absolutely continuous with respect to the Lebesgue measure and its singular measure $\mu_{f_{sc}}$

$$\mu_f =: \mu_{f_{pp}} + \mu_{f_{ac}} + \mu_{f_{sc}}.$$

Additionally we define the spaces

$$\begin{aligned}
\mathcal{H}_{pp}(H) &:= \overline{\{f \in \mathcal{H} \mid \mu_f \text{ is a pure point measure}\}} \\
\mathcal{H}_{cont}(H) &:= \{f \in \mathcal{H} \mid \mu_f \text{ is a continuous measure}\} \\
\mathcal{H}_{ac}(H) &:= \{f \in \mathcal{H}_{cont}(H) \mid \mu_f \text{ is an absolutely continuous measure}\} \\
\mathcal{H}_{sc}(H) &:= \{f \in \mathcal{H} \mid \langle f, \mathcal{H}_{ac}(H)\rangle = 0 \text{ and } \langle f, \mathcal{H}_{pp}(H)\rangle = 0\}.
\end{aligned}$$

In case of clarity, we may omit writing H.

Taking the identity for H leads to $\mathcal{H} = \mathcal{H}_{pp}$. In Lemma 2.23 we find a whole bunch of operators H with $\mathcal{H} = \mathcal{H}_{ac}$; after these examples, as can be expected, we see in Proposition 2.24 that $\mathcal{H}_{pp}, \mathcal{H}_{ac}$ and $\mathcal{H}_{sc}$ fit nicely together to form a direct sum decomposing $\mathcal{H}$. The major part of this work will later be to ensure $\mathcal{H}_{sc} = \{0\}$ for certain H.

Lemma 2.23 Let $g \in C^1((a,b))$ with $a < b$ such that $|\{g' = 0\}| \in \mathbb{N}$. Then the space $\mathcal{H}_{ac}(g(Q))$ equals $\mathcal{H} := L^2((a,b))$.

Proof: We want to show that all measures μ_f are absolutely continuous with respect to the Lebesgue measure λ. So we take $A \subset (a,b)$ with $\lambda(A) = 0$. We want to use the Measure Transformation Theorem so we sort the set

$$\{x \mid g'(x) = 0\} \cup \{a, b\} \subset [a, b]$$

by value to get distinct $t_1, .., t_n$ with $t_i < t_j$ for $i < j \leqslant n$. Then g is injective on the intervals from t_i to t_{i+1}, covering the whole interval (a, b).

Moreover we have

$$\mu_f(A) = \int_a^b f\chi_{g^{-1}(A)}\bar{f}d\lambda = \sum_i \int_{t_i}^{t_{i+1}} |f|^2\chi_{g^{-1}(A)}d\lambda$$
$$= \sum_i \int_{g(t_i)}^{g(t_{i+1})} |f\circ g|^2\chi_A|g'|d\lambda = 0,$$

i.e. μ_f is absolutely continuous with respect to λ. □

Proposition 2.24 The subspaces $\mathcal{H}_{pp}$, $\mathcal{H}_{ac}$ and $\mathcal{H}_{sc}$ are closed and

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

Proof: At first we show that $\mathcal{H}_{ac}$ is closed, so let $(f_n)_{n\in\mathbb{N}}$ be a sequence in $\mathcal{H}_{ac}$ with limit $f \in \mathcal{H}$. For every $A \in \mathcal{B}(\mathbb{R})$ with $\lambda(A) = 0$, we have

$$\mu_f(A) = \langle f, E_H(A)f\rangle = \langle \lim f_n, E_H(A)\lim f_n\rangle$$
$$= \lim \langle f_n, E_H(A)f_n\rangle = \lim \mu_{f_n}(A) = 0,$$

i.e. μ_f is absolutely continuous.

Furthermore we have to prove that $\mathcal{H}_{pp}$ and $\mathcal{H}_{cont}$ are perpendicular. So take $f_p \in \mathcal{H}_{pp}$ and $f_c \in \mathcal{H}_{cont}$. For μ_{f_p} and μ_{f_c} are singular by definition, there is $A \in \mathcal{B}(\mathbb{R})$ such that $0 = \mu_{f_c}(A) = \mu_{f_p}(\mathbb{R}\backslash A)$ and together with the definition of μ_f and the projections E_H we conclude that $E_H(A)f_c = 0$ and $E_H(\mathbb{R}\backslash A)f_p = 0$. Thus

$$\langle f_c, f_p\rangle = \langle f_c, E_H(\mathbb{R})f_p\rangle = \langle f_c, (E_H(A) + E_H(\mathbb{R}\backslash A))f_p\rangle$$
$$= \langle f_c, E_H(A)f_p\rangle + \langle f_c, E_H(\mathbb{R}\backslash A)f_p\rangle = \langle f_c, E_H(A)f_p\rangle$$
$$= \langle E_H(A)f_c, f_p\rangle = 0.$$

This implies that $\mathcal{H}_{ac}$ and $\mathcal{H}_{pp}$ are perpendicular. At last, H_{sc} is defined as the orthogonal complement of $\mathcal{H}_{ac} \oplus \mathcal{H}_{pp}$ in $\mathcal{H}$. □

All that we pull back to the spectrum by restricting H:

Definition 2.25 Let H be selfadjoint and bounded. We define the

pure point spectrum $\sigma_{pp}(H) := \sigma(H|_{\mathcal{H}_{pp}})$,

continuous spectrum $\sigma_{cont}(H) := \sigma(H|_{\mathcal{H}_{cont}})$,

absolutely continuous spectrum $\sigma_{ac}(H) := \sigma(H|_{\mathcal{H}_{ac}})$ and the

singularly continuous spectrum $\sigma_{sc}(H) := \sigma(H|_{\mathcal{H}_{sc}})$.

In a quantum mechanical context, these spectra get a physical sense; bounded states correspond to the pure point spectrum, scattering states to the continuous spectrum. To explain the difference between singularly and absolutely continuous spectrum, we look at the following lemma.

Lemma 2.26 Take a compact K, then for $f \in \mathcal{H}_{ac}(H)$ we have

$$\left\|Ke^{itH}f\right\| \to_{t\to\pm\infty} 0.$$

Proof: In general, by the Riemann-Lebesgue Lemma (see e.g. [Rud]), we know for $g \in L^1(\Omega)$ on an open interval Ω, and for its Fourier Transformation that

$$\hat{g}(t) = \int_\Omega e^{-itx} g(x) d\lambda(x) \to_{t\to\pm\infty} 0.$$

Because of the Radon-Nikodym Theorem, we find for absolutely continuous measures μ a function $f \in L^1(\mathbb{R})$ such that for every $A \in \mathcal{B}(\mathbb{R})$ we have

$$\mu(A) = \int_A f(x) dx,$$

so the above implies

$$\hat{\mu}(A)(t) := \int_A f(x) e^{-itx} dx \to_{t\to\pm\infty} 0.$$

This entails for $f \in \mathcal{H}_{ac}(H)$, and hence for μ_f from Definition 2.21

$$\hat{\mu}_f(A)(t) \to_{t\to\pm\infty} 0,$$

i.e. $e^{itH}f$ turns weakly to 0. Lemma 2.8 states that the compact K maps weakly convergent sequences to strongly convergent sequences, thus the norm of $Ke^{itH}f$ turns with large $|t|$ to 0. □

Conferring the RAGE-Theorem (see [CFKS] Theorem 5.8) we find for the continuous spectrum, covering the absolutely and singularly continuous spectrum, that for $f \in \mathcal{H}_{\text{cont}}$ and compact K the time-mean

$$\frac{1}{T}\int_0^T \left\|Ke^{-itA}f\right\|^2 dt \to_{T\to\pm\infty} 0.$$

Consider the space $\mathcal{H} = \ell^2(\mathbb{Z}^d)$. Fixing $K := \chi_A(Q)$ for compact sets A, we see in time-mean, that the state f leaves every compact neighbourhood A. More precisely, f could visit every compact neighbourhood, with time evolving, less and less frequently; taking Lemma 2.26, we see for states $f \in \mathcal{H}_{\text{ac}}$ that we even do not need the time-mean, so at some time the state wants to leave every compact neighbourhood — but beware, the converse is not true, so there may exist states in $\mathcal{H}_{\text{sc}}$ with the same property.

3 Laplace Operator

Schrödinger operators are defined as perturbations of the Laplacian. Usually the continuous Laplacian on $L^2(\mathbb{R}^n)$ is used as the kinetic energy in quantum mechanics, but, as we mentioned in the introduction, considering the discrete case and thus the tight binding method, is often sufficient.

There are different approaches to define the Laplacian on $\mathbb{Z}^d$. All carry along different properties, where the target is to mimic as many as possible of the continuous Laplacian's good properties. The standard-one introduced in Definition 3.1 is good in many respects and resembles the experience with the continuous one neatly, though it is impossible to cover all desirable properties.

This Laplacian Δ in one dimension is, by Proposition 3.5 bounded and selfadjoint with a neat multiplication representation in momentum space, has, due to Corollary 3.6, purely absolutely continuous spectrum and owns more or less easily constructable Weyl and Zhislin sequences (see Examples 3.7, 3.8 and 3.13).

The new result of this chapter, Proposition 3.12, explores the essential spectrum of $H = \Delta + V$ for anisotropic potentials V. This chapter ends with a prospect to the multidimensional setting.

3.1 Basic properties

Our goal is to investigate the properties of the discrete Laplacian in one dimension, but first we have to find out how do define it on $\mathbb{Z}$. Recollecting properties of the continuous Laplace operator will give the idea; in one dimension the Laplace operator is just the second derivative operator

$$\Delta_c := \frac{1}{2}\frac{d^2}{dt^2}$$

on $L^2(\mathbb{R})$. We first define it on the dense subspace $C_c^\infty(\mathbb{R})$ and later define it on the domain of selfadjointness. So let us have a closer look: Consider the vector space of functions $C_c^\infty(\mathbb{R})$. Taking two function $f, g \in C_0^2([0,1])$ we notice, through integration by parts, that Δ_c can be split in two

$$\begin{aligned} 2\langle f, \Delta_c g\rangle &= \int_{\mathbb{R}} f(x)\overline{\Delta_c g(x)}dx \\ &= \int_a^b \nabla_c f(x)\overline{\nabla_c g(x)}dx + \left[f\overline{\nabla_c g}\right]_b^a = \langle \nabla_c f, \nabla_c g\rangle, \end{aligned} \tag{3.1}$$

where $[a, b]$ is a compact interval containing both the supports of f and g. This double Nabla formulation is a good starting point, as we can imitate the first derivative. On $C_c^\infty(\mathbb{R})$, the derivative of f at any point x is

$$(\nabla_c f)(t) := \lim_{x\to 0} \frac{f(t+x) - f(x)}{x},$$

i.e. ∇_c is the limit of the slope y/x as x goes to 0. By fixing x at some given distance, say $x = 1$, we get a *forward difference operator* $\vec{\nabla}_c$, i.e.

$$\vec{\nabla}_c f(t) = \frac{f(t+x) - f(t)}{x}. \tag{3.2}$$

By the Mean Value Theorem, we will find $0 < \delta < x$ such that $\nabla_c f(t+\delta) = \vec{\nabla}_c f(t)$. The error introduced by the switch from ∇_c to $\vec{\nabla}_c$ is of order big O of the distance x. Moreover it is an exercise in elementary arithmetic that $\vec{\nabla}_c$ obeys the "product rule"

$$\vec{\nabla}_c(fg) = f(\vec{\nabla}_c g) + (\vec{\nabla}_c f)g + (\vec{\nabla}_c f)(\vec{\nabla}_c g). \tag{3.3}$$

On $\mathbb{Z}$ every point y has the neighbours $y \pm 1$. Due to (3.2) we are tempted to fix for $f \in \mathcal{H} := \ell^2(\mathbb{Z})$

$$\nabla f(y) := \frac{f(y+1) - f(y)}{1} \qquad \text{for all } y \in \mathbb{Z},$$

i.e. ∇ returns the slope to the right. Back to the Laplacian. Inspired by (3.1), let one ∇ change side in $\langle\nabla,\nabla\rangle$ to see what the Laplace operator in this setting looks like

$$\begin{aligned}\langle\nabla f,\nabla g\rangle &= \sum_x (f(x+1)-f(x))\left(\overline{g(x+1)-g(x)}\right)\\ &= \sum_x 2f(x)\overline{g}(x) - \left(\sum_x f(x)\overline{g(x-1)} + \sum_x f(x)\overline{g(x+1)}\right)\\ &= \sum_x f(x)\overline{(2g(x)-(g(x-1)+g(x+1)))} =: 2\langle f,\Delta g\rangle.\end{aligned}$$

It is a remarkable feature of equation (3.3) that it translates to ∇ on $\ell^2(\mathbb{Z})$ for pointwise products, that means ∇ is *no derivation* in terms of abstract algebra, i.e. Leibniz's law $\nabla(fg) = (\nabla f)g + f(\nabla g)$ does not hold. Then again, the discrete Laplacian inherits many desirable properties of the continuous Laplacian, as can be easily seen that only direct neighbours of a point contribute to the value of that point under the Laplacian leading to the fact that locally affine functions are mapped locally to 0; moreover it is translation invariant and, as we will see in Proposition 3.5, it is positive and selfadjoint.

Definition 3.1 Let $\mathcal{H}$ be the space $\ell^2(\mathbb{Z})$. We define the *Laplace operator* Δ on $\mathcal{H}$ through

$$(\Delta f)(n) := f(n) - \frac{1}{2}(f(n+1) - f(n-1)) \qquad \text{for } f \in \mathcal{H}.$$

For convenience we denote the *right shift* U and the *left shift* U^*, where $Uf(n) := f(n-1)$ so that $U^*f(n) = f(n+1)$. Then

$$\Delta = 1 - \frac{1}{2}(U + U^*) \tag{3.4}$$

can be written with the help of the shift operators.

What are consequences of this definition? Is the operator bounded, selfadjoint? What is its spectrum? We answer these questions step by step. Boundedness can easily be taken from (3.4) and the following lemma.

Lemma 3.2 The right and left shift operators U^* and U are mutually adjoint and both are unitary.

Proof: Index shift. □

For convolution operators the Fourier Transformation offers a simple method to extract the spectrum. For example the Hilbert space $\ell^2(\mathbb{Z})$ is mapped to $L^2([0,2\pi])$, where Proposition 2.17 obtains the spectrum. Besides it is often convenient to have another representation of the operator and in case of Δ, the Fourier Transform is the tool of choice, as the Laplacian is a convolution operator.

Definition 3.3 The 1-*sphere* $\mathcal{S}^1$ and the d-dimensional *torus* $\mathbb{T}^d$ are

$$\mathcal{S}^1 := \frac{\mathbb{R}}{2\pi\mathbb{Z}}$$
$$\mathbb{T}^d := \times_{k=1}^{d}\mathcal{S}^1.$$

On these we define the *Fourier Transform* $\mathcal{F} : \ell^2(\mathbb{Z}^d) \to L^2(\mathbb{T}^d)$ through

$$\mathcal{F}f(k) := \frac{1}{\sqrt{2\pi}^d}\sum_x f(x)e^{-i\langle k,x\rangle}$$

for[1] $f \in \ell^2(\mathbb{Z}^d)$. The *inverse Fourier Transform* $\mathcal{F}^{-1} : L^2(\mathbb{T}^d) \to \ell^2(\mathbb{Z}^d)$ is then given by

$$(\mathcal{F}^{-1}f)(k) = \frac{1}{\sqrt{2\pi}^d}\int_{\mathbb{T}^d} f(x)e^{i\langle k,x\rangle}dm(x),$$

where the measure dm is the Haar-measure on $\mathbb{T}^d$ such that $m(\mathbb{T}^d) = (2\pi)^d$ and $L^2(\mathbb{T}^d) := L^2(\mathbb{T}^d, m)$.

Theorem 3.4 The Fourier Transform is unitary.

For a proof and further properties, see e.g. [Rud] or [Lig]; we apply $\mathcal{F}$:

Proposition 3.5 The Laplacian is a positive, selfadjoint operator with spectrum $[0,2]$. In momentum space the Laplacian becomes a multiplication operator

$$\mathcal{F}\Delta\mathcal{F}^{-1} = 1 - \cos(Q).$$

Proof: We show the boundedness with the help of the triangle inequality

$$\|\Delta\| = \left\|1 - \frac{1}{2}(U + U^*)\right\| \leqslant \|1\| + \frac{1}{2}(\|U\| + \|U^*\|).$$

[1] First by $f \in \ell^1(\mathbb{Z}^d)$ and then by bounded extension to $\ell^2(\mathbb{Z}^d)$.

This means that the norm of the Laplacian is less or equal to 2.

We take a look at the scalar product of Δf and g

$$\begin{aligned}\langle \Delta f, g\rangle &= \langle f, g\rangle - \frac{1}{2}(\langle Uf, g\rangle + \langle U^* f, g\rangle)\\ &= \langle f, g\rangle - \frac{1}{2}(\langle f, U^* g\rangle + \langle f, Ug\rangle) = \langle f, \Delta g\rangle\end{aligned}$$

and get the symmetry of Δ. Together with the boundedness this implies that Δ is selfadjoint.

At last we use the Fourier Transform to calculate the spectrum and to prove the form $1-\cos(Q)$, applying $\mathcal{F}$; take the notation $f_-(n) := f(n-1)$ and $f_+(n) := f(n+1)$, then

$$\begin{aligned}2\sqrt{2\pi}(\mathcal{F}\Delta f)(k) &= \sum_x (2f(x) - f_+(x) - f_-(x))e^{-ikx}\\ &= \sum_x 2f(x)e^{-ikx} - \sum_x f_+(x)e^{-ikx} - \sum_x f_-(x)e^{-ikx}\\ &= \sum_x 2f(x)e^{-ikx} - \sum_x f(x)e^{-ikx}e^{ik} - \sum_x f(x)e^{-ikx}e^{-ik}\\ &= 2\sqrt{2\pi}(\mathcal{F}f)(k) - \sqrt{2\pi}(\mathcal{F}f)(k)e^{ik} - \sqrt{2\pi}(\mathcal{F}f)(k)e^{-ik}\\ &= 2\sqrt{2\pi}(\mathcal{F}f)(k)(1-\cos(k)).\end{aligned}$$

Replace f with $\mathcal{F}^{-1}g$ to obtain

$$\begin{aligned}\mathcal{F}\Delta\mathcal{F}^{-1}g &= \mathcal{F}(\Delta\mathcal{F}^{-1}g)\\ &= (\mathcal{F}\mathcal{F}^{-1}g)(1-\cos(Q)) = (1-\cos(Q))g.\end{aligned} \tag{3.5}$$

Conjugation with the unitary Fourier Transform does not affect the spectrum, so use Proposition 2.17 to see $\sigma(\Delta) = [0, 2]$. □

Equation (3.5) is worth some note as it allows to bring all the theoretic machinery in position. By Proposition 2.17 we already gained the spectrum $\sigma(\Delta)$. Looking at Example 2.18 we see that $1-\cos$ applies to it and hence $\sigma_{ess}(\Delta) = \sigma(\Delta)$ and by Lemma 2.23, we even gain that the spectrum is purely absolutely continuous, since the Fourier Transformation is unitary.

Corollary 3.6 $\sigma(\Delta) = \sigma_{ess}(\Delta) = \sigma_{ac}(\Delta)$ and $\mathcal{H} = \mathcal{H}_{ac}(\Delta)$.

Another way to extract the essential spectrum is the use of Weyl sequences. We will later need these sequences to detect the essential spectrum of the operator $H = \Delta + V(Q)$, where V is an anisotropic potential.

Example 3.7 We build a Weyl sequence for all $\lambda \in \sigma(\Delta) = \sigma_{\text{ess}}(\Delta)$. First, we construct a sequence of $(\beta_k)_{k\in\mathbb{N}}$ in $\mathcal{H}$ which we will later shift and scale to make orthogonal. We want them to have the form

$$\beta_k(n) := \begin{cases} c_n & 0 \leqslant n \leqslant k, \\ 0 & \text{otherwise,} \end{cases} \tag{3.6}$$

where $(c_n)_{n\in\mathbb{Z}}$ is a sequence to be defined later. We fix $\tau := \lambda - 1$ and set another goal for β_k, namely we want $((\Delta-\lambda)\beta_k)(n)$ to be 0 on all possible locations, so

$$\begin{aligned} (-2(\Delta - \lambda)\beta_k)(n) &= \beta_k(n+1) + \beta_k(n-1) + 2\tau\beta_k(n) \\ &= \begin{cases} c_0 & n = -1, \\ 2\tau c_0 + c_1 & n = 0, \\ 2\tau c_k + c_{k-1} & n = k, \\ c_k & n = k+1, \\ 0 & \text{otherwise.} \end{cases} \end{aligned} \tag{3.7}$$

The equations (3.6) and (3.7) lead to a recursive definition of $(c_n)_{n\in\mathbb{N}_0}$

$$c_n = -c_{n-2} - 2\tau c_{n-1}.$$

In accordance with our aims for β_k, fix $c_0 = 1$ and $c_1 = p_1$, where we fix $p_{1,2} = -\tau \pm \sqrt{\tau^2 - 1}$. The sequence's generating function C

$$C(z) = \sum_{n\in\mathbb{N}_0} c_n z^n = \frac{1 + (\tau + \sqrt{\tau^2 - 1})z}{1 + 2\tau z + z^2}$$

returns, with the help of the Expansion Theorem for Rational Generating Functions (see e.g. [GKP]) the closed form

$$c_n = 1p_1^n + 0p_2^n = p_1^n.$$

Clearly, the p_i are the roots of the quotient of $C(z)$ and its reflected polynomial and, with p_1, c_n is of absolute value 1. Therefore we can easily bound the norm of $(\Delta - \lambda)\beta_k$ through equation (3.7) by a global constant and the norm of β_k

$$\|\beta_k\|^2 = \sum_{i=0}^{k} |c_i|^2 = 1 + k. \tag{3.8}$$

The β_k have bounded supports, so we can shift them in a way their supports do not overlap, or, stating it differently, to get them orthogonal. Normalizing them, together with (3.8) and (3.7) creates orthonormal

$$f_k = \frac{\beta_k}{\|\beta_k\|}$$

such that $\|(\Delta - \lambda)f_k\| \to 0$. Therefore $(f_k)_{k\in\mathbb{N}}$ is a Weyl sequence and even a Zhislin sequence.

Example 3.8 Another way to gain a Weyl sequence is to search for solutions $c_\pm$ of $\Delta c = \lambda c$. By reason of equation (3.5), we make the ansatz

$$c_\pm(n) := e^{\pm ikn} \qquad \text{for } k \in (0, \pi).$$

Then we have

$$\lambda c_\pm = \Delta c_\pm = c_\pm(1 - \cos(k))$$

and therefore $\cos(\pm k) = 1 - \lambda$.

This eigenvector lies in $\ell^\infty(bZ)$ and not in $\mathcal{H}$. Evade this drawback through defining

$$\beta_m := \frac{\chi_{[0,m]}c_+}{\left\|\chi_{[0,m]}c_+\right\|}.$$

As $\left\|\chi_{[0,m]}c_+\right\| = \sqrt{1+m}$, the sequence $(\beta_m)_{m\in\mathbb{N}}$ lies in $\mathcal{H}$ and it is easy to check that we have found a Weyl sequence, being similar to the sequence we constructed in the example above.

3.2 Isotropic and Anisotropic Potentials

In this section we examine the spectrum of $H := \Delta + V$ for an anisotropic potential V. Proposition 3.12 provides that the essential spectrum of H is the spectrum of Δ shifted by the limits of V. For the lack of a suitable tool-kit, we have to postpone questions regarding $\mathcal{H}_{ac}(H)$ and $\mathcal{H}_{sc}(H)$ to a later chapter. However, we have not treated potentials yet, so we do much good in beginning with a review of isotropic potentials and advance to anisotropic ones thereafter.

Definition 3.9 We define the set $C_\infty(\mathbb{Z})$ as the set of $V \in \ell^\infty(\mathbb{Z}, \mathbb{R})$ such that the limits $\lim_{n\to\pm\infty} V(n) = l_\pm$ exist and are finite.

These functions will form our anisotropic potentials. But let us start with isotropic potentials:

Corollary 3.10 Let $V \in C_\infty(\mathbb{Z})$, with $\lim_{n\to\pm\infty} V(n) = 0$. Then

i) $V(Q)$ is compact,

ii) $\sigma(V(Q)) = \sigma_{pp}(V(Q)) = \overline{V(\mathbb{Z})}$,

iii) $\sigma_{ess}(\Delta + V(Q)) = \sigma_{ess}(\Delta)$.

Proof: i)$V(Q)$ is compact, for the sequence $V_n(Q) := V(Q)\chi_{[-n,n]}(Q)$ is a sequence of finite dimensional range operators such that

$$\|V_n(Q) - V(Q)\| = \limsup_{n\to\infty, |m|>n} |V(m)|$$

converges, with n going to ∞, to 0. Use [Wer] Korollar II.3.3.

ii) For $0 \neq \lambda \in V(\mathbb{Z})$, the set of points $\{x \mid V(x) = \lambda\}$ is finite, implying that the dimension of $\ker(V-\lambda)$ is finite. But as $V(n)$ converges to 0 when $|n| \to \infty$, λ is isolated and thus $\lambda \in \sigma_{disc}(V(Q))$.

iii) We use Corollary 2.13 with $H_1 := \Delta + V(Q)$ and $H_2 := \Delta$. Then $H_1 - H_2 = V(Q)$ is compact and $\sigma_{ess}(\Delta + V(Q)) = \sigma_{ess}(\Delta)$. □

Example 3.11 We assume the settings of the preceding corollary. To construct a Weyl sequence for $\Delta + V(Q)$, we can reuse the sequence from Example 3.7, since we got orthogonality of the f_n by shifting the β_n with n farther away from 0, where the influence of V vanishes to 0.

From here it is not hard to get to the point: The essential spectrum of $\Delta + V$ for anisotropic V is that of Δ shifted by the limits of V.

Proposition 3.12 Let $V \in C_\infty(\mathbb{Z})$ and denote $l_\pm := \lim_{n\to\pm\infty} V(n)$. Then

$$\sigma_{ess}(\Delta + V(Q)) = \sigma_{ess}(\Delta) + \{l_\pm\}.$$

We divide the proof in two. We begin with the inclusion

$$\sigma_{ess}(\Delta + V(Q)) \supset \sigma_{ess}(\Delta) + \{l_\pm\},$$

by constructing suitable Weyl sequences. For the other inclusion we want to use Proposition 2.20 and thus need a short intermezzo with multiplication operators $\theta(Q)$ in Example 3.13.

Proof: Let $\lambda \in [0,2]+l_+$ and define $\lambda' := \lambda - l_+$. Then for λ' we construct a Weyl sequence $(f_n)_{n\in\mathbb{N}}$ for Δ as in Example 3.7, where we make sure, that the applied shifts are always right shifts. For the sequence $(V(n))_{n\in\mathbb{N}}$ converges to l_+, we have for $\varepsilon > 0$ an $n = n(\varepsilon)$ such that $|V(m) - l_+| < \varepsilon$ for all $m > n$. Then we have for $k > n$

$$\|(V(Q) - l_+)f_k\|^2 = \sum_{x>n} |(V(x) - l_+)|^2 |f_k(x)|^2 \leqslant \varepsilon^2 \|f_k\| = \varepsilon^2.$$

Therefore

$$\begin{aligned}\|(\Delta + V(Q) - \lambda)f_k\| &= \|(\Delta - \lambda' + V(Q) - l_+)f_k\| \\ &\leqslant \|(\Delta - \lambda')f_k\| + \|(V(Q) - l_+)f_k\| \\ &\leqslant \|(\Delta - \lambda')f_k\| + \varepsilon^2,\end{aligned}$$

so we found a Weyl sequence for $\Delta + V(Q)$ with $\lambda \in [0,2] + l_+$. Similarly we construct Weyl sequences for $\lambda \in [0,2] + l_-$. □

The other inclusion is left over. To show it, let us prepare a sequence $(\theta_n)_{n\in\mathbb{N}}$ to be used in Proposition 2.20.

Example 3.13 For any bounded multiplication operator $\theta(Q)$ we have

$$\begin{aligned}2\,[\Delta, \theta(Q)] &= \theta(Q)(U + U^*) - (U + U^*)\theta(Q) \\ &= (\theta(Q) - \theta(Q+1))U + (\theta(Q) - \theta(Q-1))U^*\end{aligned}$$

Let $a, b \in \mathbb{Z}$ and $a < b$. With the above, we explore

$$\begin{aligned}2\big[\Delta, \chi_{[a,b]}(Q)\big] f(x) &= \chi_{[a,b]}(x) f(x-1) + \chi_{[a,b]}(x) f(x+1) \\ &\quad - \chi_{[a,b]}(x-1) f(x-1) - \chi_{[a,b]}(x+1) f(x+1).\end{aligned}$$

We perform a shift and one element separations on the $\chi_{[\cdot]}$ to get

$$2\big[\Delta, \chi_{[a,b]}(Q)\big] = (\chi_{\{a\}}(Q) - \chi_{\{b+1\}}(Q))U + (\chi_{\{a-1\}}(Q) - \chi_{\{b\}}(Q))U^*, \tag{3.9}$$

$$2\big[\Delta, \chi_{\{a\}}(Q)\big] = (\chi_{\{a\}}(Q) - \chi_{\{a+1\}}(Q))U + (\chi_{\{a-1\}}(Q) - \chi_{\{a\}}(Q))U^*. \tag{3.10}$$

We are ready to define the sequence $(\theta_n)_{n\in\mathbb{N}}$

$$\theta_n := \chi_{[-n,n]} + \sum_{k=-2n}^{-n-1} (\frac{1}{n}k + 2)\chi_{\{k\}} + \sum_{k=n+1}^{2n} (-\frac{1}{n}k + 2)\chi_{\{k\}}.$$

Equations (3.9), (3.10), collecting expressions and index shifts, displays

$$2[\Delta, \theta_n(Q)] = \frac{1}{n}\left((\chi_{[-2n+1,n]} + \chi_{[n+1,2n]})U + (\chi_{[-2n,-n-1]} + \chi_{[n,2n-1]})U^*\right).$$

Therefore $\|[\Delta, \theta_n(Q)]\|$ converges with $n \to \infty$ to 0.

Proof of Proposition 3.12: We are going to show that $\sigma_{\mathsf{ess}}(\Delta + V(Q))$ is subset of $[0,2] + \{l_\pm\}$. As $[\Delta + V(Q), \theta(Q)] = [\Delta, \theta(Q)]$, Proposition 2.20 in conjunction with Example 3.13 hold, we have for $\lambda \in \sigma_{\mathsf{ess}}(\Delta + V(Q))$ a corresponding Zhislin sequence $(f_n)_{n\in\mathbb{N}}$.

Fix $H := \Delta + V(Q)$ and define orthogonal projections $\pi_\pm$ onto

$$\mathcal{H}_\pm := \{x \in \mathcal{H} \mid x(\mp k) = 0 \text{ for all } k \in \mathbb{N}_0\},$$

to project the Zhislin sequence on "one side". Clearly there is a subsequence $(f_{n_k})_{k\in\mathbb{N}}$ such that $\|\pi_- f_{n_k}\| \geqslant \frac{1}{2}$ or $\|\pi_+ f_{n_k}\| \geqslant \frac{1}{2}$ for all k. Without loss of generality we assume the latter and define sequences

$$g_k := \frac{\pi_+ g_{n_k}}{\|\pi_+ g_{n_k}\|} \text{ and } d_k := \frac{1}{\|\pi_+ g_{n_k}\|},$$

where $(g_k)_{k\in\mathbb{N}}$ is still a Zhislin sequence, since

$$(H - \lambda)g_k = (H - \lambda)\pi_+ d_k f_{n_k} = \chi_{\{-1\}} g(0) + \pi_+ d_k (H + V(Q) - \lambda) f_{n_k}$$

is clearly converging strongly to 0. To get the result, we clip l_+ from λ through $\lambda_\Delta := \lambda - l_+$ and hence get

$$(H - \lambda)g_k = (\Delta - \lambda_\Delta)g_k + (V(Q) - l_+)g_k.$$

The rightmost summand converges to 0, as $(g_k)_{k\in\mathbb{N}}$ is a Zhislin sequence and as $V(n) - l_+$ converges to 0 for large n. As the whole expression converges to 0, so does $(\Delta - \lambda_\Delta)g_k$ and, as we know the essential spectrum of Δ, is $[0,2]$ we get $\lambda_\Delta \in [0,2]$. □

3.3 Multidimensional Laplace Operator

As a prospect we enlarge the concept of the Laplace operator from $\mathbb{Z}$ to $\mathbb{Z}^d$ and Proposition 3.15 inspects its spectrum, but, as we will not return to that subject later, will only serve as an invitation to further investigation. Similarly to the one dimensional case, we construct in Example 3.16 corresponding Weyl sequences.

Definition 3.14 Let $d \in \mathbb{N}$ and $\mathcal{H} := \ell^2(\mathbb{Z}^d)$. We define the d-*dimensional Laplacian* $\Delta^{(d)}$

$$\Delta^{(d)} := \sum_{j=1}^{d} \Delta_j,$$

where we put the operators Δ_j

$$\Delta_j f(k) := f(k) - \frac{1}{2}(f(k+e_j) + f(k-e_j))$$

for $f \in \mathcal{H}$, $j \in \{1,..,d\}$ and $k \in \mathbb{Z}^d$. The e_j are the j-th standard unit direction in $\mathbb{Z}^d$.

Similarly to the one dimensional Laplacian, $\Delta^{(d)}$ on $\mathbb{Z}^d$ is bounded, but its spectrum is somewhat extended:

Proposition 3.15 The spectrum and the essential spectrum of $\Delta^{(d)}$ coincide and form the interval $[0, 2d]$.

Proof: As in the proof of Proposition 3.5, we use the Fourier Transform

$$\mathcal{F}\Delta^{(d)}\mathcal{F}^-1 = \mathcal{F}(\sum_{j=1}^{d} \Delta_j)\mathcal{F}^-1 = \sum_{j=1}^{d} \mathcal{F}\Delta_j\mathcal{F}^-1 = \sum_{j=1}^{d}(1-\cos(Q_k))$$

and thus Proposition 2.17 to get $\sigma(\Delta^{(d)}) = [0, 2d]$. Extending Example 2.18 to $\mathbb{R}^n$ concludes $\sigma(\Delta^{(d)}) = \sigma_{\text{ess}}(\Delta^{(d)})$. Moreover we refer to Proposition 2.11 in conjunction with Example 3.16. □

Example 3.16 Again we want to construct Weyl sequences for $\Delta^{(d)}$. First we construct an "eigenvector". To do so, we fragment $\lambda \in (0, 2d)$ in a sum of λ_i, such that $\lambda_i \in (0, 2)$. Then we define $\tau_i := \lambda_i - 1$ and $p_i := -\tau_i - \sqrt{\tau_i^2 - 1}$ and define

$$f_i(n_i) := p_i^{n_i} \qquad \text{for } n_i \in \mathbb{Z}.$$

According to Example 3.7 we get $\Delta f_i = \lambda_i f_i$. This enables us to construct a $f \in l^\infty(\mathbb{Z}^d)$ with $\Delta^{(d)} f = \lambda f$, through putting

$$f(n) := \prod_{i=1}^{d} f_i(n_i) \qquad \text{for } n \in \mathbb{Z}^d$$

Now we apply $\Delta^{(d)}$ to f and strengthen our arithmetic skills

$$\begin{aligned}(\Delta^{(d)}f)(n) &= \sum_j \Delta_j f(n) = \sum_j f(n) - \frac{1}{2}(f(n+e_j) + f(n-e_j)) \\ &= \sum_j \prod_i f_i(n_i) - \frac{1}{2}(f_j(n+1) + f_j(n-1))(\prod_{i\neq j} f_i(n_i)) \\ &= \sum_j (f_j(n_j) - \frac{1}{2}(f_j(n_j+1) + f_j(n_j-1))) \prod_{i\neq j} f_i(n_i) \\ &= \sum_j \lambda_j f_j(n_j) \prod_{i\neq j} f_i(n_i) = \sum_j \lambda_j f(n) = \lambda f(n).\end{aligned}$$

To get a Weyl sequence, we bound the support of f and through shifting the normalized result, we get things orthonormal.

Another interesting approach is explored in [GG05], which we only want to fringe here. Let $\Gamma = (E, V)$ be an undirected graph and $f : E \to \mathbb{C}$. We denote the relation of neighbourhood of two edges $x, y \in E$ by $x \sim y$. The Laplace operator is then defined according to

$$(\Delta^{(\Gamma)}f)(x) := \sum_{y\sim x} (f(y) - f(x)) \qquad \text{for } x \in E.$$

Spectral analysis and scattering theory of operators $\Delta^{(\Gamma)} + V$ on $\ell^2(\Gamma)$ is discussed in the cited paper. Directed graphs Γ may also be of interest.

4 Mourre Theory

This chapter explores the Mourre Theory of the operator couple (H, A). H is taken bounded, A unbounded but selfadjoint. Definitions 4.4 and 4.6 begin with the introduction of the One-Commutator $[H, A]_\circ$; Propositions 4.5, 4.7 and Lemma 4.8 deal with the investigation of its existence and heredity of existence for certain H. We find the Virial Theorem 4.11 letting us, in the next section when we advance to Mourre Estimates, count the number of eigenvalues of H. The chapter closes with the the Limiting Absorption Principle, i.e. Theorem 4.15, providing the absence of singularly continuous spectrum of H, when a suitable Mourre Estimate is present and H obeys "enough smoothness".

But first of all, we want to motivate the Mourre Theory through its initial inspiration.

4.1 Motivation

What is the idea behind Mourre Estimates? Putnam's Theorem, i.e. Lemma 4.2, provides us with the idea that for a given H we seek a suitable A such that $[H, iA]$ is positive in some sense, then H has purely absolutely continuous spectrum. Putnam's Theorem forces us to use bounded A, which are hard to find in most settings, so the Mourre Theory is all about loosening that restriction. Proposition 4.1 shows that a suitable estimate on the resolvent of H implies that its spectrum is purely absolutely continuous. Putnam's Theorem and the main result of this chapter, the Limiting Absorption Principle (see Theorem 4.15), will henceforth estimate the resolvent. Notice that this section is derived and in the proofs partly identical to the corresponding chapter in [CFKS], incidentally even taking up the same numbering.

Proposition 4.1 Suppose H selfadjoint and bounded, take an open interval $I = (a, b)$ and suppose for every $f \in D$ in a dense set $D \subset \mathcal{H}$ that there is a constant $c(f) < \infty$ such that

$$\sup_{\varepsilon>0, \lambda\in I} \left|\operatorname{Im}\left\langle f, (H - \lambda - i\varepsilon)^{-1} f\right\rangle\right| \leqslant c(f).$$

Then H has purely absolutely continuous spectrum in I.

The fact that $c(f)$ usually depends on f, makes perturbation theory hard, but Putnam's Theorem as well as the Limiting Absorption Principle will return independent constants. We will exploit that in Chapter 6.

Proof: We use Stone's Formula (see [RS] Volume I, Theorem VII.13), i.e. for intervals $I' := (a', b') \subset (a, b) = I$ we have

$$\frac{1}{2}\left\langle f, (E_{[a',b']}(H) + E_{(a',b')}(H))f\right\rangle = \lim_{\varepsilon\searrow 0} \frac{1}{\pi}\int_{I'} \operatorname{Im}\left\langle f, (H - \lambda - i\varepsilon)^{-1} f\right\rangle d\mu.$$

As $E_{[a',b']}(H) \geqslant E_{(a',b')}(H)$ that equation implies

$$\langle f, E_{I'}(H) f\rangle \leqslant \frac{1}{\pi}\int_{I'} c(f) d\mu = \frac{c(f)}{\pi}|I'|$$

for $f \in D$. We can easily proceed to finite unions of disjoint open intervals, so let $I'_\infty := \cup_{i=1}^{\infty}(a'_i, b'_i)$ be a union consisting of disjoint open intervals in I and $I'_u := \cup_{i=1}^{u}(a'_i, b'_i)$ a finitely united subset of I'_∞. Then

$$\left\langle f, E_{I'_\infty} f\right\rangle = \lim_{u\to\infty}\left\langle f, E_{I'_u} f\right\rangle \leqslant \frac{c(f)}{\pi}\lim_{u\to\infty}|I'_u| = \frac{c(f)}{\pi}|I'_\infty|$$

Now take $S \subset I$ with $|S| = 0$. Then by outer regularity of the Lebesgue measure, we can find open sets S_k with $S \subset S_k$ and $\|S_k\| \leqslant 1/k$. Then

$$\langle f, E_S f\rangle \leqslant \inf_k \langle f, E_{S_k} f\rangle \leqslant \frac{c(f)}{\pi} \inf_k |S_k| = 0,$$

i.e. we have continuity with respect to the Lebesgue measure. As D is dense, H has absolutely continuous spectrum in I. □

Lemma 4.2 (Putnam's Theorem) Suppose H and A are bounded, self-adjoint operators such that there is an operator C with Ker $C = \{0\}$ and

$$[H, iA] = C^*C, \tag{4.1}$$

then H has purely absolutely continuous spectrum.

Proof: We notate the resolvent of H by $R(z) := (H - z)^{-1}$. Then for $\mu \in \mathbb{R}$ and $\varepsilon > 0$ we find

$$\begin{aligned}\|CR(\mu \pm i\varepsilon)\|^2 &= \|R(\mu \mp i\varepsilon)C^*CR(\mu \pm i\varepsilon)\| \\ &= \|R(\mu \mp i\varepsilon)[H, iA]R(\mu \pm i\varepsilon)\| \\ &= \|R(\mu \mp i\varepsilon)[H - \mu \mp i\varepsilon, iA]R(\mu \pm i\varepsilon)\| \\ &\leqslant \|AR(\mu \pm i\varepsilon)\| + \|R(\mu \mp i\varepsilon)A\| + 2\varepsilon\|R(\mu \mp i\varepsilon)AR(\mu + i\varepsilon)\| \\ &\leqslant 4\varepsilon^{-1}\|A\|\end{aligned}$$

and therefore

$$2\|C\mathrm{Im}R(\mu + i\varepsilon)C^*\| = \|CR(\mu + i\varepsilon)(2i\varepsilon)R(\mu - i\varepsilon)C^*\| \leqslant 8\|A\|. \tag{4.2}$$

Since the image of C^* is dense, the above returns the statement using Proposition 4.1. □

This proof shows by equation (4.2) for bounded A and H that the inequality $[H, iA] \geqslant \alpha I$ is impossible, since this would make $R(z)$ bounded, i.e. H had no spectrum. This hints that we have to extend our search for suitable A to unbounded operators. The arising problems with the involved commutators are dealt with in the next section. Both [ABG] and [PSS] even explain that Mourre Theory can be extended to unbounded H.

4.2 One-Commutator Properties

In the following we will make heavy use of commutators of selfadjoint, unbounded operators A with bounded operators H. This raises basic questions about the definition of commutators; for illustrative purposes, let us take up the usual definition of the commutator for A and H

$$[H, A]f := HAf - AHf. \tag{4.3}$$

As A is unbounded, we have to consider its domain. For the HAf term take $f \in D(A)$, then Af and HAf are well defined. Problems arise on the right: Hf is defined, but what about $Hf \in D(A)$? To postpone this question we place the scalar product around (4.3) and move over to the adjoint of A and H

$$\begin{aligned} \langle f, [H, A]f \rangle &= \cancel{\langle f, HAf \rangle - \langle f, AHf \rangle} \\ &:= \langle H^* f, Af \rangle - \langle Af, Hf \rangle . \end{aligned} \tag{4.4}$$

Now we can take $f \in D(A)$ and things look fine. Actually, this is the usual approach to tackle this problem; [ABG] serves as reference.

Example 4.3 The features of this definition are easily provided in case of unbounded A and H. Consider the space $\mathcal{H} = L^2(\mathbb{R})$ and the operators $H := \Delta$, defined on $C_c^2(\mathbb{R})$. For A take $A := i\partial Q + iQ\partial$, defined on $C_c^1(\mathbb{R})$. Then $D(H) \cap D(A) = D(H)$, thus the sesquilinearform of (4.4) is defined on $D(H)$. If we would want to define the commutator through $HA - AH$, we would, roughly speaking, need three times differentiable functions, which is quite far away from $D(H)$.

Yet we are not sure if (4.4) actually defines an operator $[H, A]$; to gain that insight, we need to tighten our knots around A and H.

Definition 4.4 Let A be selfadjoint and H be bounded. We say H *is of class* $\mathcal{C}^1(A)$ if there is $c > 0$ such that

$$|\langle H^* f, Af \rangle - \langle Af, Hf \rangle| \leqslant c\|f\|^2 \qquad \text{for } f \in D(A). \tag{4.5}$$

We will examine the structure of this class in Proposition 4.7 and Lemma 4.8; Lemma 4.9 uncovers why we choose the ambiguous notation $\mathcal{C}^1$, but beforehand we find out how the existence of the commutator follows from it, so how gears (4.5) into (4.4)?

Proposition 4.5 Let A be selfadjoint and $H \in \mathcal{C}^1(A)$. Define the sesquilinearform $\Phi : D(A)^2 \to \mathbb{C}$ by

$$\Phi(f,g) := \frac{1}{4}\sum_{k=1}^{4} i^k \left(\left\langle H^*(g+i^k f), A(g+i^k f)\right\rangle - \left\langle A(g+i^k f), H(g+i^k f)\right\rangle\right)$$

for all $f, g \in D(A)$. Then Φ defines a bounded operator $T_\circ$ such that

$$\Phi(f,g) = \langle f, T_\circ g\rangle .$$

Proof: Fix $f_k := g + i^k f$ for $k = 1, \dots, 4$ and $\Phi^{(g)} : D(A) \to \mathbb{C}$ with $\Phi^{(g)}(f) := \Phi(f,g)$. We want to see boundedness of $\Phi^{(g)}$ for all $g \in D(A)$, which is clear for $g = 0$, so for $g \neq 0$

$$\left\|\Phi^{(g)}\right\| = \sup_{0\neq f\in D(A)} \frac{\left\|\Phi^{(g)}f\right\|}{\|f\|} = \sup_{f\in D(A),\|f\|=\|g\|} \frac{\left\|\Phi^{(g)}f\right\|}{\|g\|}$$

and as for $\|f\| = \|g\|$ we have $\|f_k\| \leqslant 2\|g\|$, we get from $H \in \mathcal{C}^1(A)$

$$\left\|\Phi^{(g)}\right\| = \sup_{f\in D(A),\|f\|=\|g\|} \frac{\left\|\Phi^{(g)}f\right\|}{\|g\|} \leqslant \frac{4c4\|g\|}{4\|g\|} = 4c.$$

The Bounded Linear Transformation Theorem therefore guarantees the existence of an extension $\Phi_\circ^{(g)}$ of $\Phi^{(g)}$ on $\mathcal{H}$. By the Riesz Lemma we then receive for every $f \in D(A)$ a unique $y \in \mathcal{H}$ complying $\Phi_\circ^{(g)} = \langle f, y\rangle$ for all $f \in D(A)$. Call $y := Ty$. It is easy to see that T is linear and from the bound of $\Phi_\circ^{(g)}$ that $\|T\| \leqslant 4c$. Again, extend T with the Bounded Linear Transformation Theorem to $T_\circ$ on $\mathcal{H}$. □

In the definition of Φ we used the polarization identity to tackle the definition of $\mathcal{C}^1(A)$; unpacking this sum leads for $f, g \in D(A)$

$$\langle f, T_\circ g\rangle = \langle H^* f, Ag\rangle - \langle Af, Hg\rangle ,$$

looking much like equation (4.4), so give $T_\circ$ its deserved name:

Definition 4.6 Let A be selfadjoint and $H \in \mathcal{C}^1(A)$. We define the *commutator* $[H, A]$ on $D(A)$ in the form sense by

$$\langle f, [H,A]f\rangle := \langle H^* f, Af\rangle - \langle Af, Hf\rangle \qquad \text{for } f \in D(A). \tag{4.6}$$

We denote $[H, A]$ on $\mathcal{H}$ by $[H, A]_\circ$. Moreover we say H is of *class* $\mathcal{C}^2$ *of* A, if $H \in \mathcal{C}^1(A)$ and $[H, A]_\circ \in \mathcal{C}^1(A)$.

Up to this point, checking that H is of class $\mathcal{C}^1(A)$ is finding the estimate (4.5), which may be a tedious undertaking. Luckily the scalar product $\langle\cdot,\cdot\rangle$ is sesquilinear and in a way stable with respect to the adjoint, so having several different operators in $\mathcal{C}^1(A)$ raises hope that we can easily expand our repertoire of $\mathcal{C}^1$ operators. And indeed

Proposition 4.7 The class $\mathcal{C}^1(A)$ is an $*$-algebra and the definition of the commutator fits well, that is for $H_1, H_2 \in \mathcal{C}^1(A)$ we have that

i) $H_1 + H_2 \in \mathcal{C}^1(A)$ and $[H_1 + H_2, A]_\circ = [H_1, A]_\circ + [H_2, A]_\circ$,

ii) $H_1 H_2 \in \mathcal{C}^1(A)$ and $[H_1 H_2, A]_\circ = [H_1, A]_\circ H_2 + H_1 [H_2, A]_\circ$,

iii) $H_1^* \in \mathcal{C}^1(A)$ and $[H_1^*, A]_\circ = [H_1, A]_\circ^*$.

Proof: In this proof we use $[H, A]$ in the form sense. As H_1 and H_2 are in $\mathcal{C}^1(A)$ there are some constants c_1, c_2 such that for $f \in D(A)$ the estimate $|\langle f, [H_i, A]f\rangle| \leqslant c_i \|f\|^2$ holds.

i) We calculate

$$\begin{aligned}\langle f, [(H_1 + H_2), A]f\rangle &= \langle (H_1 + H_2)^* f, Af\rangle - \langle Af, (H_1 + H_2)f\rangle \\ &= \langle H_1^* f, Af\rangle - \langle Af, H_1 f\rangle + \langle H_2^* f, Af\rangle - \langle Af, H_2 f\rangle \\ &= \langle f, [H_1, A]f\rangle + \langle f, [H_2, A]f\rangle\,.\end{aligned} \tag{4.7}$$

In absolute terms this means

$$|\langle f, [(H_1 + H_2), A]f\rangle| \leqslant |\langle f, [H_1, A]f\rangle| + |\langle f, [H_2, A]f\rangle| \leqslant (c_1 + c_2)\|f\|^2$$

providing that $H_1 + H_2 \in \mathcal{C}^1(A)$. As $D(A)$ is a dense set, we can use equation (4.7) to see $[H_1 + H_2, A]_\circ = [H_1, A]_\circ + [H_2, A]_\circ$.

ii) We repeat the steps of i)

$$\begin{aligned}\langle f, [H_1 H_2, A]f\rangle &= \langle (H_1 H_2)^* f, Af\rangle - \langle Af, H_1 H_2 f\rangle \\ &= \langle (H_1 H_2)^* f, Af\rangle - \langle Af, H_1 H_2 f\rangle + \langle H_1^* f, AH_2 f\rangle - \langle AH_1^* f, H_2 f\rangle \\ &= \langle f, [H_1, A]H_2 f\rangle + \langle f, H_1 [H_2, A]f\rangle \\ &= \langle f, [H_1, A]H_2 f\rangle + \langle H_1^* f, [H_2, A]f\rangle\,.\end{aligned} \tag{4.8}$$

In absolute terms we get

$$|\langle f, [H_1 H_2, A]f\rangle| \leqslant (c_1 \|H_2\| + c_2 \|H_1\|)\|f\|^2,$$

read that $H_1H_2 \in \mathcal{C}^1(A)$ and from (4.8) the equation for $[H_1H_2, A]_\circ$.

iii) Clear from Definitions 4.4 and 4.6. □

This proposition obviously makes polynomials of $\mathcal{C}^1$ operators $\mathcal{C}^1$, so an nearby idea is to use the Stone-Weierstrass Theorem to obtain this property for the whole reminder of functional calculus with compactly supported, continuous functions. This does not work out, since the estimation constants in the proof of Proposition 4.7 defend controlling. However, for smooth function we can regularize A to command the needed bound.

Lemma 4.8 Let $H \in \mathcal{C}^1(A)$ be selfadjoint and $\varphi \in C_c^\infty(\mathbb{R})$. Then $\varphi(H)$ is of class $\mathcal{C}^1(A)$, i.e. $[A, \varphi(H)]_\circ$ is bounded and, moreover, the sets $\varphi(H)D(A)$, $(H+i)^{-1}D(A)$ are subsets of $D(A)$.

Proof: To circumvent domain questions, we begin with regularizing A with $R_\lambda := \lambda(iA+\lambda)^{-1}$ for $\lambda \neq 0$. Due to the spectral theorem, R_λ is bounded on $\mathcal{H}$ with an image contained in $D(A)$ and so $A_\lambda := AR_\lambda$ is bounded. Recollecting the boundedness of $[H, A]_\circ$ and as we can, by Definition 4.6, drop the subscript $\circ$ in $D(A)$, we can write for $f, g \in \mathcal{H}$

$$\begin{aligned}
\langle f, R_\lambda[H,A]_\circ R_\lambda g\rangle &= \langle R_\lambda^* f, [H,A]R_\lambda g\rangle = \langle HR_\lambda^* f, AR_\lambda g\rangle - \langle AR_\lambda^* f, HR_\lambda g\rangle \\
&= \langle HR_\lambda^* f, AR_\lambda g\rangle - \big\langle (i/\bar\lambda)HAR_\lambda^* f, AR_\lambda g\big\rangle \\
&\quad - \langle AR_\lambda^* f, HR_\lambda g\rangle - \langle AR_\lambda^* f, (i/\lambda)HAR_\lambda g\rangle \\
&= \big\langle (H(R_\lambda^* - (i/\bar\lambda)AR_\lambda^*)f, A_\lambda g\big\rangle - \langle A_\lambda^* f, H(R_\lambda + (i/\lambda)AR_\lambda)g\rangle \\
&= \big\langle (H(1/\bar\lambda)(\bar\lambda - iA)R_\lambda^* f, A_\lambda g\big\rangle - \langle A_\lambda^* f, H(1/\lambda)(\lambda - iA)R_\lambda)g\rangle \\
&= \langle Hf, A_\lambda g\rangle - \langle A_\lambda^* f, Hg\rangle = \langle f, [H, A_\lambda]g\rangle\,.
\end{aligned}$$

In short $[H, A_\lambda] = R_\lambda[H,A]_\circ R_\lambda$ and with that both are uniformly bounded for large λ. Having said this, we start the actual proof by writing

$$\begin{aligned}
e^{itH}A_\lambda - A_\lambda e^{itH} &= (e^{itH}A_\lambda e^{-itH} - A_\lambda)e^{itH} \\
&= \left(\int_0^t e^{ixH}[H, A_\lambda]e^{-ixH}dx\right)e^{itH}.
\end{aligned} \tag{4.9}$$

We note that with R_λ is $[H, A_\lambda] = R_\lambda[H, iA]_\circ R_\lambda$ uniformly bounded for large λ. Taking this bound into (4.9) we see that there is a constant $C > 0$ independent of λ such that

$$\big\|[A_\lambda, e^{itH}]\big\| \leqslant Ct. \tag{4.10}$$

Take $\varphi \in C_c^\infty(\mathbb{R})$ and denote its Fourier Transform by $\hat{\varphi}$. We gain by the inverse Fourier Transform

$$\varphi(H) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{\varphi}(s) e^{isH} ds$$

and from (4.10) thus

$$\|[A_\lambda, \varphi(H)]\| \leqslant C(\varphi). \tag{4.11}$$

The constant $C(\varphi)$ now depends on φ, still not on λ. We let λ grow to ∞ and read $\varphi(H) \in \mathcal{C}^1(A)$.

By definition we have

$$\langle f, [\varphi(H), A]_\circ g\rangle = \langle \varphi^*(H)f, Ag\rangle - \langle Af, \varphi(H)g\rangle \text{ for all } f, g \in D(A).$$

Since $\varphi(H) \in \mathcal{C}^1(A)$, we find $c \geqslant 0$ resulting in

$$|\langle Af, \varphi(H)g\rangle| \leqslant c\|f\| \cdot \|Ag\|.$$

So there is $B \in \mathcal{B}(D(A), \mathcal{H})$ complying with

$$\langle Af, \varphi(H)g\rangle = \langle f, Bg\rangle$$

and therefore $\varphi(H)D(A) \subset D(A)$. □

This lemma is an interesting one, as it contradicts Example 4.3. If H is bounded and $H \in \mathcal{C}^1(A)$, then $HD(A) \subset D(A)$ and therefore $HA - AH$ is well defined on $D(A)$, thus increasing the user friendliness of $[H, A]_\circ$, but soothingly we would not have known that without the theory.

The usual association of $\mathcal{C}^1$ with differentiability is intended and apt, since $[H, A]_\circ$ can be written as the strong limit of $t \mapsto t^{-1}(e^{-itA}He^{itA} - H)$ with t tending to 0 for any $H \in \mathcal{C}^1(A)$. We also defined $\mathcal{C}^2(A)$ which is clearly linked to the second derivative of this mapping, but for lacking need to do so, we do not iterate this game.

Lemma 4.9 Let A be a selfadjoint operator and H be bounded. H is of class $\mathcal{C}^1(A)$ if and only if the limit of $t^{-1}(e^{-itA}He^{itA} - H)$ exists strongly for t tending to 0. For those H this strong limit is equal to $[H, iA]_\circ$.

Proof: In general take $f, g \in D(A)$. By Stone's Theorem we know the function $t \mapsto \langle e^{iAt}f, He^{iAt}g\rangle$ is C^1. Hence by partial integration we have

$$\left\langle f, \frac{e^{-iAt}He^{iAt} - H}{-it} g \right\rangle = \frac{1}{t}\int_0^t \left(\langle Ae^{iAy}f, He^{iAy}g\rangle - \langle e^{iAy}f, HAe^{iAy}g\rangle\right) dy$$
$$= \frac{1}{t}\int_0^t \langle e^{iAy}f, [A,H]e^{iAy}g\rangle \, dy. \tag{4.12}$$

We assume that the strong limit of $t^{-1}(e^{-iAt}He^{iAt} - H)$ exists. By the Banach-Steinhaus principle of uniform boundedness there is $c \geqslant 0$ satisfying for all $0 < |t| \leqslant 1$

$$\left\| |t|^{-1}\left(e^{-iAt}He^{iAt} - H\right)\right\| \leqslant c.$$

Since the integrand in equation (4.12) is continuous for $f, g \in D(A)$ for all y, we acquire through letting t tend to 0 that $|\langle f, [A,H]g\rangle| \leqslant c\|f\| \cdot \|g\|$ and by fixing the relation $g = f$ proved half the game.

On the other hand suppose $H \in \mathcal{C}^1(A)$, i.e.

$$|\langle H^* f, Af\rangle - \langle Af, Hf\rangle| \leqslant c\|f\|^2 \qquad \text{for } f \in D(A).$$

Then, there is $[H,A]_\circ$ on $\mathcal{H}$ satisfying $\langle g, [A,H]h\rangle = \langle g, [A,H]_\circ f\rangle$ for all $g, h \in D(A)$. Using the Lebesgue Dominated Convergence Theorem on equation (4.12), we gain for all $f, g \in \mathcal{H}$

$$\left\langle f, \frac{e^{-iAt}He^{iAt} - T}{-it} g \right\rangle = \frac{1}{t}\int_0^t \langle e^{iAy}f, [A,H]_\circ e^{iAy}g\rangle \, dy,$$

implying that the weak derivative of $ie^{iAt}He^{iAt}$ exists at $t = 0$ and equals $[A,H]_\circ$. This also holds strongly, since differentiation shows that

$$i\frac{d}{dx}e^{-itA}He^{itA} = e^{-itA}[A,H]_\circ e^{itA}$$

weakly and weakly differentiable functions with strongly continuous derivatives are strongly C^1 (see [ABG] Lemma 5.A.2 b). □

Example 4.10 Take $f \in D(A)$, assume that $Hf = \lambda f$ and consider

$$\langle f, [H,A]_\circ f\rangle = \langle f, [H-\lambda, A]_\circ f\rangle = \langle (H-\lambda)f, Af\rangle - \langle Af, (H-\lambda)f\rangle = 0.$$

This seems to be a very fine property, but it is well posed on $D(A)$ only. The following Virial Theorem solves this problem. You may consult [GG99] for various variants of the Virial Theorem.

Lemma 4.11 (Virial Theorem) Let H be a bounded and selfadjoint operator of class $\mathcal{C}^1(A)$ of a selfadjoint operator A. For $\lambda \in \mathbb{R}$ we have

$$E_{\{\lambda\}}(H)[H, A]_\circ E_{\{\lambda\}}(H) = 0.$$

Proof: For $u \in \mathcal{H}$ we know from Lemma 4.9 that

$$[H, t^{-1}e^{itA}]u \to_{t\to 0} [H, iA]_\circ u, \tag{4.13}$$

as

$$[H, t^{-1}e^{itA}]u = t^{-1}\left(He^{itA} - e^{itA}H\right)u = e^{itA}t^{-1}\left(e^{-itA}He^{itA} - H\right)u.$$

This demonstrates for eigenvectors v_1, v_2 with $\lambda \in \mathbb{R}$ and $Hv_i = \lambda v_i$ of H the equality

$$\begin{aligned}\langle v_1, [H, iA]_\circ v_2\rangle &= \lim_{t\to 0}\frac{1}{t}\left\langle v_1, [H, e^{itA}]v_2\right\rangle = \lim_{t\to 0}\frac{1}{t}\left\langle v_1, [H-\lambda, e^{itA}]v_2\right\rangle \\ &= \lim_{t\to 0}\frac{1}{t}\left(\left\langle (H-\lambda)v_1, e^{itA}v_2\right\rangle - \left\langle e^{-itA}v_1, (H-\lambda)v_2\right\rangle\right) = 0,\end{aligned}$$

which proves the lemma. □

4.3 Mourre Estimates

Mourre Estimates act as a central pivot to deduce the absence of singularly continuous spectrum for a given operator H. To achieve that, the estimate must be "strict". By Proposition 4.14 it is possible to render any Mourre Estimate strict as long as H has no eigenvalue in the concerned part of the spectrum; incidentally Proposition 4.13 keeps the count of eigenvalues finite, so through restriction to the eigenvalue free parts of the spectrum we obtain a strict Mourre Estimate and we land at the intended place, so let us introduce where about we are talking. [CFKS] serves as reference.

Definition 4.12 Let $H \in \mathcal{C}^1(A)$. We say that a *Mourre estimate* for the couple (H,A) holds on an interval J if there is a constant $c > 0$ and a compact operator K such that

$$E_J(H)[H, iA]_\circ E_J(H) \geqslant cE_J(H) + K \tag{4.14}$$

holds. We say that the Mourre estimate is *strict*, if $K = 0$, i.e.

$$E_J(H)[H, iA]_\circ E_J(H) \geqslant cE_J(H) \tag{4.15}$$

holds.

Looking at the differences between equations (4.14) and (4.15) we notice they encircle the operator K; to cope with our problems we have to conquer properties of compact operators, which we already did in Lemma 2.8.

To open the door to strict Mourre Estimates and thus to get rid of compact perturbations, we have to rid the estimate of eigenvalues λ, as from the Virial Theorem

$$E_{\{\lambda\}}(H)[H, A]_\circ E_{\{\lambda\}}(H) = 0,$$

so without a compact $K \neq 0$ in (4.14) there is no possibility to ever reach a true statement as long as eigenvalues are part of the considered spectrum.

Proposition 4.13 Let H be selfadjoint and of class $\mathcal{C}^1(A)$ and assume that a Mourre Estimate (4.14) holds on an interval J. Then the span of all eigenvectors of H corresponding to eigenvalues in J is of finite dimension.

Proof: We suppose that the span had dimension infinite. For H is selfadjoint we can take a sequence $(e_n)_{n\in\mathbb{N}}$ of orthonormal eigenvectors with a corresponding sequence $(\lambda_n)_{n\in\mathbb{N}}$ of eigenvalues in J, i.e. $He_n = \lambda_n e_n$. With the Virial Theorem (Lemma 4.11) and the estimate of (4.14) we gain

$$0 = E_{\{\lambda_n\}}(H)[H, iA]_\circ E_{\{\lambda_n\}}(H) \geqslant c\|e_n\|^2 + \langle e_n, Ke_n\rangle = c + \langle e_n, Ke_n\rangle$$

As the e_n are orthonormal, their sequence converges weakly to 0 and as K is compact, Ke_n converges, by Lemma 2.8, strongly to 0. In the last equation we let n tend to infinity, so we have

$$-c \geqslant \langle e_n, Ke_n\rangle \rightarrow_{n\to\infty} 0.$$

In a way false statements tell the truth; we conclude that there can not be infinitely many orthonormal eigenvectors for eigenvalues in J. □

Finally, due to the last proposition, we find only finitely many eigenvalues, which we simply remove from consideration — remember that the ultimate goal is to find some estimate of the resolvent of H (see Theorem 4.15), which implies $\mathcal{H}_{sc}(H) = \{0\}$; eigenvalues contribute only to the pure point spectrum, therefore

Proposition 4.14 Suppose that H is selfadjoint and $H \in \mathcal{C}^1(A)$. Assume an interval J_0 containing no eigenvalues of H and suppose a Mourre Estimate (4.14) with constant c holds on J_0. For any ε in $(0, c)$ and for any $x \in J_0$ there is an interval $J \subset J_0$ containing x such that

$$E_J(H)[H, iA]_\circ E_J(H) \geqslant (c - \varepsilon)E_J(H). \tag{4.16}$$

Proof: Let $(J_n)_{n\in\mathbb{N}}$ be a sequence of intervals with $x \in J_{n+1} \subset J_n$ for all n including 0 and $|J_n| \to_{n\to\infty} 0$. Then, by assumption, there is $c > 0$ such that for all n

$$E_{J_n}(H)[H, iA]_\circ E_{J_n}(H) \geqslant cE_{J_n}(H) + E_{J_n}(H)KE_{J_n}(H). \tag{4.17}$$

For we can write $\|E_{J_n}(H)f\|^2 = \int_{J_n} 1 d\mathbb{E}_{n,f}(\lambda)$ where, as there is no eigenvalue of H in $J_n \subset J_0$, the measure $\mathbb{E}_{n,f}$ is purely continuous, $E_{J_n}(H)$ converges strongly to 0. Additionally with Lemma 2.8 iii), $E_{J_n}(H)KE_{J_n}(H)$ converges uniformly to 0. So we can increase n until the equation

$$\|E_{J_n}(H)KE_{J_n}(H)\| \leqslant \varepsilon\|E_{J_n}(H)\|$$

holds and define $J := J_n$. We plug that into (4.17) to deduce (4.16). □

4.4 Limiting Absorption Principle

Finally, we want to deduce the absence of singularly continuous spectrum wherever a Mourre Estimate holds, being a consequence of Theorem 4.15.

We follow the proof of [PSS] Theorem 7.8, which is similar to the proof in [CFKS]. However we replace the weights in $|A|+1$ with a smooth version $\langle A\rangle$, where

$$\langle x\rangle := \sqrt{1 + |x|^2}. \tag{4.18}$$

Theorem 4.15 Assume that H is of class $\mathcal{C}^2(A)$ and suppose I is an open interval such that a strict Mourre Estimate holds. Take $\alpha > \frac{1}{2}$, then

$$\sup_{\delta>0,\mu\in I} \left\| \langle A\rangle^{-\alpha} (H - \mu - i\delta)^{-1} \langle A\rangle^{-\alpha} \right\| \leqslant C \tag{4.19}$$

holds for some C, thus H has purely absolutely continuous spectrum in I.

The proof of this theorem is quite demanding. With Proposition 4.1, the purely absolutely continuous spectrum of H in I is an outcome of (4.19).

To convince oneself of the validity of a statement, it is often convenient to try it at its extreme conditions. Sometimes these tests already draw the map of the proof for the remaining cases. This feat will show up here, so fix $\alpha = 1$, then Theorem 4.15 still takes a long proof. We split it into the forthcoming propositions and lemmas and their corresponding proofs, so all these take the same assumptions as Theorem 4.15.

The route: Lemma 4.16 introduces a pair of differential inequalities which are sufficient to prove Theorem 4.15 for $\alpha = 1$; therefore this proof is called the *differential inequality method.* The remaining lemmas then concentrate on showing the validity of the estimates for the given hypotheses on H and its Mourre Estimate.

We also need some sets, operators and functions that we do not want to define every time we use them. Let $\varphi \in C_c^\infty(I; \mathbb{R})$ with $0 \leqslant \varphi \leqslant 1$ and $\varphi(I') = \{1\}$ for some open interval $I' \subset I$. Fixing φ, we define

$$M^2 := \varphi(H)[H, iA]_\circ \varphi(H) \geqslant c(I)\varphi^2(H)$$

and fix for $\varepsilon > 0$ and $\mathrm{Im}(z) > 0$

$$G_\varepsilon(z) := (H - i\varepsilon M^2 - z)^{-1}.$$

Then, by the Spectral Theorem, $\langle A \rangle^{-1} = \sqrt{1 + A^2}^{\,-1}$ is bounded and its image is contained in $D(A)$. Finally fix

$$F_\varepsilon := F_\varepsilon(z) := \langle A \rangle^{-1} G_\varepsilon(z) \langle A \rangle^{-1}.$$

Lemma 4.16 Assume $\varepsilon_0 > 0$ such that for $0 < \varepsilon < \varepsilon_0$ both the estimates

$$\|F_\varepsilon\| \leqslant \frac{C}{\varepsilon} \tag{4.20}$$

$$\left\| \frac{dF_\varepsilon}{d\varepsilon} \right\| \leqslant C \left(\|F_\varepsilon\| + \frac{\sqrt{\|F_\varepsilon\|}}{\sqrt{\varepsilon}} + 1 \right) \tag{4.21}$$

hold for some constant C independent of $\mathrm{Re}(z) = \mu \in I'$, then they imply Theorem 4.15 for $\alpha = 1$.

Proof: We plug (4.20) into (4.21) to see for small $\varepsilon > 0$ that

$$\left\| \frac{dF_\varepsilon}{d\varepsilon} \right\| \leqslant \frac{C}{\varepsilon} \left(C + \sqrt{C} + \varepsilon \right) \leqslant \frac{C^{(1)}}{\varepsilon}$$

for some $C^{(1)} > 0$ independent of μ. We integrate and gain that $\|F_\varepsilon\|$ is bounded by $C^{(2)}|\ln(\varepsilon)|$. We plug that another time into (4.21) to find for small ε

$$\left\|\frac{dF_\varepsilon}{d\varepsilon}\right\| \leqslant C^{(3)}\frac{|\ln(\varepsilon)|}{\sqrt{\varepsilon}}. \tag{4.22}$$

The function $\varepsilon \mapsto |\ln(\varepsilon)|/\sqrt{\varepsilon}$ with the antiderivative $\varepsilon \mapsto 4\sqrt{\varepsilon} - 2\ln(\varepsilon)\sqrt{\varepsilon}$ on $(0,1]$, is absolutely Riemann integrable on $(0,1]$ with existing improper integral and, hence, lies in $L^1([0,1])$, so integrate (4.22) once to see that $\|F_\varepsilon\|$ does not blow up for ε tending to 0. Taking this into the definition of F_ε returns equation (4.19). □

Lemma 4.16 thus is the key to Theorem 4.15 and we will from here concentrate on the differential estimates (4.20) and (4.21); in preparation we need to see $M^2 \in \mathcal{C}^1(A)$:

Lemma 4.17 Suppose that $H \in \mathcal{C}^2(A)$, then $[A, M^2]_\circ$ is bounded.

Proof: We fix $B := [H, iA]_\circ$ and , with Proposition 4.7 in mind, calculate

$$[A, M^2]_\circ = [A, \varphi(H)]_\circ B\varphi(H) + \varphi(H)[A, B]_\circ\varphi(H) + \varphi(H)B[A, \varphi(H)]_\circ.$$

This is, according to Lemma 4.8, bounded. □

Both (4.20) and (4.21) are estimates on F_ε. For F_ε is based on G_ε, we start estimating G_ε and move on to F_ε later.

Lemma 4.18 Take the assumptions from Theorem 4.15. Then

i) for $\varepsilon > 0$ and $\mathrm{Im}(z) > 0$, the inverse $G_\varepsilon(z)$ of $(H - i\varepsilon M^2 - z)$ exists and is continuous for $\varepsilon \in [0, \infty]$ and C^1 for $\varepsilon \in (0, \infty)$ such that

$$\frac{dG_\varepsilon}{d\varepsilon} = iG_\varepsilon M^2 G_\varepsilon, \tag{4.23}$$

ii) for all $\varepsilon > 0$ and $\mathrm{Im}(z) > 0$ and $\mathrm{Re}(z) \in I'$ the estimate

$$\|\varphi(H)G_\varepsilon(z)f\| \leqslant C\frac{\sqrt{|\langle f, G_\varepsilon(z)f\rangle|}}{\sqrt{\varepsilon}} \tag{4.24}$$

holds for all $f \in \mathcal{H}$,

iii) there is $\varepsilon_0 > 0$ such that for all $\varepsilon \in (0, \varepsilon_0)$ and $\mathrm{Re}(z) \in I'$ we have

$$\|(1-\varphi(H))G_\varepsilon(z)\| \leqslant C, \tag{4.25}$$

$$\|G_\varepsilon(z)\| \leqslant \frac{C}{\varepsilon}, \tag{4.26}$$

$$\left\|G_\varepsilon(z)\langle A\rangle^{-1}\right\| \leqslant C\left(1+\frac{\sqrt{\|F_\varepsilon\|}}{\sqrt{\varepsilon}}\right). \tag{4.27}$$

Proof: For shorter notation we denote $T(z,\varepsilon) := H - i\varepsilon M^2 - z$.

i) Decomposing z into $z = \mu + i\delta$ yields for $f \in \mathcal{H}$

$$\begin{aligned}\left\|(H-i\varepsilon M^2-z)f\right\|^2 &= \left\langle (H-i\varepsilon M^2-\mu-i\delta)f, (H-i\varepsilon M^2-\mu-i\delta)f\right\rangle \\ &= \left\|(H-i\varepsilon M^2-\mu)f\right\|^2 + \delta^2\|f\|^2 + 2\delta\varepsilon\|Mf\|^2.\end{aligned} \tag{4.28}$$

Taking $\delta > 0$ and noting that a similar estimate holds for the adjoint $T(z,\varepsilon)^* = T(z^*,\varepsilon)$ shows that $\mathrm{Ker}\, T(z,\varepsilon) = \mathrm{Ker}\, T(z,\varepsilon)^* = \{0\}$ providing us with $\overline{\mathrm{Ran}\, T(z,\varepsilon)} = \mathcal{H}$. Now assume a Cauchy-Sequence $(g_n)_{n\in\mathbb{N}}$ in $\mathrm{Ran}\, T(z,\varepsilon)$, carrying unique f_n with $g_n = T(z,\varepsilon)f_n$. We fetch from (4.28)

$$\begin{aligned}\|f_n - f_m\|^2 &= \frac{1}{\delta^2}\|g_n-g_m\|^2 - \frac{1}{\delta^2}\left\|(H-i\varepsilon M^2-\mu)(f_n-f_m)\right\| \\ &\quad - 2\frac{\varepsilon}{\delta}\|M(f_n-f_m)\|^2 \leqslant \frac{1}{\delta^2}\|g_n-g_m\|^2,\end{aligned}$$

that is $(f_n)_{n\in\mathbb{N}}$ is a Cauchy Sequence and thus $\mathrm{Ran}\, T(z,\varepsilon)$ is closed.

Fixing z and recollecting that M and H are bounded, we get the required strong differentiability and continuity for $\varepsilon \mapsto G_\varepsilon(z)$, as $G_\varepsilon(z)$ is the inverse of a polynomial of bounded operators. Finally, assuming $f \in \mathcal{H}$ we have $f = G_\varepsilon(z)T(z,\varepsilon)f$ that we differentiate with respect to ε using the product rule to obtain (4.23).

ii) We note the equality

$$\begin{aligned}&G_\varepsilon^*(2ieM^2 + 2i\mathrm{Im}(z))G_\varepsilon \\ &\quad = G_\varepsilon^*(H - H + 2ieM^2 + \mathrm{Re}(z) - \mathrm{Re}(z) + 2i\mathrm{Im}(z))G_\varepsilon \\ &\quad = G_\varepsilon^*(H + i\varepsilon M^2 + z)G_\varepsilon - G_\varepsilon^*(H - i\varepsilon M^2 + \bar{z})G_\varepsilon \\ &\quad = G_\varepsilon^* - G_\varepsilon\end{aligned}$$

and thence use the Mourre Estimate to get

$$\begin{aligned}\|\varphi(H)G_\varepsilon f\|^2 &= \left\langle f, G_\varepsilon^*\varphi(H)^2G_\varepsilon f\right\rangle \leqslant (2c(I)\varepsilon)^{-1}\left\langle f, G_\varepsilon^* 2\varepsilon M^2 G_\varepsilon f\right\rangle \\ &\leqslant (2c(I)\varepsilon)^{-1}\left\langle f, G_\varepsilon^* 2(\varepsilon M^2 + \mathrm{Im}(z))G_\varepsilon f\right\rangle \\ &= (2c(I)\varepsilon)^{-1}\langle f, (G_\varepsilon^* - G_\varepsilon)f\rangle \\ &\leqslant (c(I)\varepsilon)^{-1}|\langle f, G_\varepsilon f\rangle|.\end{aligned}$$

iii) We can express G_ε in terms of G_0

$$(1-\varphi(H))G_\varepsilon(z) = (1-\varphi(H))G_0(z)(1+i\varepsilon M^2 G_\varepsilon(z)).$$

For $\mathrm{Re}(z) \in I'$, $(1-\varphi(H))G_0(z)$ is bounded and hence

$$\|(1-\varphi(H))G_\varepsilon\| \leqslant C(1+\varepsilon\|G_\varepsilon\|), \tag{4.29}$$

i.e. equation (4.25) follows from (4.26) and (4.29). Well, to see (4.26) we use (4.24) and estimate

$$\begin{aligned}\|G_\varepsilon\| + 1 &\leqslant \|\varphi(H)G_\varepsilon\| + \|(1-\varphi(H))G_\varepsilon\| + 1 \\ &\leqslant C\varepsilon^{-1/2}\|G_\varepsilon\|^{1/2} + C_1(1+\varepsilon\|G_\varepsilon\|) + 1.\end{aligned}$$

Taking $C_1\varepsilon \leqslant 1/2$ and $C_1 + 1/2 \leqslant C\varepsilon^{-1/2}$, we can further estimate

$$\begin{aligned}\|G_\varepsilon\| + 1 &\leqslant C\varepsilon^{-1/2}(\|G_\varepsilon\|^{1/2} + 1) + \frac{1}{2}(\|G_\varepsilon\| + 1) \\ &\leqslant 2C\varepsilon^{-1/2}(\|G_\varepsilon\| + 1)^{1/2} + \frac{1}{2}(\|G_\varepsilon\| + 1),\end{aligned}$$

and therefore $\|G_\varepsilon\| \leqslant 16C^2/\varepsilon$, i.e. (4.26) is true for

$$\varepsilon \leqslant \varepsilon_0 := \min\left\{(2C_1)^{-1}, C^2(C_1+1/2)^{-2}\right\}.$$

For the remaining equation we take (4.24) and plug in $f := \langle A\rangle^{-1} g$ and have

$$\left\|\varphi(H)G_\varepsilon \langle A\rangle^{-1} g\right\| \leqslant C\varepsilon^{-1/2}|\langle g, F_\varepsilon g\rangle|^{1/2},$$

on which we apply Cauchy-Schwarz to get

$$\left\|\varphi(H)G_\varepsilon \langle A\rangle^{-1}\right\| \leqslant C\varepsilon^{-1/2}\|F_\varepsilon\|^{1/2}.$$

Moreover, since $\left\|\langle A\rangle^{-1}\right\| \leqslant 1$ and by (4.25),

$$\left\|(1-\varphi(H))G_\varepsilon \langle A\rangle^{-1}\right\| \leqslant \|(1-\varphi(H))G_\varepsilon\|$$

is bounded. Writing $G_\varepsilon = (1-\varphi(H))G_\varepsilon + \varphi(H)G_\varepsilon$ returns thus (4.27). □

To complete the proof of Theorem 4.15, exchange G_ε with F_ε.

Lemma 4.19 Under the assumptions of Theorem 4.15, the inequalities (4.21) and (4.20) hold.

Proof: By the definition of F_ε, we get (4.20) from (4.26) by left and right multiplication of the bounded $\langle A\rangle^{-1}$. Deriving (4.21) is somewhat more painful; we commence with (4.23)

$$-i\frac{dF_\varepsilon}{d\varepsilon} = \langle A\rangle^{-1} G_\varepsilon M^2 G_\varepsilon \langle A\rangle^{-1} = T_1 + T_2 + T_3,$$

where we place the operators T_i through

$$\begin{aligned} T_1 &:= -\langle A\rangle^{-1} G_\varepsilon(1-\varphi(H))[H,iA]_\circ(1-\varphi(H))G_\varepsilon \langle A\rangle^{-1}, \\ T_2 &:= -\langle A\rangle^{-1} G_\varepsilon(1-\varphi(H))[H,iA]_\circ(1-\varphi(H))G_\varepsilon \langle A\rangle^{-1} \\ &\quad - \langle A\rangle^{-1} G_\varepsilon\varphi(H)[H,iA]_\circ\varphi(H)G_\varepsilon \langle A\rangle^{-1}, \\ T_3 &:= \langle A\rangle^{-1} G_\varepsilon[H,iA]_\circ G_\varepsilon \langle A\rangle^{-1}. \end{aligned}$$

We remember that $[H,iA]_\circ$ and by (4.25) that $(1-\varphi(H))G_\varepsilon \langle A\rangle^{-1}$ are bounded, i.e. there is $C_1 > 0$ such that $\|T_1\| \leqslant C_1$. We continue this argument and, moreover, take (4.27) into account and hence have

$$\begin{aligned} \|T_2\| &\leqslant C_2''\left\|\varphi(H)G_\varepsilon \langle A\rangle^{-1}\right\| \leqslant C_2'\left\|G_\varepsilon \langle A\rangle^{-1}\right\| \\ &\leqslant C_2(1+\varepsilon^{-1/2}\|F_\varepsilon\|^{1/2}). \end{aligned}$$

We further guillotine the remaining operator T_3

$$\begin{aligned} T_3 &= T_4 + T_5, \\ T_4 &:= \langle A\rangle^{-1} G_\varepsilon[H-i\varepsilon M^2 - z, iA]_\circ G_\varepsilon \langle A\rangle^{-1}, \\ T_5 &:= \langle A\rangle^{-1} G_\varepsilon[i\varepsilon M^2, iA]_\circ G_\varepsilon \langle A\rangle^{-1}. \end{aligned}$$

Taking the commutator in T_4 into Definition 4.6, we see

$$\|T_4\| \leqslant 2\left\|\langle A\rangle^{-1} AG_\varepsilon \langle A\rangle^{-1}\right\| \leqslant 2\left\|G_\varepsilon \langle A\rangle^{-1}\right\| \leqslant 2C(1+\varepsilon^{-1/2}\|F_\varepsilon\|^{1/2}),$$

where we recall $\left\|\langle A\rangle^{-1} A\right\| \leqslant 1$. The remaining T_5 is estimated with the help of (4.27) and Lemma 4.17

$$\begin{aligned} \|T_5\| &\leqslant \varepsilon\left\|G_\varepsilon \langle A\rangle^{-1}\right\|^2 \left\|[M^2,iA]\right\| \leqslant C_5'(\varepsilon^{1/2}+\|F_\varepsilon\|^{1/2})^2 \\ &\leqslant C_5(1+\|F_\varepsilon\|). \end{aligned}$$

The combination of all these estimates validate (4.21). □

Since we provided the proof of Theorem 4.15 for $\alpha = 1$, we want to loose the reins on α. A very basic technical lemma offers the path through the required estimates:

Lemma 4.20 The recurrence $\beta_0 = 1$, $\beta_{n+1} = -(\alpha - (\beta_n \alpha + 1)/2)$ becomes for $\alpha > 1/2$ and large n negative and is solved through the expression

$$\beta_n = 1 - \frac{2^n - 1}{2^{n-1}} \alpha. \tag{4.30}$$

Proof: Clearly (4.30) is true for $n = 0$. Let us assume that the equation holds for n. Then

$$\beta_{n+1} = -\left(\alpha - \frac{\beta_n \alpha + 1}{2}\right) = -\left(\alpha - 1 + \frac{2^n - 1}{2^n}\alpha\right) = 1 - \frac{2^{n+1} - 1}{2^n}\alpha$$

inductively shows (4.30). Look into the α factor of β_n

$$-\frac{2^n - 1}{2^{n-1}} = \frac{2}{2^n} - 2$$

to see the convergence to -2, so for $\alpha > 1/2$ the β_n get negative. □

Proof of Theorem 4.15: Assume $\varepsilon \leqslant 1$ Define $D_\varepsilon := \langle A \rangle^{-\alpha} \langle \varepsilon A \rangle^{\alpha - 1}$. Due to the Spectral Theorem we have $\|D_\varepsilon A\| \leqslant 1$ and

$$\left\| \frac{dD_\varepsilon}{d\varepsilon} \right\| = (1 - \alpha) \left\| \varepsilon A^2 \langle A \rangle^{-\alpha} \langle \varepsilon A \rangle^{\alpha - 3} \right\| \leqslant \varepsilon^{\alpha - 1}(1 - \alpha). \tag{4.31}$$

Moreover replace $F_\varepsilon = \langle A \rangle^{-1} G_\varepsilon \langle A \rangle^{-1}$ with

$$F'_\varepsilon := D_\varepsilon G_\varepsilon D_\varepsilon.$$

For not taking use of the structure of $\langle A \rangle^{-1}$ in the proof of (4.27), we gain

$$\|G_\varepsilon D_\varepsilon\| \leqslant C^{(1)} \left(1 + \frac{\sqrt{F'_\varepsilon}}{\sqrt{\varepsilon}}\right)$$

and therefore conclude with (4.31) that

$$\left\| \frac{dD_\varepsilon}{d\varepsilon} G_\varepsilon D_\varepsilon + D_\varepsilon G_\varepsilon \frac{dD_\varepsilon}{d\varepsilon} \right\| \leqslant C^{(2)} \varepsilon^{\alpha - 1}(1 + \varepsilon^{-1/2} \|F_\varepsilon\|^{1/2} + \|F'_\varepsilon\|).$$

Similarly to Lemma 4.19 we can estimate $D_\varepsilon G_\varepsilon D_\varepsilon$ and can thus put everything together to have

$$\left\|\frac{dF'_\varepsilon}{d\varepsilon}\right\| \leqslant C^{(3)}\varepsilon^{\alpha-1}(1+\varepsilon^{-1/2}\|F'_\varepsilon\|^{1/2}+\|F'_\varepsilon\|). \tag{4.32}$$

Let us now start an iterative process. Assume that $\|F'_\varepsilon\| \leqslant C\varepsilon^{-\beta_n}$ for some $\beta_n \leqslant 1$, which, taken into 4.32, yields to

$$\left\|\frac{dF'_\varepsilon}{d\varepsilon}\right\| \leqslant C_n^{(4)}\varepsilon^{\alpha-1}(1+\varepsilon^{-1/2-\beta_n/2}).$$

and through integration shows

$$\|F'_\varepsilon\| \leqslant C_n^{(5)}(1+\varepsilon^{\alpha-\beta_n\alpha/2-1/2}).$$

By (4.26) we can start with $\beta_0 = 1$ and by Lemma 4.20 gain uniform boundedness of F'_ε in a finite number of steps. Considering $\varepsilon = 0$ leaves equation (4.19). □

5 Application of the Mourre Theory

This chapter further develops the ideas of the Laplace chapter. Using the Mourre Theory we conclude, in Theorem 6.5, the absence of singularly continuous spectrum for $H_s = \Delta + L(Q) + V_s(Q)$, where $L|_{\mathbb{Z}_\pm} = l_\pm$ forms a *Barrier potential*, introducing anisotropy, and V_s is taken in $O(1/n^2)$. Therefore we seek a suitable A to be used in the commutator $[H_s, A]_\circ$, leading to a strict Mourre Estimate, i.e. Corollary 5.19, which we plug into the Limiting Absorption Principle. The fact that L describes an anisotropic potential poses some obstacle, we thus commence with examining $H := \Delta + L$. Definition 5.2 deals with this obstacle by splitting the space $\mathcal{H} = \ell^2(\mathbb{Z})$ into the left and right sides $\ell^2(\mathbb{Z}_-)$ and $\ell^2(\mathbb{Z}_+)$; subsequently Propositions 5.5, 5.10, 5.11 build up a Mourre Estimates for (H, A) restricted to theses spaces, concluding in Corollary 5.12. Finally Proposition 5.14 glues the estimate.

On this way we will perturb the Laplacian, so Section 5.5 recovers the Laplacian. The last section then deals with adding V_s to H.

5.1 A suitable conjugate operator on $\ell^2(\mathbb{Z})$

Our initial task is to find a selfadjoint A such that a strict Mourre Estimate holds for $[\Delta, iA]_\circ$ and, then, take a step towards $[H, iA]_\circ$. The realization of this is heavily inspired by ideas and notions gathered from [GG05]. Actually, some trouble arises when placing anisotropic potentials, forcing us to split $\mathcal{H} = \ell^2(\mathbb{Z})$ and to find appropriate A on the splinters. The Fourier Transformation maps Δ to a multiplication operator, which makes a good starting point, so we commence with considering general A for multiplication operators.

Proposition 5.1 Consider $\mathcal{H} = L^2(I)$, where I is an interval. Let $\varphi(Q)$ be a multiplication operator with $\varphi \in C^1(I)$. Fix $A := i\varphi'(Q)\partial + i\partial\varphi'(Q)$, which we first define on $C^1(I)$ and then move on to the closure. Then

$$[\varphi(Q), iA]_\circ = 2\varphi'(Q)^2.$$

Proof: We expand on $C^1(I)$

$$\begin{aligned}[\varphi(Q), iA] &= [\varphi(Q), -\varphi'(Q)\partial - \partial\varphi'(Q)] \\ &= [\varphi(Q), -\varphi'(Q)\partial] + [\varphi(Q), -\partial\varphi'(Q)].\end{aligned} \tag{5.1}$$

We separately expand both addends of the right side of (5.1), to see their positivity, beginning with the left

$$\begin{aligned}[\varphi(Q), -\varphi'(Q)\partial]_\circ &= [\varphi(Q), -\varphi'(Q)]_\circ\partial + \varphi'(Q)[\varphi(Q), -\partial]_\circ \\ &= \varphi'(Q)[\varphi(Q), -\partial]_\circ = \varphi'(Q)[\partial, \varphi(Q)]_\circ.\end{aligned}$$

We note that $[\partial, \varphi(Q)]_\circ = \varphi'(Q)$, since for f in $D([\partial, \varphi(Q)]_\circ)$, we have

$$[\partial, \varphi(Q)]_\circ f = \partial(\varphi f) - \varphi\partial f = \varphi' f + \varphi f' - \varphi f' = \varphi'(Q) f$$

and therefore

$$[\varphi(Q), -\varphi'(Q)\partial]_\circ = \varphi'(Q)^2.$$

Similarly we continue with the second summand in (5.1)

$$\begin{aligned}[\varphi(Q), -\partial\varphi'(Q)]_\circ &= [\varphi(Q), -\partial]_\circ\varphi'(Q) - \partial[\varphi(Q), \varphi'(Q)]_\circ \\ &= [\varphi(Q), -\partial]_\circ\varphi'(Q) = \varphi'(Q)^2,\end{aligned}$$

resembling the stated result. □

In momentum space, Proposition 3.5 gave the form $1 - \cos(Q)$ to the Laplacian. So with Proposition 5.1 we construct $A_{\mathbb{Z}}$ with $[\Delta, iA_{\mathbb{Z}}]_\circ \geqslant 0$. Place $\varphi := 1 - \cos$ and get $\varphi' = \sin$. So fix

$$\tilde{A}_{\mathbb{Z}} := \frac{i\sin(Q)\partial + i\partial\sin(Q)}{2}.$$

on the 2π-periodic functions in $C^\infty(\mathbb{R})$. We want to sketch how this plays together: The Fourier Coefficients of such functions fall, in absolute terms, faster than any polynomial. The derivation in the definition of $\tilde{A}$ will introduce a multiplication by Q, so the dwindling of the coefficients does not change under $\tilde{A}$.

Of course the inverse Fourier Transform $\mathcal{F}^{-1}$ is the tool to bring $\tilde{A}_{\mathbb{Z}}$ back to $\ell^2(\mathbb{Z})$. For convenience we define $c := (2\pi)^{-\frac{1}{2}}$ and see for $f \in C^\infty(\mathcal{S}^1)$

$$\begin{aligned}
(\mathcal{F}^{-1}\tilde{A}_{\mathbb{Z}}f)(k) &= c\int_0^{2\pi} (\tilde{A}_{\mathbb{Z}}f)(x)e^{ikx}dx \\
&= \frac{ic}{2}\int_0^{2\pi} (\sin(x)f'(x) + \cos(x)f(x) + \sin(x)f'(x))e^{ikx}dx \qquad (5.2)\\
&= \frac{ic}{2}\int_0^{2\pi} (2\sin(x)f'(x) + \cos(x)f(x))e^{ikx}dx.
\end{aligned}$$

Integration by parts allows drawing f from f'

$$\begin{aligned}
\int_0^{2\pi} \sin(x)e^{ikx}f'(x)dx = [\sin(x)e^{ikt}f(x)]_0^{2\pi} \\
- \int_0^{2\pi} f(x)(\cos(x) + ik\sin(x))e^{ikx}dx \\
= -\int_0^{2\pi} f(x)(\cos(x) + ik\sin(x))e^{ikx}dx.
\end{aligned}$$

We put this result into (5.2) and get a quite compact form

$$(\mathcal{F}^{-1}\tilde{A}_{\mathbb{Z}}f)(k) = -\frac{ic}{2}\int_0^{2\pi} f(x)\cos(x)e^{ikx}dx + kc\int_0^{2\pi} f(x)\cos(x)e^{ikx}dx.$$

Using Euler's Formulas for sine and cosine reveals that they act as shifting operators when used within the inverse Fourier Transformation

$$\begin{aligned}
(\mathcal{F}^{-1}\tilde{A}_{\mathbb{Z}}f)(k) = &-\frac{ic}{4}\int_0^{2\pi} f(x)(e^{i(k+1)x} + e^{i(k-1)x})dx \\
&-\frac{ick}{2}\int_0^{2\pi} f(x)(e^{i(k+1)x} - e^{i(k-1)x})dx,
\end{aligned}$$

which can be easily expressed in terms of the operators U, U^* and Q

$$\mathcal{F}^{-1}\tilde{A}_{\mathbb{Z}} = -\frac{i}{2}\left[\frac{1}{2}(U^* + U) + Q(U^* - U)\right]\mathcal{F}^{-1}.$$

Thus on the aborting sequences $\ell^2_c(\mathbb{Z})$, which are subset of $\mathcal{F}^{-1}C^\infty(\mathcal{S}^1)$ we want to define

$$\begin{aligned} A_{\mathbb{Z}} &:= -\frac{i}{2}\left[\frac{1}{2}(U^* + U) + Q(U^* - U)\right] \\ &= \frac{i}{2}\left[U\left(Q + \frac{1}{2}\right) - \left(Q + \frac{1}{2}\right)U^*\right] \end{aligned} \tag{5.3}$$

and then close the operator. This closure exists, since $A_{\mathbb{Z}}$ is symmetric and the domain of $A^*_{\mathbb{Z}}$ contains the dense subspace $\ell^2_c(\mathbb{Z})$. This $A_{\mathbb{Z}}$ would suit our needs, except for anisotropic potentials. For the isotropic case we could stick to this $A_{\mathbb{Z}}$ and most of the following properties and their proofs hold without major changes.

5.2 A suitable conjugate operator on $\ell^2(\mathbb{Z}_\pm)$

Now we have the general idea to find an A with $[H, iA]_\circ \geqslant 0$, so the next step is to split $\ell^2(\mathbb{Z})$ into $\ell^2(\mathbb{Z}_-) \oplus \ell^2(\mathbb{Z}_+)$ in a way that enables us to easily bring the Barrier potential L into play.

Definition 5.2 We split $\mathcal{H} = \ell^2(\mathbb{Z})$ into $\ell^2(\mathbb{Z}_-) \oplus \ell^2(\mathbb{Z}_+)$, where we choose $\mathbb{Z}_+ := \mathbb{N}_0$ and $\mathbb{Z}_- := \mathbb{Z}\backslash\mathbb{Z}_+$. In the following a subscribed $+$ and $-$ indicates on which space we operate. We begin with splitting Q, as found in Definition 2.14, into $Q_\pm$. So for $f \in \ell^2(\mathbb{Z}_+)$ and $g \in \ell^2(\mathbb{Z}_-)$

$$\begin{aligned} (Q_+f)(k) &:= kf(k) \text{ for } k \in \mathbb{Z}_+, \\ (Q_-g)(l) &:= lf(l) \text{ for } l \in \mathbb{Z}_-. \end{aligned}$$

In consequence we gain $Q = Q_- \oplus Q_+$ on $\ell^2(\mathbb{Z}_-) \oplus \ell^2(\mathbb{Z}_+)$. Similarly we split multiples of the identity $c\mathbb{1}$ into $c\mathbb{1} = c_- \oplus c_+$ on $\ell^2(\mathbb{Z}_-) \oplus \ell^2(\mathbb{Z}_+)$.

The following operators, defined in the same manner, will not fit as seamlessly into this scheme. So, the *shift operators* $U_\pm, U^*_\pm$ are defined by

$$(U_+f)(k) = \begin{cases} f(k-1) & k > 0, \\ 0 & k = 0, \end{cases} \quad \text{and } U^*_+(k) = f(k+1) \quad \text{for } k \in \mathbb{Z}_+,$$

$$(U^*_-g)(l) = \begin{cases} g(l+1) & l < 1, \\ 0 & l = 1, \end{cases} \quad \text{and } U_-(l) = g(l-1) \quad \text{for } l \in \mathbb{Z}_-.$$

Then $U_{\pm}^*$ and $U_{\pm}^*$ are mutually adjoint. We easily verify

$$U_+U_+^* = \chi_{\mathbb{N}}(Q) \text{ and } U_+^*U_+ = 1_+$$

and similarly for U_- and U_-^*. So $U_{\pm}$ are partial isometries, in particular $\|U_{\pm}\| = 1$, but beware $U \neq U_- \oplus U_+$.

Hence define the *perturbed Laplacians* $\Delta_{\pm}$ on $\ell^2(\mathbb{Z}_{\pm})$ through

$$\Delta_{\pm} := 1_{\pm} - \frac{1}{2}(U_{\pm} + U_{\pm}^*) \tag{5.4}$$

There is only a meagre difference between Δ and $\Delta_- \oplus \Delta_+$:

Corollary 5.3 By the definition of $\Delta_{\pm}$ it is clear that

$$\Delta = \Delta_+ \oplus \Delta_- - \frac{1}{2}(\chi_{\{-1\}}(Q)U^* + \chi_{\{0\}}(Q)U),$$

so we can express Δ on $\ell^2(\mathbb{Z}_-) \oplus \ell^2(\mathbb{Z}_+)$ by writing

$$\Delta = \left(\begin{array}{c|c} \Delta_- & -\frac{1}{2}\chi_{\{-1\}}(Q)U^* \\ \hline -\frac{1}{2}\chi_{\{0\}}(Q)U & \Delta_+ \end{array}\right).$$

The operators $\Delta_{\pm}$ and Δ carry, by Proposition 5.5, similar properties, which is of course desirable. To examine them, we want to get $\Delta_{\pm}$ into a multiplication operator — we used the Fourier Transformation on Δ, but, because it does not work out exactly the same on $\Delta_{\pm}$, have to switch to other transformations $\mathcal{G}_{\pm}$:

Lemma 5.4 We define the operators $\mathcal{G}_{\pm} : \ell^2(\mathbb{Z}_{\pm}) \to L^2_{\mathrm{odd}}([-\pi, \pi])$ by

$$(\mathcal{G}_+f_+)(x) = \frac{1}{\sqrt{\pi}} \sum_{l \in \mathbb{Z}_+} f(l) \sin((l+1)x)$$

$$(\mathcal{G}_-f_-)(x) = \frac{1}{\sqrt{\pi}} \sum_{l \in \mathbb{Z}_-} f(l) \sin(lx)$$

for all $f_+ \in \ell^2(\mathbb{Z}_+)$ and $f_- \in \ell^2(\mathbb{Z}_-)$. Then $\mathcal{G}_{\pm}$ are unitary transformations.

Proof: We show this proof on the $\mathbb{Z}_+$ side. For shorter notation fix $\mathcal{G} := \mathcal{G}_+$. We begin by calculating the value of two integrals. Let $p, q \in \mathbb{N}$, and $p \neq q$, then

$$\int_{-\pi}^{\pi} \sin^2(px)dx = \int_{-p\pi}^{p\pi} \sin^2(y)\frac{dx}{p} = \left[\frac{1}{2p}(y - \sin(y)\cos(y))\right|_{-p\pi}^{p\pi} = \pi,$$

$$\begin{aligned}\int_{-\pi}^{\pi} \sin(px)\sin(qx) &= \int_{-\pi}^{\pi} \cos((p-q)x) - \cos((p+q)x)\frac{dx}{2} \\ &= \left[\frac{\sin(y)}{2(p-q)}\right|_{-(p-q)\pi}^{(p-q)\pi} + \left[\frac{\sin(y)}{2(p+q)}\right|_{(p+q)\pi}^{(p+q)\pi} = 0.\end{aligned}$$

At first Take $f \in \ell^1(\mathbb{Z}_+)$, then, with the above,

$$\begin{aligned}\langle \mathcal{G}f, \mathcal{G}f\rangle &= \pi^{-1}\int_{-\pi}^{\pi}\left(\sum_{j\in\mathbb{Z}_+}\sin((j+1)x)f(j)\right)\left(\sum_{k\in\mathbb{Z}_+}\sin((k+1)x)\overline{f(k)}\right)dx \\ &= \pi^{-1}\sum_{j\in\mathbb{Z}_+}\sum_{k\in\mathbb{Z}}\int_{-\pi}^{\pi}\sin((j+1)x)\sin((k+1)x)f(j)\overline{f(l)}dx \\ &= \sum_{i\in\mathbb{Z}_+}|f(i)|^2 = \langle f, f\rangle .\end{aligned}$$

We are left to show that this transformation is surjective. From the Fourier transformation we know that its sinus terms ($e^{ikx} = \cos(kx) + i\sin(kx)$) cover the full space L^2_{odd}, hence does our transformation. □

Proposition 5.5 The operators $\Delta_\pm$ are bounded and selfadjoint and unitarily equivalent to $(1-\cos(Q))$ and therefore $\sigma(\Delta_\pm) = \sigma_{ess}(\Delta_\pm) = [0,2]$ is purely absolutely continuous.

Proof: Boundedness and selfadjointness are shown as in Proposition 3.5. Fix $\mathcal{G} := \mathcal{G}_+$. For $x, y \in \mathbb{Z}_+$ we say x is neighbour of y if $|x-y| = 1$ and denote that by $x \sim y$. Then for $f \in L^1(\mathbb{Z}_+)$

$$\begin{aligned}-2\sqrt{\pi}(\mathcal{G}\Delta_+ f)(k) &= -2\sqrt{\pi}\mathcal{G}f(k) + \sum_{j\in\mathbb{Z}_+}\sum_{j\sim y} f(y)\sin((j+1)k) \\ &= -2\sqrt{\pi}\mathcal{G}f(k) + f(0)\sin 2k \\ &\qquad + \sum_{j\geqslant 1}(f(j-1)+f(j+1))\sin((j+1)k) \\ &= -2\sqrt{\pi}\mathcal{G}f(k) + \sum_{z\in\mathbb{Z}_+} f(z)\sin((z+2)k) + \sum_{z\in\mathbb{Z}_+} f(z)\sin(zk) \\ &= -2\sqrt{\pi}\mathcal{G}f(k) + \sum_{z\in\mathbb{Z}_+} f(z)(\sin((z+2)k) + \sin(zk)).\end{aligned}$$

Since

$$\begin{aligned}\sin((z+2)k) &= \sin((z+1)k+k)\\ &= \sin((z+1)k)\cos(k)+\cos((z+1)k)\sin(k), \text{ and}\\ \sin(zk) &= \sin((z+1)k-k)\\ &= \sin((z+1)k)\cos(k)-\cos((z+1)k)\sin(k),\end{aligned}$$

we gain

$$\begin{aligned}-2\sqrt{\pi}(\mathcal{G}\Delta_+ f)(k) &= -2\sqrt{\pi}\mathcal{G}f(k)+\sum_{z\in\mathbb{Z}_+} f(z)(\sin((z+2)k)+\sin(zk))\\ &= -2\sqrt{\pi}\mathcal{G}f(k)+2\sqrt{\pi}(\mathcal{G}f)(k)\cos(k)\\ &= -2\sqrt{\pi}(\mathcal{G}f)(k)(\cos(k)-1).\end{aligned}$$

We read by Proposition 2.17 and Lemma 2.23 the spectrum of Δ_+. A similar calculation for Δ_- proves the claim. □

Next we deal with the conjugate operators $A_\pm$, so from (5.3) we derive:

Definition 5.6 On the space of aborting sequences $\ell^2_c(\mathbb{Z}_\pm)$ we fix

$$\begin{aligned}A_\pm|_{\ell^2_c(\mathbb{Z}_\pm)} &:= -\frac{i}{2}\left[\frac{1}{2}(U^*_\pm+U_\pm)+Q_\pm(U^*_\pm-U_\pm)\right]\\ &= \frac{i}{2}\left[U_\pm\left(Q_\pm+\frac{1}{2}_\pm\right)-\left(Q_\pm+\frac{1}{2}_\pm\right)\right].\end{aligned}$$

The last equation can be taken from the next lemma. For $A_\pm$ we take the closure of these operators, which exist, as the operators are symmetric and the domains of $(A_\pm)^*$ contain the dense subspace $\ell^2_c(\mathbb{Z}_\pm)$. Again, beware that $A_\mathbb{Z} \neq A_- \oplus A_+$.

To retrieve Mourre Estimates for $(\Delta_\pm, A_\pm)$, we need that $A_\pm$ are selfadjoint. To show that we need to commute $U_\pm$,$U^*_\pm$ with $Q_\pm$. The following lemma will clear the path.

Lemma 5.7 On the space of aborting sequences $\ell^2_c(\mathbb{Z}_\pm)$, the following relations hold

$$\begin{aligned} Q_\pm U_\pm &= U_\pm(Q_\pm + 1_\pm), \qquad Q_\pm U^*_\pm = U^*_\pm(Q_\pm - 1_\pm), \\ U^*_\pm Q_\pm U_\pm &= U^*_\pm U_\pm(Q_\pm + 1_\pm), \\ U_\pm Q_\pm U^*_\pm &= U_\pm U^*_\pm(Q - 1_\pm), \\ U^*_\pm Q_\pm U^*_\pm &= U^{*2}_\pm(Q_\pm - 1_\pm), \\ U_\pm Q_\pm U_\pm &= U^2_\pm(Q_\pm + 1_\pm). \end{aligned}$$

Proof: Let $f \in \ell^2_c(\mathbb{Z}_+)$. For $k \in \mathbb{Z}_+\backslash\{0\}$ we have

$$\begin{aligned} (Q_+U_+f)(k) &= kf(k-1) = (k-1)f(k-1) + f(k-1) \\ &= (U_+(Q_+ + 1)f)(k), \end{aligned}$$

and for $k = 0$, we have on both sides 0, so we got the first relation. The second one is similar. All subsequent relations are consequences of the prior and we conclude similarly for $\mathbb{Z}_-$. □

From here we can read without effort:

Corollary 5.8 The operators $U_\pm$ and $U^*_\pm$ are elements of $\mathcal{C}^2(Q_\pm)$.

But actually we are interested in properties of the operators $A_\pm$, which we will earn easier, now.

Proposition 5.9 The operators $A_\pm$ are essentially selfadjoint on $\ell^2_c(\mathbb{Z}_\pm)$.

Proof: Define $B_- := -Q_-$ and $B_+ := Q_+ + 1_+$. At first we show that $\ell^2_c(\mathbb{Z}_\pm)$ is a core for $B_\pm$, i.e. $\ell^2_c(\mathbb{Z}_\pm)$ is dense in $D(B_\pm)$ under the graph norm $\|\cdot\|+\|B_\pm\cdot\|$. Take $f \in D(B_\pm)$ and for $n \in \mathbb{N}$ define $f_n := \chi_{I_\pm}(Q_\pm)f \in \ell^2_c(\mathbb{Z}_\pm)$, where the intervals $I_+ := [0, n]$ and $I_- := [-n, -1]$. Clearly $\|f - f_n\| \to_{n\to\infty} 0$ and

$$B_\pm(f - f_n) = \chi_{\mathbb{Z}_\pm\backslash I_\pm}(Q_\pm)B_\pm f.$$

Thus the above converges strongly to 0, implying that $\|B_\pm(f - f_n)\|$ goes to 0, so all relevant terms turn to 0.

For the main part, we want to use [RS] Volume II, Theorem X.36' c) to show that $A_\pm$ are essentially selfadjoint on any core of $D(B_\pm)$. First, by Lemma 5.7 we see that $A_\pm$ are symmetric and therefore $(f, g) \mapsto \langle f, A_\pm g\rangle$ are quadratic forms on $D(B_\pm)$ and we are left to support that

i) $|\langle f, A_\pm g\rangle| \leqslant c_1\left\|B_\pm^{1/2}f\right\| \cdot \left\|B_\pm^{1/2}g\right\|$ for all $f, g \in D(B_\pm^{1/2})$, and

ii) $|\langle B_\pm f, A_\pm g\rangle - \langle f, A_\pm B_\pm g\rangle| \leqslant c_2\left\|B_\pm^{1/2}f\right\|\cdot\left\|B_\pm^{1/2}g\right\|$ for all $f, g \in D(B_\pm^{3/2})$.

i) By the definition of $B_\pm$ we also see for $f \in \ell^2_c(\mathbb{Z}_\pm)$ that

$$\left\|Q_\pm^{1/2}f\right\| \leqslant \left\|B_\pm^{1/2}f\right\|.$$

Also, since $(B_\pm^{1/2}U_\pm f)(k) = \pm(k+1)^{1/2}f(k-1)$ for $k \in \mathbb{Z}_\pm\backslash\{0\}$ and by a similar equation for $U_\pm^*$, we obtain $c_{(1)} > 0$ such that

$$\begin{aligned}\left\|B^{1/2}U_\pm f\right\| &\leqslant c_{(1)}\left\|B^{1/2}f\right\| \text{ and}\\ \left\|B^{1/2}U_\pm^* f\right\| &\leqslant c_{(1)}\left\|B^{1/2}f\right\|.\end{aligned}$$

Taking these inequalities we estimate for $f, g \in \ell^2_c(\mathbb{Z}_\pm)$

$$\begin{aligned}2|\langle f, A_\pm g\rangle| &= \left|\left\langle f, \left[\frac{1}{2}(U_\pm + U_\pm^*) + Q_\pm(U_\pm^* - U_\pm)\right] g\right\rangle\right|\\ &\leqslant \|f\|\cdot\|g\| + \left\|Q_\pm^{1/2}f\right\|\cdot\left\|Q_\pm^{1/2}(U_\pm^* - U_\pm)g\right\|\\ &\leqslant c_1\left\|B_\pm^{1/2}f\right\|\cdot\left\|B_\pm^{1/2}g\right\|,\end{aligned}$$

where $c_1 := 1 + 2c_{(1)}$.

ii) At first we point out $U_\pm, U_\pm^* \in \mathcal{C}^1(B_\pm)$ due to Corollary 5.8. Hence there is a constant $c_{(2)} > 0$ complying

$$\left|\left\langle f, [U_\pm^* + U_\pm, B_\pm]_\circ g\right\rangle\right| \leqslant c_{(2)}\|f\|\cdot\|g\| \leqslant c_{(2)}\left\|B_\pm^{1/2}f\right\|\cdot\left\|B_\pm^{1/2}g\right\|,$$

which is already half of the inequality we seek. Furthermore, since $Q_\pm$ and $B_\pm$ commute, we have $c_{(3)}$ such that

$$\begin{aligned}|\langle f, [Q_\pm U_\pm, B_\pm]g\rangle| \leqslant |\langle f, Q_\pm[U_\pm, B_\pm]g\rangle| &= \left|\left\langle Q_\pm^{1/2}f, Q_\pm^{1/2}[U_\pm, \pm Q_\pm]g\right\rangle\right|\\ &\leqslant \left\|B^{1/2}f\right\|\cdot\left\|Q_\pm^{1/2}Ug\right\| \leqslant c_{(3)}\left\|B_\pm^{1/2}f\right\|\cdot\left\|B_\pm^{1/2}g\right\|.\end{aligned}$$

The same for $U_\pm^*$ instead of $U_\pm$, and hence provided the full estimate. □

5.3 Mourre estimate for the free operator on $\ell^2(\mathbb{Z}_\pm)$

The construction of A with Proposition 5.1 nurtures our expectation on an easy form of $[\Delta, iA]_\circ$, which is preferable, as finding a corresponding Mourre Estimate in Proposition 5.11 becomes easy. Still we do not want to leave the $(\Delta_\pm, A_\pm)$ path, since anisotropy will be linked directly to $\Delta_\pm$ not before Corollary 5.12. A good starting point is to find out, what $[\Delta_\pm, A_\pm]_\circ$ effectively are:

Proposition 5.10 Remember Definition 5.2. $\Delta_\pm$ is of class $\mathcal{C}^2(A_\pm)$ and

$$[\Delta_\pm, iA_\pm]_\circ = \Delta_\pm(2 - \Delta_\pm).$$

Proof: By Corollary 5.8 $U_\pm$, the operators $U_\pm^*$ are of class $\mathcal{C}^2(A_\pm)$, so the perturbed Laplacians $\Delta_\pm = 1_\pm + \frac{1}{2}(U_\pm + U_\pm^*)$ are, by Proposition 4.7, of class $\mathcal{C}^2(A_\pm)$. In this proof we denote $\langle B, C\rangle_f := \langle Bf, Cf\rangle$. So for $f \in \ell^2_c(\mathbb{Z}_+)$, where $\ell^2_c(\mathbb{Z}_+)$ is a core for A_+ by Proposition 5.9, calculate

$$\begin{aligned}\langle f, [\Delta_+, A_+]f\rangle &= \frac{1}{2}\left(\langle A_+, U_+ + U_+^*\rangle_f - \langle U_+ + U_+^*, A_+\rangle_f\right)\\ &= \frac{1}{2}\left(\langle (U_+ + U_+^*)A_+, 1\rangle_f - \langle 1, (U_+ + U_+^*)A_+\rangle_f\right).\end{aligned} \tag{5.5}$$

With Lemma 5.7 we dig out

$$A_+ = -\frac{i}{2}\left[(U_+^* - U_+)Q_+ - \frac{1}{2}(U_+^* + U_+)\right],$$

which helps us to gain the equations on $\ell^2_c(\mathbb{Z}_+)$

$$\begin{aligned}U_+A_+ &= -\frac{i}{2}\left[(\chi_\mathbb{N} - U_+^2)Q_+ - \frac{1}{2}(\chi_\mathbb{N} + U_+^2)\right]\\ U_+^*A_+ &= -\frac{i}{2}\left[(U_+^{2*} - 1)Q_+ - \frac{1}{2}(U_+^{2*} + 1)\right]\end{aligned}$$

and thence

$$\begin{aligned}(U_+^* + U_+)A_+ &= -\frac{i}{2}\left[(U_+^{2*} - U_+^2)Q_+ - 1 - \frac{1}{2}(\chi_{\{0\}} + U_+^2 + U_+^{2*})\right],\\ [(U_+^* + U_+)A_+]^* &= \frac{i}{2}\left[Q_+(U_+^2 - U_+^{2*}) - 1 - \frac{1}{2}(\chi_{\{0\}} + U_+^2 + U_+^{2*})\right]\\ &= \frac{i}{2}\left[(U_+^2 - U_+^{2*})Q_+ + \frac{3}{2}(U_+^2 + U_+^{2*}) - 1 - \frac{1}{2}\chi_{\{0\}}\right].\end{aligned}$$

We plug that knowledge back into (5.5), so

$$\begin{aligned}\langle f, [\Delta_+, A_+]f\rangle &= \left\langle 1, \frac{i}{4}(-2 - \chi_{\{0\}} + (U_+^2 + U_+^{2*}))\right\rangle_f \\ &= \langle 1, -i\Delta_+(2-\Delta_+)\rangle_f ,\end{aligned}$$

which is what we wanted to check. $[\Delta_-, A_-]_\circ$ works similarly.

Since $[\Delta_\pm, A_\pm]_\circ$ are polynomials in $\Delta_\pm$ we learn from Lemma 4.8 that $[\Delta_\pm, A_\pm]_\circ \in \mathcal{C}^1(A_\pm)$, i.e. $\Delta_\pm \in \mathcal{C}^2(A_\pm)$. □

It is a very remarkable feature of Proposition 5.10 that $[\Delta_\pm, A_\pm]_\circ$ are functions in $\Delta_\pm$, which allows, through functional calculus, the extraction of the sought Mourre Estimate.

Proposition 5.11 Let $I = (a, b) \subset\subset (0, 2)$ be an interval. Then

$$E_I(\Delta_\pm)[\Delta_\pm, iA_\pm]_\circ E_I(\Delta_\pm) \geqslant c(I)E_I(\Delta_\pm),$$

where $c(I)$ is strictly positive

$$c(I) := \min\left\{2a - a^2, 2b - b^2\right\}. \tag{5.6}$$

Proof: We define a function $f : \mathbb{R} \to \mathbb{R}$ with $f : x \mapsto x(2-x)$ such that $[\Delta_\pm, iA_\pm] = f(\Delta_\pm)$. Functional calculus then works as the tool

$$\begin{aligned}E_I(\Delta_\pm)[\Delta_\pm, iA]_\circ E_I(\Delta_\pm) &= \Delta_\pm(2-\Delta_\pm)E_I(\Delta_\pm) = f(\Delta_\pm)E_I(\Delta_\pm) \\ &\geqslant \inf\left(f(I)\right)\, E_I(\Delta_\pm).\end{aligned}$$

As f describes a parabola and as I is an interval we get $\inf(f(I)) = c(I)$ and hence have proved the proposition. □

This makes it easy to introduce anisotropy:

Corollary 5.12 Take $l_\pm \in \mathbb{R}$ and fix $H_\pm := \Delta_\pm + l_\pm$ on $\ell^2(\mathbb{Z}_\pm)$. For every interval $J \subset\subset (0, 2) + \{l_\pm\}$, we find $c(J) > 0$ such that

$$E_J(H_\pm)[H_\pm, iA_\pm]_\circ E_J(H_\pm) \geqslant c(J)E_J(H_\pm).$$

The constant $c(J)$ can be taken from Proposition 5.11, with the interval shifted by $l_\pm$.

Proof: Similar to Proposition 5.11. □

5.4 Mourre estimate for the free operator on $\ell^2(\mathbb{Z})$

Corollary 5.12 introduced the aimed anisotropy, Proposition 5.14 then glues Mourre Estimates on the separated spaces $\ell^2(\mathbb{Z}_\pm)$, followed, in the next section, by the restoration of the Laplacian from the perturbed Laplacians.

Now we glue spaces:

Definition 5.13 Let $l_\pm \in \mathbb{R}$ and fix $H_\pm := \Delta_\pm + l_\pm$ on $\ell^2(\mathbb{Z}_\pm)$. On the whole space $\ell^2(\mathbb{Z}_-) \oplus \ell^2(\mathbb{Z}_-)$ define

$$\begin{aligned} L_{jt} &:= l_- \oplus l_+ =: \left(\begin{array}{c|c} l_- & 0 \\ \hline 0 & l_+ \end{array}\right), \\ \Delta_{jt} &:= \Delta_- \oplus \Delta_+ =: \left(\begin{array}{c|c} \Delta_- & 0 \\ \hline 0 & \Delta_+ \end{array}\right), \\ H_{jt} &:= \Delta_{jt} + L_{jt}, \\ H &:= \Delta + L_{jt}, \\ A := A_{jt} &:= A_- \oplus A_+ =: \left(\begin{array}{c|c} A_- & 0 \\ \hline 0 & A_+ \end{array}\right). \end{aligned}$$

The rightmost notation of the first two and the last operators aids readability in the following proofs, while the meaning is clear through the definition on $\ell^2(\mathbb{Z}_-) \oplus \ell^2(\mathbb{Z}_+)$. The operator L_{jt} forms a *Barrier potential*, introducing the sought anisotropy. In the end, we want to retrieve Mourre Estimates for H, although in this section we keep sticking to H_{jt}.

The transition form $H_\pm$ to H_{jt} creates a set D_1 of *thresholds*, i.e. the points were the constant $c(J)$ in the Mourre Estimate turns to 0. Near these points the constant of the Limiting Absorption Principle will blow up, so we must avoid them. The thresholds consist of no more than four points, thence we do not risk to overlook singularly continuous spectrum. So fix the sets

$$\begin{aligned} D_1 &:= \{l_-, l_- + 2, l_+, l_+ + 2\} \\ F_1 &:= ([l_+, l_+ + 2] \cup [l_-, l_- + 2]) \setminus D_1. \end{aligned}$$

By Proposition 5.5 and Corollary 5.12, the set F_1 is the union of the essential spectra of $\Delta_\pm + l_\pm$ excluding the thresholds.

We can mine the Mourre Estimates for $H_\pm$ to find one for H_{jt}, i.e. we glue $\ell^2(\mathbb{Z}_-) \oplus \ell^2(\mathbb{Z}_+)$ and thus reclaim our grip on $\mathcal{H}$:

Proposition 5.14 For every interval $J \subset\subset F_1$, there is $c(J) > 0$ such that

$$E_J(H_{jt})[H_{jt}, iA]_\circ E_J(H_{jt}) \geqslant c(J)E_J(H_{jt}).$$

Writing the bounds $a < b$ of J and fixing $a_\pm := a - l_\pm$ and $b_\pm := b - l_\pm$ returns $c(J)$ explicitly by

$$c(J) = \min\{c_-(J), c_+(J)\}, \text{ where}$$
$$c_\pm(J) := \begin{cases} \min\left\{2a_\pm - a_\pm^2, 2b_\pm - b_\pm^2\right\} & 0 < a_\pm < b_\pm < 2, \\ \infty & \text{otherwise.} \end{cases}$$

Proof: It is obvious that

$$E_J(H_{jt}) = \left(\begin{array}{c|c} E_J(H_-) & 0 \\ \hline 0 & E_J(H_+) \end{array}\right)$$

so

$$\begin{aligned} &E_J(H_{jt})[H_{jt}, iA]_\circ E_J(H_{jt}) \\ &\quad = \left(\begin{array}{c|c} E_J(H_-)[H_-, A_-]_\circ E_J(H_-) & 0 \\ \hline 0 & E_J(H_+)[H_+, A_+]_\circ E_J(H_+). \end{array}\right) \end{aligned}$$

If J intersects both $(0, 2) + l_-$ and $(0, 2) + l_+$, then take c the minimum of $c_\pm$ taken from Corollary 5.12 and read

$$E_J(H_{jt})[H_{jt}, iA]_\circ E_J(H_{jt}) \geqslant c \left(\begin{array}{c|c} E_J(H_+) & 0 \\ \hline 0 & E_J(H_-) \end{array}\right) = cE_J(H_{jt}).$$

Otherwise let J intersect $(0, 2) + l_+$, only. Then

$$\begin{aligned} E_J(H_{jt})[H_{jt}, iA]_\circ E_J(H_{jt}) &= \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & E_J(H_+)[H_+, A_+]_\circ E_J(H_+) \end{array}\right) \\ &\geqslant c \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & E_J(H_+) \end{array}\right) = cE_J(H_{jt}), \end{aligned}$$

which similarly holds true for l_-. By the choice of J there are no other types of intersection. □

5.5 Mourre estimate for the Laplacian

In the last section we linked anisotropy to the Barrier potential L_{jt} and gained a strict Mourre Estimate for $H_{jt} = \Delta_{jt} + L_{jt}$. The next step is to recover the Laplacian Δ, although from Corollary 5.3, we know that we only have to deal with some finite rank perturbation. All the notation in this section is based on Definition 5.13.

Corollary 5.15 $H \in \mathcal{C}^2(A)$ and $[\Delta - \Delta_{jt}, iA]$ is compact.

Proof: Proposition 5.10 explored that $\Delta_{jt} \in C^2(A_{jt})$. l_- and l_+ as parts of L_{jt} are identities respectively on $\ell^2(\mathbb{Z}_-)$ and on $\ell^2(\mathbb{Z}_+)$, thus we gain that $A_{jt} = A_- \oplus A_+$ and L_{jt} commute, so $L_{jt} \in \mathcal{C}^2(A_{jt})$ and hence deduce that $H_{jt} = \Delta_{jt} + L_{jt} \in \mathcal{C}^2(A_{jt})$.

By Corollary 5.3,

$$K := \Delta - \Delta_{jt} = -\frac{1}{2}\left(\chi_{\{-1\}}U^* + \chi_{\{0\}}U\right)$$

is of finite rank. Thus K maps $\mathcal{H}$ into $\ell^2_c(\mathbb{Z})$, i.e. by Proposition 5.9 into $D(A_{jt})$, so $[K, iA_{jt}]_\circ$ exists and is bounded.

Consider $A_\pm$ from Definition 5.6. Commuting K with $(U_\pm^* + U_\pm)$ easily returns finite rank operators. Moreover on $\ell^2_c(\mathbb{Z})$ $\chi_{\{0\}}UQ_\pm = U\chi_{\{-1\}}Q_\pm$ and $\chi_{\{0\}}U^*Q_\pm = U^*\chi_{\{1\}}Q_\pm$ are of rank 0 or of rank 1, so the closures of $KA_\pm$ are of finite rank. Using Lemma 5.7 and applying the above trick on $A_\pm K$ reveals that $A_\pm K$ is also of finite rank, thus $[K, iA_{jt}]_\circ$ is a finite rank operator, thus $[K, iA_{jt}]_\circ$ maps into $D(A)$ and hence $[[K, iA_{jt}]_\circ, iA_{jt}]_\circ$ is bounded, that is $K \in C^2(A)$. Taking all that together, we gain with Proposition 4.7 from $H = H_{jt} + K$ that $\Delta + L_{jt} \in \mathcal{C}^2(A)$. □

Since we have a strict Mourre Estimate for (H_{jt}, A_{jt}), the compact perturbation $\Delta - \Delta_{jt}$ will, at first, remove the adjective strict in the Mourre Estimate for (H, A_{jt}):

Proposition 5.16 Remember Definition 5.13. Then for every interval $J \subset\subset I$, where $I \subset\subset F_1$ is an interval with bounds in F_1, there is $c > 0$ such that the estimate

$$E_J(H)[H, iA]_\circ E_J(H) \geqslant cE_J(H) + K \tag{5.7}$$

holds, whereas K is a compact operator.

Proof: Fix $K' := \Delta - \Delta_{jt}$. By Corollary 5.15, K' is of finite rank. Examine with Proposition 4.7

$$[H, iA]_\circ = [H_{jt}, iA]_\circ + [K', iA]_\circ.$$

We multiply this equation from left and right with $E_I(H_{jt})$ and use Proposition 5.14

$$E_I(H_{jt})[H, iA]_\circ E_I(H_{jt}) \geqslant cE_I(H_{jt}) + K^{(1)} \tag{5.8}$$

with $K^{(1)} = E_I(H_{jt})[K', iA]E_I(H_{jt})$ compact, as $E_I(H_{jt})$ is bounded. We want to reformulate equation (5.8) equivalently in terms of quadratic forms and play with its arguments, moving us more the less directly to the desired result, thence for $g \in \ell^2(\mathbb{Z})$

$$\langle g, E_I(H_{jt})[H, iA]_\circ E_I(H_{jt})g\rangle \geqslant c\,\langle g, E_I(H_{jt})g\rangle + \left\langle g, K^{(1)}g\right\rangle. \tag{5.9}$$

In several steps we get from I to J and from $E_J(H_{jt})$ to $E_J(H)$. To do so we pick up $\varphi \in C_c^\infty(\mathbb{R}, \mathbb{R})$ with $\varphi \leqslant 1$, $\operatorname{supp}(\varphi) \subset I$ and $\varphi|_J = 1$ and define $\Phi_{jt} := \varphi(H_{jt})$, $\Phi_H := \varphi(H)$ and $f := \Phi_{jt}g$. We exchange g with f in (5.9) and hence have

$$\begin{aligned}\langle g, \Phi_{jt}[H, iA]_\circ \Phi_{jt}g\rangle &= \langle f, E_I(H_{jt})[H, iA]_\circ E_I(H_{jt})f\rangle \\ &\geqslant c\,\langle f, E_I(H_{jt})f\rangle + \left\langle f, K^{(1)}f\right\rangle \\ &= c\,\langle \Phi_{jt}g, \Phi_{jt}g\rangle + \left\langle g, K^{(2)}g\right\rangle.\end{aligned} \tag{5.10}$$

Again $K^{(2)} = \Phi_{jt}K^{(1)}\Phi_{jt}$ is compact.

Corollary 2.13 tells us that $\Phi_{jt} - \Phi_H$ is compact, offering a path in (5.10) from Φ_{jt} to Φ_H. We consider the leftmost term

$$\begin{aligned}\langle g, \Phi_{jt}[H, iA]_\circ \Phi_{jt}g\rangle &= \langle g, (\Phi_{jt} - \Phi_H + \Phi_H)[H, iA]_\circ \Phi_{jt}g\rangle \\ &= \langle g, (\Phi_{jt} - \Phi_H)[H, iA]_\circ \Phi_{jt}g\rangle + \langle g, \Phi_H[H, iA]_\circ \Phi_{jt}g\rangle.\end{aligned}$$

We repeat this with the Φ_{jt} on the right and obtain

$$\langle g, \Phi_{jt}[H, iA]_\circ \Phi_{jt}g\rangle = \left\langle g, K^{(3)}g\right\rangle + \langle g, \Phi_H[H, iA]_\circ \Phi_H g\rangle \tag{5.11}$$

with some compact $K^{(3)}$. Moreover, subtracting (5.11) from (5.10) is equivalent to

$$\langle g, \Phi_H[H, iA]_\circ \Phi_H g\rangle \geqslant c\,\langle \Phi_{jt}g, \Phi_{jt}g\rangle + \left\langle g, K^{(4)}g\right\rangle \tag{5.12}$$

with a compact $K^{(4)}$. We apply that trick once more on the factor Φ_{jt} on the right side and (5.12) advances to

$$\langle g, \Phi_H[H, iA]_\circ \Phi_H g \rangle \geqslant c \langle \Phi_H g, \Phi_H g \rangle + \left\langle g, K^{(5)} g \right\rangle . \qquad (5.13)$$

Again, $K^{(5)}$ is compact.

To get the result, we repeat the very first step; we fix $\nu := E_J(H)g$ and use ν instead of g in (5.13) and use that $\varphi|_J = 1$, i.e.

$$\begin{aligned} \langle g, E_J(H)[H, iA]_\circ E_J(H)g \rangle &= \langle \nu, \Phi_H[H, iA]_\circ \Phi_H \nu \rangle \\ &\geqslant c \langle \Phi_H \nu, \Phi_H \nu \rangle + \left\langle \nu, K^{(5)} \nu \right\rangle \\ &= c \langle g, E_J(H) g \rangle + \left\langle g, K^{(6)} g \right\rangle . \end{aligned}$$

This is equation (5.7). □

5.6 Perturbation by potentials

Finally, we want to perturb the Mourre Estimate somewhat further, i.e. to add to $H = \Delta + L_{jt}$ a *short range potential* $V_s(Q)$ with $V_s \in O(1/n^2)$ and find that the Limiting Absorption Principle applies to $H_s := H + V_s$, thus gaining the absence of singularly continuous spectrum.

Lemma 5.17 Take $A_\pm$ from Definition 5.6 and its domain form Proposition 5.9. Then for mappings $V_\pm : \mathbb{Z}_\pm \to \mathbb{C}$

i) $V_\pm \in O(1/|n|)$ implies $V_\pm(Q_\pm) \in \mathcal{C}^1(A_\pm)$,

ii) $V_\pm \in o(1/|n|)$ makes $[V_\pm(Q), iA_\pm]_\circ$ compact,

iii) $V_\pm \in O(1/|n|^2)$ assures $V_\pm \in \mathcal{C}^2(A_\pm)$.

Proof: i,iii) Take $f \in \ell^2_c(\mathbb{Z}_\pm)$, where $\ell^2_c(\mathbb{Z}_\pm)$ is a core for $A_\pm$ by Proposition 5.9. Then

$$\begin{aligned} \langle f, [V_\pm(Q), A_\pm] f \rangle &= \left\langle V^*_\pm(Q) f, A_\pm f \right\rangle - \langle A_\pm f, V_\pm(Q) f \rangle \\ &= -\frac{i}{2} \left\langle f, \left[V_\pm(Q) \frac{1}{2}(U^*_\pm + U_\pm) + V_\pm(Q) Q_\pm (U^*_\pm - U_\pm) \right] f \right\rangle \\ &\quad + \frac{i}{2} \left\langle f, \left[\frac{1}{2}(U^*_\pm + U_\pm) V_\pm(Q) + Q_\pm (U^*_\pm - U_\pm) V_\pm(Q) \right] f \right\rangle . \end{aligned} \qquad (5.14)$$

As $V_\pm(x) \to 0$ for $x \to \pm\infty$, we find c_∞ such that both

$$\left|\left\langle f, V_\pm(Q)\frac{1}{2}(U_\pm^* + U_\pm)f\right\rangle\right| \leqslant c_\infty \|f\|^2 \text{ and}$$
$$\left|\left\langle f, \frac{1}{2}(U_\pm^* + U_\pm)V_\pm(Q)f\right\rangle\right| \leqslant c_\infty \|f\|^2.$$

As $V_\pm \in O(1/|n|)$ we have that mappings $x \mapsto t_1(x)V_\pm(x)$, where t_1 is a translation $x \mapsto x + b$, keep bounded for large x and can therefore bound $V_\pm(Q)Q(U_\pm^* - U_\pm)$ and $Q(U_\pm^* - U_\pm)V_\pm(Q)$, so we just justified i). Considering $V_\pm \in O(1/|n|^2)$ and expanding

$$\langle [V_\pm(Q), A_\pm]^* f, A_\pm f\rangle - \langle A_\pm f, [V_\pm(Q), A_\pm] f\rangle$$

leads to terms like the ones above. Then again mappings $x \mapsto t_2(x)V(x)$, where t_2 is of the form $(x+b)^2 + c$, keep bounded with large x and we can thus bound all terms.

ii) From equation (5.14) consider the last line and the last addend

$$Q_\pm(U_\pm^* - U_\pm)V_\pm(Q) = \left([Q, U_\pm^*] + U_\pm^* Q - [Q, U_\pm] - U_\pm Q\right) V.$$

Using Corollary 5.8, i.e. $[Q, U_\pm]_\circ$ and $[Q, U_\pm^*]_\circ$ are bounded, we see that the whole question can be reduced to the question whether $V_\pm Q_\pm = Q_\pm V_\pm$ is compact. We know that if there is a sequence $(T_n)_{n\in\mathbb{N}}$ of continuous, finite rank operators, with $\|T_n - V_\pm Q_\pm\| \to_{n\to\infty} 0$, then $V_\pm Q_\pm$ is compact (see [Wer] Korollar II.3.3). We define the functions

$$T_n(x) := \begin{cases} V_\pm(x)x & |x| \leqslant n \\ 0 & |x| > n \end{cases} \qquad \text{for } x \in \mathbb{Z}_\pm.$$

Then

$$(V_\pm Q_\pm - T_n)(x) = \begin{cases} 0 & |x| \leqslant n \\ V_\pm(x)x & |x| > n \end{cases} \qquad \text{for } x \in \mathbb{Z}_\pm$$

and, as $V_\pm \in o(1/|x|)$, we know $(V_\pm Q_\pm - T_n)(x) \to_{|x|\to\infty} 0$ and therefore $\|V_\pm Q_\pm - T_n\|$ turns with growing n to 0. □

For all these Potentials V, we have $[V(Q), iA]_\circ$ compact, allowing us to obtain a Mourre Estimate for $(\Delta + L_{jt} + V(Q), A)$, using the Mourre Estimate for $(\Delta + L_{jt}, A)$.

Proposition 5.18 Remember Definition 5.13. Let $V_\pm$ be mappings on $\mathbb{Z}_\pm$ with $V_\pm \in o(1/|x|)$. Fix

$$V := \left(\begin{array}{c|c} V_-(Q) & 0 \\ \hline 0 & V_+(Q) \end{array}\right).$$

Then for every interval $J \subset I$, where $I \subset\subset F_1$ is an interval with bounds in F_1, there is $c > 0$ such that the estimate

$$E_J(H+V)[H+V, iA]_\circ E_J(H+V) \geqslant cE_J(H+V) + K \tag{5.15}$$

holds, whereas K is a compact operator.

Proof: In the proof of Proposition 5.7 replace the definition of K' with $K' := V$ and apply Lemma 5.17 where needed. □

To apply Theorem 4.15, we also need a strict Mourre estimate; from the Mourre Theory we know that removing eigenvalues frees a direct path:

Corollary 5.19 Take up the settings of Proposition 5.18 and assume an open interval $J_0 \subset F_1$ such that $H + V$ has no eigenvalue in J_0 and take $x \in J_0$. Then there is an open interval $J \subset J_0$ with $x \in J$ and some constant $c > 0$ obeying a strict Mourre Estimate

$$E_J(H+V)[H+V, iA]_\circ E_J(H+V) \geqslant cE_J(H+V). \tag{5.16}$$

Proof: Apply Proposition 4.14 on 5.18. □

This corollary introduced some new thresholds that we need to remove.

Definition 5.20 Take D_2 the set of eigenvalues of $H + V$. Fix

$$F_2 := F_1 \backslash D_2.$$

F_1 can be found in Definition 5.13. Beware, V changes roles in the following.

Theorem 5.21 Look up Definition 5.13. Take $H_s := H + V_s$, whereas $V_s \in O(1/n^2)$. Then for every interval $J \subset\subset F_2$, where F_2 belongs to H_s, we find a constant $C > 0$ such that for all $\alpha > 1/2$ and for all $z \in \mathbb{C}$ with $\mathrm{Re}(z) \in J$ and $\mathrm{Im}(z) > 0$ we have

$$\left\| \langle A \rangle^{-\alpha} (H_s - z)^{-1} \langle A \rangle^{-\alpha} \right\| \leqslant C,$$

so the spectrum of H_s in J and thus in F_2 is purely absolutely continuous.

Proof: First we assume that J is an interval as found in Corollary 5.19, i.e. we find $c > 0$ such that

$$E_J(H_s)[H_s, iA]_\circ E_J(H_s) \geqslant cE_J(H_s).$$

With Lemma 5.17 find $V_s \in \mathcal{C}^2(A)$. As by Corollary 5.15, $H \in \mathcal{C}^2(A)$ we get, using Proposition 4.7, that $H_s \in \mathcal{C}^2(A)$. This allows us to apply Theorem 4.15 with the above Mourre Estimate, i.e. there is a constant C' such that for $\text{Re}(z) \in J$ and $\text{Im}(z) > 0$ we have

$$\left\| \langle A \rangle^{-\alpha} (H_s - z)^{-1} \langle A \rangle^{-\alpha} \right\| \leqslant C',$$

which is the claim.

For intervals J not suited to Corollary 5.19, we find by the choice of J that $\bar{J} \subset F_2$. Then for every $j \in \bar{J}$ we find an open interval J_j and c_j following

$$E_{J_j}(H_s)[H_s, iA]_\circ E_{J_j}(H_s) \geqslant c_j E_{J_j}(H_s)$$

and with the above for $\text{Re}(z) \in J_j$ and $\text{Im}(z) > 0$

$$\left\| \langle A \rangle^{-\alpha} (H_s - z)^{-1} \langle A \rangle^{-\alpha} \right\| \leqslant C_{J_j}.$$

As $\bar{J}$ is compact, we find a finite set $N \subset \bar{J}$ such that

$$\cup_{j \in N} J_j \supset \bar{J},$$

so take $C := \max\left\{ C_{J_j} \mid j \in N \right\}$, then

$$\left\| \langle A \rangle^{-\alpha} (H_s - z)^{-1} \langle A \rangle^{-\alpha} \right\| \leqslant C,$$

which is what we wanted to show. □

6 Perturbation of the L.A.P.

For $H_s := \Delta + L_{jt} + V_s$ with the short range $V_s \in O(1/n^2)$ we managed to deduce the absence of singularly continuous spectrum. This chapter wants to dig out more information by adding another potential V, so

$$H := H_s + V, \text{ where } V \in o(1/|n|^{1+\varepsilon}).$$

Notice that this H is different from the H of Definition 5.13. For that we will need to compare V to $\langle A \rangle$, which we solve by first comparing $\langle A \rangle$ to

$\langle Q \rangle$, thus allowing us to compare V to $\langle Q \rangle$. This is prepared through the following two lemmas, subsequented by Proposition 6.4, rewriting the estimate of Theorem 5.21 on the resolvent of H_s in the weights $\langle Q \rangle$ instead of $\langle A \rangle$. This is applied in Theorem 6.5 and, using some continuity arguments, further mined into Proposition 6.7. Throughout this chapter, remember the thresholds from Definition 5.20 and take A from Definition 5.13.

Lemma 6.1 For all $x \in \mathbb{R}$ we have $(x \pm 2)^2 \leqslant 5(1 + x^2)$.

Proof: Examine the graphs of $f_\pm : \mathbb{R} \to \mathbb{R}$, $x \mapsto (x \pm 2)^2 - 5(1 + x^2)$. □

Recall that A is given by Defition 5.13.

Lemma 6.2 For all $\alpha \in [0, 1]$ and all $f \in D(\langle A \rangle^\alpha)$ we have

$$\|\langle A \rangle^\alpha f\| \leqslant C\|\langle Q \rangle^\alpha f\|.$$

Proof: From Proposition 5.9 we know that $D(\langle A \rangle^\alpha) \subset D(\langle Q \rangle^\alpha)$. At first, let $\alpha = 1$. Since $Q = Q_- \oplus Q_+$ and since $A = A_- \oplus A_+$, following Definitions 5.2 and 5.6, we can restrict the proof to the spaces $\ell^2(\mathbb{Z}_\pm)$, so we consider the $\mathbb{Z}_+$ side; the $\mathbb{Z}_-$ side is similar. By Proposition 5.9 we know $\ell^2_c(\mathbb{Z})$ is a core for A_+. Take $f \in \ell^2_c(\mathbb{Z})$, then

$$\|\langle A_+ \rangle f\|^2 = \left\langle f, \langle A_+ \rangle^2 f \right\rangle = \left\langle f, (A_+^2 + 1)f \right\rangle. \tag{6.1}$$

Consider

$$A_+ = \frac{i}{2}\left[U_+(Q_+ + \frac{1}{2}_+) - (Q_+ + \frac{1}{2}_+)U_+^*\right]. \tag{6.2}$$

We have $\|A_+ f\| \leqslant \left\|(Q_+ + \frac{1}{2}_+)f\right\|$ so that

$$\|A_+^2 f\| \leqslant \left\|(Q_+ + \frac{1}{2}_+)^2 f\right\|.$$

This results in

$$\|(A_+^2 + 1_+)f\| \leqslant \left\|\left(Q_+^2 + Q_+ + \frac{5}{4}_+\right) f\right\| \leqslant \frac{3}{2}\|(Q_+^2 + 1)f\|.$$

Now drop the restriction $\alpha = 1$: Since $\langle A \rangle$ is selfadjoint and positive, it is unitarily equivalent to a positive multiplication operator and we can thus use Theorem 9.1 to obtain the result for all $\alpha \in [0, 1]$. □

We are therefore able to compare $\langle A \rangle$ to $\langle Q \rangle$. We now recall and define some sets and operators we will need throughout the rest of this chapter:

Definition 6.3 Recall A and L_{jt} from Definition 5.13. Let $V, V_s : \mathbb{Z} \to \mathbb{R}$ be potentials, obeying $V_s \in o(1/n^2)$ and $V \in o(1/|n|^{1+\varepsilon})$ for some $\varepsilon \in (0,1)$. Set the operators $H_s := \Delta + L_{jt} + V_s(Q)$ and $H_\kappa := H_s + \kappa V(Q)$ for $\kappa \in \mathbb{R}$. Fix an interval $J \subset\subset F_2$, where F_2 corresponds to H_s and can be found in Definition 5.20.

Proposition 6.4 For every $\alpha > 1/2$ there is a constant C such that for all z with $\mathrm{Re}(z) \in J$ and $\mathrm{Im}(z) > 0$ we have

$$\left\| \langle Q \rangle^{-\alpha} (H_s - z)^{-1} \langle Q \rangle^{-\alpha} \right\| \leqslant C.$$

Proof: Because of Theorem 5.21 we find $C' > 0$ such that for all $f \in \mathcal{H}$ and uniformly in z we have

$$\left| \left\langle \langle A \rangle^{-\alpha} f, (H_s - z)^{-1} \langle A \rangle^{-\alpha} f \right\rangle \right| \leqslant C' \|f\|^2.$$

This returns for $g \in D(\langle A \rangle^\alpha)$ and by Lemma 6.2 a constant C complying

$$\left| \left\langle g, (H_s - z)^{-1} g \right\rangle \right| \leqslant C' \|\langle A \rangle^\alpha g\|^2 \leqslant C \|\langle Q \rangle^\alpha g\|^2,$$

so for all $h \in \mathcal{H}$

$$\left| \left\langle h, \langle Q \rangle^{-\alpha} (H_s - z)^{-1} \langle Q \rangle^{-\alpha} h \right\rangle \right| \leqslant C \|h\|^2,$$

resembling the claim. □

Now, we can put everything together to perturb the above estimate on the resolvent with another potential.

Theorem 6.5 Recall Definiton 6.3. Assume that $|\kappa| \leqslant q(J)$, where the constant $q(J) > 0$ is sufficiently small. Then for $\alpha \in (1/2, (1+\varepsilon)/2)$

$$\sup_{\mathrm{Re}(z) \in J, \mathrm{Im}(z) > 0} \left\| \langle Q \rangle^{-\alpha} (H_\kappa - z)^{-1} \langle Q \rangle^{-\alpha} \right\| < \infty.$$

Hence H_κ has purely absolutely continuous spectrum in J.

Proof: We want to estimate

$$\left\| \langle Q \rangle^{-\alpha} (H_\kappa - z)^{-1} \langle Q \rangle^{-\alpha} \right\|$$

uniformly in z and draw the absence of singularly continuous spectrum from Proposition 4.1. Observe for $z \in \mathbb{C}$ with $\mathrm{Im}(z) > 0$ and $\mathrm{Re}(z) \in J$

$$\begin{aligned} H_s - z &= (H_\kappa - z) - \kappa V, \text{ thus} \\ 1 &= (H_\kappa - z)(1 - (H_\kappa - z)^{-1} \kappa V)(H_s - z)^{-1} \end{aligned}$$

and

$$\begin{aligned}(H_\kappa - z)^{-1} &= (1 - (H_\kappa - z)^{-1}\kappa V)(H_s - z)^{-1} \\ &= (H_s - z)^{-1} - (H_\kappa - z)^{-1}\kappa V(H_s - z)^{-1}.\end{aligned}$$

Hence

$$(H_\kappa - z)^{-1}(1 + \kappa V(H_s - z)^{-1}) = (H_s - z)^{-1}.$$

Take $\alpha \in (1/2, (1+\varepsilon)/2)$ and multiply with $\langle Q\rangle^{-\alpha}$, then

$$\begin{aligned}&\langle Q\rangle^{-\alpha}(H_\kappa - z)^{-1}\langle Q\rangle^{-\alpha}\langle Q\rangle^{\alpha}(1 + \kappa V(H_s - z)^{-1})\langle Q\rangle^{-\alpha} \\ &\quad = \langle Q\rangle^{-\alpha}(H_s - z)^{-1}\langle Q\rangle^{-\alpha}.\end{aligned} \tag{6.3}$$

That looks familiar to the equations of Proposition 6.4. If the operator $\langle Q\rangle^{\alpha}(1 + \kappa V(H_s - z)^{-1})\langle Q\rangle^{-\alpha}$ is invertible, we will be able to bound $\langle Q\rangle^{-\alpha}(H_\kappa - z)^{-1}\langle Q\rangle^{-\alpha}$ uniformly in z. Remember that $V \in o(1/|n|^{1+\varepsilon})$, so by the above choice of α we know that $\langle Q\rangle^{\alpha}\kappa V\langle Q\rangle^{\alpha}$ is compact — so we get invertibility by the Fredholm Alternative (see e.g. [RS] Volume I, Theorem VI.14 and following corollary) and thus have to deal with injectivity, i.e. find f such that

$$\begin{aligned}(1 + \langle Q\rangle^{\alpha}\kappa V(H_s - z)^{-1})\langle Q\rangle^{-\alpha} f = 0, \text{ so} \\ \langle Q\rangle^{\alpha}\kappa V(H_s - z)^{-1}\langle Q\rangle^{-\alpha} f = -f.\end{aligned}$$

Define $g := (H_s - z)^{-1}\langle Q\rangle^{-\alpha} f$, then

$$\begin{aligned}\langle Q\rangle^{\alpha}\kappa V g = -\langle Q\rangle^{\alpha}(H_s - z)g, \text{ which is} \\ \langle Q\rangle^{\alpha}(H_s + \kappa V - z)g = 0.\end{aligned}$$

$\langle Q\rangle^{\alpha}$ is invertible and, since $H_s + \kappa V$ is selfadjoint, also $H_s + \kappa V - z$ is invertible as $\operatorname{Im}(z) \neq 0$. Therefore $g = 0$, implying $f = 0$, i.e. we have injectivity and hence the awaited invertibility; thus move from (6.3) to

$$\begin{aligned}&\langle Q\rangle^{-\alpha}(H_\kappa - z)^{-1}\langle Q\rangle^{-\alpha} \\ &\quad = \langle Q\rangle^{-\alpha}(H_s - z)^{-1}\langle Q\rangle^{-\alpha}\langle Q\rangle^{\alpha}(1 + \kappa V(H_s - z)^{-1})^{-1}\langle Q\rangle^{-\alpha}.\end{aligned} \tag{6.4}$$

Since we want to estimate the left side, we deal with $\langle Q\rangle^{-\alpha}(H_s - z)^{-1}\langle Q\rangle^{-\alpha}$ through Proposition 6.4 uniformly in z; call the obtained bound c, and we are obliged to cope with the remains

$$\begin{aligned}&\langle Q\rangle^{\alpha}(1 + \kappa V(H_s - z)^{-1})\langle Q\rangle^{-\alpha} \\ &\quad = 1 + \langle Q\rangle^{\alpha}\kappa V\langle Q\rangle^{\alpha}\langle Q\rangle^{-\alpha}(H_s - z)^{-1}\langle Q\rangle^{-\alpha} =: 1 + M.\end{aligned}$$

Clearly, $\|M\| < 1$ suffices. We know $\left\|\langle Q\rangle^{-\alpha}(H_s - z)^{-1}\langle Q\rangle^{-\alpha}\right\| \leqslant c$, so we need to find out $\|\langle Q\rangle^{\alpha}\kappa V\langle Q\rangle^{\alpha}\| < 1/c$, which is true, as $\langle Q\rangle^{\alpha} V\langle Q\rangle^{\alpha}$ is bounded through the choice of α and, $|\kappa| \leqslant q(J)$ was chosen sufficiently small. □

In Theorem 6.5 we expect that it is possible to drop the restriction $|\kappa| \leqslant q(J)$. Solving this problem following the ideas of [ABG] or [GG05] would blow up the intended extent of this thesis, so we contend here with partial results of Proposition 6.7.

Lemma 6.6 Take Definiton 6.3. Fix $\alpha \in (1/2, (1+\varepsilon)/2)$. Then for every $f \in D(\langle Q\rangle^{\alpha})$ and all $\lambda \in J$

i) the limit

$$\left\langle f, (H_s - \lambda - i0^+)^{-1} f\right\rangle := \lim_{\eta \downarrow 0^+} \left\langle f, (H_s - \lambda - i\eta)^{-1} f\right\rangle$$

exists.

ii) the mapping $\lambda \mapsto \langle f, (H_s - \lambda - i0^+)^{-1} f\rangle$ is continuous and bounded.

Proof: Fix $G_\varepsilon(z) := (H_s - z - i\varepsilon E_I(H_s)[H_s, iA]E_I(H_s))^{-1}$. We know from Proposition 6.4 that

$$\sup_{\lambda \in J, \varepsilon > 0} \left\|\langle Q\rangle^{-\alpha}(H_s - \lambda - i\varepsilon)^{-1}\langle Q\rangle^{-\alpha}\right\| \leqslant C,$$

i.e. following the proof of the Limiting Absorption Principle we have uniformly in ε that

$$|\langle f, G_\varepsilon(z) f\rangle| \leqslant C\|\langle Q\rangle^{\alpha} f\|^2. \tag{6.5}$$

We would like to let ε tend to 0; notice from Lemma 4.18 that $G_\varepsilon(z)$ is continuous and differentiable in ε on $(0, \infty)$. Fix $\varepsilon_0 > 0$, then

$$\langle f, G_0(z) f\rangle = \langle f, G_{\varepsilon_0}(z) f\rangle - \int_{\varepsilon_0}^{0} \left\langle f, \frac{d}{d\epsilon} G_\epsilon(z) f\right\rangle d\epsilon. \tag{6.6}$$

Since resolvents of bounded operators are holomorphic, we notice that the mapping $z \mapsto G_{\varepsilon_0}(z)$ is holomorphic, providing us with continuity in z for the left term. We can thus mimic the proof for Lemma 4.16, using the estimates of Lemma 4.18 iii) to get that we can bound the integrand of (6.6) uniformly in z, thus with the Lebesgue Dominated Convergence Theorem

$$\lim_{z\to\lambda+0^+}\int_{\varepsilon_0}^{0}\left\langle f,\frac{d}{de}G_e(z)f\right\rangle de=\int_{\varepsilon_0}^{0}\lim_{z\to\lambda+0^+}\left\langle f,\frac{d}{de}G_e(z)f\right\rangle de.$$

Therefore we are able to let ε tend to 0 without losing continuity in z. □

With this continuity information we can revisit the proof of Theorem 6.5 to deduce some more.

Proposition 6.7 Take Definition 6.3. Fix

$$1+K(\lambda):=1+\langle Q\rangle^{\alpha}V\langle Q\rangle^{\alpha}\langle Q\rangle^{-\alpha}(H_0-\lambda-i0^+)^{-1}\langle Q\rangle^{-\alpha},$$

and choose $\lambda_0\subset J$ such that $1+K(\lambda_0)$ is injective. Then there is a set $K\subset\mathbb{R}$, with $\mathbb{R}\backslash K$ discrete, such that for $\kappa\in K$ there is an interval I around λ_0 where H_κ has purely absolutely continuous spectrum, in particular

$$\sup_{\mathrm{Re}(z)\in I,\mathrm{Im}(z)>0}\left\|\langle Q\rangle^{-\alpha}(H_\kappa-z)^{-1}\langle Q\rangle^{-\alpha}\right\|<\infty.$$

Proof: First notice that H_κ obeys $H_0=H_s$ and $H_1=H_0+V$. We remember from the proof of Theorem 6.5, that $\langle Q\rangle^{\alpha}\kappa V\langle Q\rangle^{\alpha}$ is compact, so $K(\lambda)$ is compact. Moreover we write equation (6.3)

$$\begin{aligned}&\langle Q\rangle^{-\alpha}(H_\kappa-z)^{-1}\langle Q\rangle^{-\alpha}\langle Q\rangle^{\alpha}(1+\kappa V(H_0-z)^{-1})\langle Q\rangle^{-\alpha}\\&\quad=\langle Q\rangle^{-\alpha}(H_0-z)^{-1}\langle Q\rangle^{-\alpha}.\end{aligned}\tag{6.7}$$

Here we let z tend to $\lambda+i0^+$, where we know from the above lemma, that the term $\langle Q\rangle^{\alpha}(1+\kappa V\langle Q\rangle^{\alpha}\langle Q\rangle^{-\alpha}(H_0-\lambda-i0^+)^{-1})\langle Q\rangle^{-\alpha}=1+\kappa K(\lambda)$ is continuous in λ.

With $K(\lambda_0)$ being compact, we notice $\sigma(K(\lambda_0))$ is dense at most at 0. As for $\kappa\neq 0$

$$1+\kappa K(\lambda_0)=\kappa\left(K(\lambda_0)+\kappa^{-1}\right),$$

the set

$$\tilde{G}:=\{k\mid 0\in\sigma(1+kK(\lambda_0))\}$$

is discrete. Putting $G:=\mathbb{R}\backslash\tilde{G}$, implies for $\kappa\in G$ that $1+\kappa K(\lambda)$ is invertible. Fix $\kappa\in G$, then there is a constant $c>0$ obeying

$$\|(1+\kappa K(\lambda_0))f\|\geqslant c\|f\|.$$

For we have continuity in λ, we know there is a neighbourhood I around λ_0 such that for a given $0 < \delta < c$, we find for all $\lambda \in I$

$$\|1 + \kappa K(\lambda) f\| \geqslant \delta \|f\|,$$

preserving invertibility. Therefore we are able to go from (6.7) to

$$\begin{aligned}
&\langle Q\rangle^{-\alpha} (H_\kappa - \lambda)^{-1} \langle Q\rangle^{-\alpha} \\
&\quad = \langle Q\rangle^{-\alpha} (H_0 - \lambda)^{-1} \langle Q\rangle^{-\alpha} \langle Q\rangle^{\alpha} (1 + \kappa V (H_0 - \lambda)^{-1})^{-1} \langle Q\rangle^{-\alpha},
\end{aligned}$$

and can estimate the right side to be bounded for $\lambda \in I$, which explains our claim. □

7 Scattering Theory

Scattering experiments usually involve a scatterer, e.g. a crystal, and a test particle. At the beginning the crystal and the particle are a vast distance off and, with time evolving, getting nearer until they interact. After a while the particle leaves the scatterer and moves away, enlarging the distance and thus the scatterer is expected to exercise no more influence on the particle, which is then free again. In terms of quantum mechanics, we express this with the interacting time evolution e^{-itH} and the free time evolution e^{-itH_0}, where often $H_0 = \Delta$ and $H = H_0 + V$ for some "fast decaying" potential V. A state f getting asymptotically free in the long term means there is a state f_+ such that for t near ∞ we have

$$e^{-itH} f \approx e^{-itH_0} f_+.$$

Similarly looking æons in the past, and thereby neglecting any particle sources we would meet in real experiments, we have for t near $-\infty$ a state f_+ complying

$$e^{-itH} f \approx e^{-itH_0} f_-.$$

Multiplying both to the left with e^{itH} lets us expect

$$f = \lim_{t \to -\infty} e^{itH} e^{-itH_0} f_- = \lim_{t \to \infty} e^{itH} e^{-itH_0} f_+.$$

If the particle is instead subjected to long term forces, i.e. the potential V is long range (e.g. the Coulomb Potential), we can not assume that the particle will become free in the future.

This chapter wants to examine these ideas with more mathematical rigour. First we introduce the vocabulary and advance to completeness and existence. The results of this chapter can be found in [CFKS] Chapter 5, [Kit] and [RS] Volume III, Chapter XI.

7.1 Generalized Wave Operator Properties

Now, we define suitable operators $\Omega^\pm$ to examine this behaviour. After that, assuming their existence, Proposition 7.3 examines some properties.

Definition 7.1 Let A and B be self-adjoint operators on $\mathcal{H}$ and let $P_{ac}(B)$ be the orthogonal projection on $\mathcal{H}_{ac}(B)$. We say that the *generalized wave operators* $\Omega^\pm(A, B)$ exist, if the strong limits

$$\Omega^\pm(A, B) := \text{s-}\lim_{t\to\mp\infty} e^{iAt}e^{-iBt}P_{ac}(B)$$

exist. In that case we define

$$\mathcal{H}_+ := \operatorname{Ran}\Omega^+ \text{ and } \mathcal{H}_- := \operatorname{Ran}\Omega^-,$$

and if $\mathcal{H}_+ = \mathcal{H}_- = \operatorname{Ran} P_{ac}(A)$, we say that $\Omega^\pm(A, B)$ are complete.

Remark 7.2 For the the wave operators $\Omega^\pm(A, B)$ there exist two conventions regarding the strong limit over $t \to \mp\infty$ or respectively over $t \to \pm\infty$. Here we stick to the first, which is also used in [RS] Chapter XI.

The purpose of the projections $P_{ac}(B)$ is to avoid eigenvalues, which do not play a role in scattering. By keeping the idea of $A = H$ and $B = H_0$ we get, assuming that $\Omega^\pm$ exists, the interpretation of the state $f = \Omega^+ f_-$ that developed to the past, looks asymptotically like a the state f_-, which was not subjected to the scatter. The spaces $\mathcal{H}_+$ and $\mathcal{H}_-$ are therefore called the sets of *incoming* and *outgoing states*. In Proposition 7.3 we see that $\Omega^\pm$ are partial isometries, hence the definition of completeness is a word for the phenomenon that every incoming state has exactly one corresponding outgoing state and vice versa.

Proposition 7.3 Suppose that $\Omega^\pm$ exist, then

i) the operators $\Omega^\pm$ are partial isometries from $\mathcal{H}_{ac}(B)$ to $\mathcal{H}_\pm$,

ii) the spaces $\mathcal{H}_\pm$ are invariant under A and

$$\Omega^\pm(D(B)) \subset D(A), \qquad A\Omega^\pm(A,B) = \Omega^\pm(A,B)B, \tag{7.1}$$

iii) the spaces $\mathcal{H}_\pm$ are subspaces of $\mathcal{H}_{ac}(A)$.

Proof: i) The operators e^{iAt} and e^{-iBt} are unitary and $P_{ac}(B)$ is an orthogonal projection.
ii) For any $s \in \mathbb{R}$ we can shift the limit of $\Omega^\pm(A,B)$

$$\begin{aligned}\Omega^\pm(A,B) &= \text{s-}\lim_{t\to\mp\infty} e^{iAt}e^{-iBt}P_{ac}(B) = \text{s-}\lim_{t\to\mp\infty} e^{iA(t+s)}e^{-iB(t+s)}P_{ac}(B)\\ &= e^{iAs}\text{s-}\lim_{t\to\mp\infty} e^{iAt}e^{-iBt}P_{ac}(B)e^{-iBs} = e^{iAs}\Omega^\pm(A,B)e^{-iBs}.\end{aligned}$$

We multiply from left with e^{-iAs} and note that strong differentiation with respect to s is digestible and

$$e^{iAs}\Omega^\pm(A,B) = \Omega^\pm(A,B)e^{iBs}. \tag{7.2}$$

From the above we get, with the help of Stone's Theorem, that equation (7.1) holds and furthermore that $\mathcal{H}_\pm$ are invariant subspaces for e^{iAs}.

iii) We already know that $\Omega^\pm$ are partial isometries

$$A = \Omega^\pm(A,B)B\Omega^\pm(A,B)^*.$$

So $A|_{\mathcal{H}_\pm}$ is unitarily equivalent to $B|_{\mathcal{H}_{ac}(B)}$ and hence $A|_{\mathcal{H}_\pm}$ is purely absolutely continuous, so $\mathcal{H}_\pm \subset \mathcal{H}_{ac}(A)$. □

7.2 Completeness

By the initial physical argumentation we expect that the generalized wave operators exist in several contexts and are usually complete. Mathematically it is harder to gain that result and we have to take much care of domains and convergence. There is a Chain Rule 7.4 that allows easy mating of wave operators, so if we know $\Omega^\pm(A,B)$ and $\Omega^\pm(B,C)$ exist, we derive the existence of $\Omega^\pm(A,C)$, which will serve in Proposition 7.5 through factoring $\Omega^\pm(A,A)$ as a joint to completeness, which becomes equivalent to the existence of both $\Omega^\pm(A,B)$ and $\Omega^\pm(B,A)$. We postpone nice existence criteria to the next section.

Proposition 7.4 (Chain Rule) Suppose that $\Omega^\pm(A, B), \Omega^\pm(B, C)$ exist. Then $\Omega^\pm(A, C)$ exists and can be written as

$$\Omega^\pm(A, C) = \Omega^\pm(A, B)\Omega^\pm(B, C).$$

Proof: First, we expand the limit argument of $\Omega^\pm(A, C)$

$$\begin{aligned} e^{itA}e^{-itC}P_{ac}(C) &= e^{itA}e^{-itB}P_{ac}(B)e^{itB}e^{itC}P_{ac}(C) \\ &\quad + e^{itA}e^{-itB}(1 - P_{ac}(B))e^{itB}e^{itC}P_{ac}(C). \end{aligned}$$

The first summand converges to $\Omega^\pm(A, B)\Omega^\pm(B, C)$ as the product of uniformly bounded and strongly convergent operators is strongly convergent; the second summand vanishes, since $e^{itA}e^{-itB}$ is bounded and, from Proposition 7.3, $\operatorname{Ran}\Omega^\pm(B, C) \subset \mathcal{H}_{ac}(B)$, so

$$\lim_{t\to\mp\infty} \left\|(1 - P_{ac}(B))e^{itB}e^{-itC}P_{ac}(C)f\right\| = 0$$

for any $f \in \mathcal{H}$. □

Proposition 7.5 Completeness of $\Omega^\pm(A, B)$ is equivalent to the existence of $\Omega^\pm(B, A)$.

Proof: We assume that both $\Omega^\pm(A, B)$ and $\Omega^\pm(B, A)$ exist. With the Chain Rule 7.4 we calculate

$$P_{ac}(A) = \Omega^\pm(A, A) = \Omega^\pm(A, B)\Omega^\pm(B, A)$$

and read that $\mathcal{H}_{ac} \subset \operatorname{Ran}\Omega^\pm(A, B)$. The latter range is, by Proposition 7.3, subset of $\mathcal{H}_{ac}$ and $\Omega^\pm(A, B)$ are therefore complete.

Conversely $\Omega^\pm(A, B)$ exist and are complete. For any $f \in \mathcal{H}_{ac}(A)$ there is a $g \in \mathcal{H}$ with $f - \Omega^\pm(A, B)g = 0$, as $\mathcal{H}_{ac}(A)$ is the range of $\Omega^\pm(A, B)$. Since e^{iAt} and e^{iBt} are unitary this implies that

$$\left\|e^{iBt}e^{-iAt}f - P_{ac}(B)g\right\| \to_{t\to-\infty} 0,$$

so $\lim_{t\to-\infty} e^{iBt}e^{-iAt}f = P_{ac}(B)g$, i.e. $\Omega^\pm(B, A)$ exist. □

7.3 Existence

To this point we have the unsatisfying existence of $\Omega^\pm(A, A)$ and of chained $\Omega^\pm$. Cook's Method 7.6 can be applied more generally, but involves a lot of estimation and does not return completeness. If we know the difference of A and B is "small", e.g. of trace class, as we would have in the initially described physical contexts for fast enough decaying potentials, we anticipate existence and completeness, which the Kato-Rosenblum Theorem 7.10 consequently returns.

All existence criteria found on Cook's Method 7.6, involving the sometimes tedious search for some estimates. The later criteria of Theorem 7.9 and especially 7.10 hide that search through abstract means.

Theorem 7.6 (Cook's Method) Let A and B be selfadjoint. If there is a subset $\mathcal{D}$ of $D(B) \cap \mathcal{H}_{ac}(B)$ dense in $\mathcal{H}_{ac}(B)$ such that for any $f \in \mathcal{D}$ there exists t_0 with

i) For $|t| > t_0$, $e^{-iBt}f$ lies in $D(A)$,

ii) $\displaystyle\int_{t_0}^{\infty} \left[\left\|(B-A)e^{-iBt}f\right\| + \left\|(B-A)e^{iBt}f\right\|\right] dt < \infty,$

then $\Omega^{\pm}(A, B)$ exists.

Proof: Take $f \in \mathcal{D}$ and define $\varphi_f(t) := e^{iAt}e^{-iBt}f$, being differentiable on (t_0, ∞) as by i) $e^{-itB}f$ is contained in $D(A) \cap D(B)$. We then use its derivative to estimate the behaviour of φ_f near infinity, so let $t, s > t_0$ then

$$\frac{d}{dt}\varphi_f(t) = -ie^{iAt}(B-A)e^{-iBt}f,$$
$$\|\varphi_f(t) - \varphi_f(s)\| \leqslant \int_s^t \left|\frac{d}{du}\varphi_t(u)\right| du \leqslant \int_s^t \left\|(B-A)e^{-iBu}f\right\| du.$$

Hypothesis ii) tells us that with s going to infinity, the latter distance approaches zero, so $\lim_{t\to\infty} \varphi_f(t)$ exists for all $\varphi \in \mathcal{D}$. Since $\mathcal{D}$ is dense in $D(B) \cap \mathcal{H}_{ac}(B)$, we can make use of the Bounded Linear Transformation Theorem to extend this on $D(B) \cap \mathcal{H}_{ac}(B)$. On the orthogonal subspace we assign the value 0 and have thus found $\Omega^{\pm}(A, B)$. □

We mentioned that trace class operators are key to our potentials.

Definition 7.7 Let $\mathcal{H}$ be a separable Hilbert space and $(f_n)_{n\in\mathbb{N}}$ an orthonormal basis of $\mathcal{H}$. For positive operators A on $\mathcal{H}$ we define the *trace*

$$\operatorname{tr}(A) := \sum_{n=1}^{\infty} \langle f_n, Af_n \rangle .$$

All operators with $\operatorname{tr}(\sqrt{A^*A}) < \infty$ define the *trace class* $\mathcal{T}_1$. We also call the set $\mathcal{T}_2$ of all A with $\operatorname{tr}(A^*A) < \infty$ *Hilbert-Schmidt.*

Proposition 7.8 The trace of A is independent of the chosen basis. Furthermore we have for positive $A, B \in \mathcal{T}_1$ that

i) $\operatorname{tr}(A + B) = \operatorname{tr}A + \operatorname{tr}B$.

ii) $\operatorname{tr}(\lambda A) = \lambda \operatorname{tr}A$ for $\lambda \geqslant 0$.

iii) $\operatorname{tr}(UAU^*) = \operatorname{tr}A$ for unitary U.

iv) if $0 \leqslant A \leqslant B$, then $\operatorname{tr}A \leqslant \operatorname{tr}B$.

Proof: Properties i), ii) and iv) are obvious.
Let $(f_n^{(i)})_{n\in\mathbb{N}}$ $(i \in \{1, 2\})$ be orthonormal bases of $\mathcal{H}$. Then we have

$$\begin{aligned}\operatorname{tr}_1 A &:= \sum_n \left\langle f_n^{(1)}, A f_n^{(1)} \right\rangle = \sum_n \left\| \sqrt{A} f_n^{(1)} \right\|^2 \\ &= \sum_n \sum_m \left| \left\langle f_m^{(2)}, \sqrt{A} f_n^{(1)} \right\rangle \right|^2 = \sum_n \sum_m \left| \left\langle \sqrt{A} f_m^{(2)}, f_n^{(1)} \right\rangle \right|^2.\end{aligned}$$

The series consist solely of positive summands and are therefore absolutely convergent and hence we can interchange summation over m and n; we invert the unpacking of the trace and get $\operatorname{tr}_1(A) = \operatorname{tr}_2(A)$. From this independence we also get iii), as the orthonormal base property is preserved under unitary transformation. □

The following theorem explains how fast decaying potentials lead to existence of the wave operators. Actually Theorem 7.9 gives a little more freedom, whereas the Kato-Rosenblum Theorem 7.10 is a restriction inescapably resulting in completeness.

Theorem 7.9 (Pearson) Let A and B be self-adjoint operators and let J be a bounded operator. Suppose that there exists $C \in \mathcal{T}_1$ such that $C = AJ - JB$ in the sense that for all $f \in D(A)$ and $g \in D(B)$

$$\langle f, Cg \rangle = \langle Af, Jg \rangle - \langle f, JBg \rangle$$

then

$$\Omega^{\pm}(A, B; J) := \text{s-}\lim_{t\to\mp\infty} e^{iAt} J e^{-iBt} P_{ac}(B)$$

exist.

Proof: For being lengthy, we only want to sketch the proof without getting into all details of the involved estimates and domains. An almost complete proof can be obtained from [RS] Volume III, Theorem XI.7. Define $W(t) := e^{iAt}Je^{-iBt}$ and consider t approaching ∞. The density argument of Theorem 7.6 makes it sufficient to show that

$$\lim_{t\to\infty, t<s} \|(W(t) - W(s))f\|^2 = 0 \tag{7.3}$$

for all $f \in \mathcal{D}$, for some suitable dense set $\mathcal{D}$. That we take as the set of all $f \in \mathcal{H}$ such that there is $\varphi \in L^\infty(\mathbb{R})$ and such for all measurable M we have the identity

$$\langle f, E_M(B)f\rangle = \int_M |\varphi(s)|^2 d\lambda(s).$$

Denote the L^∞-norm of φ by $\|f\|_{\mathcal{D}}$. It is then easy to see that $\|\cdot\|_{\mathcal{D}}$ is a norm and that $\mathcal{D}$ is dense in $\mathcal{H}_{ac}(B)$.

We want to divide (7.3) into two factors that we control separately. For bounded X and $a < b$ define

$$\begin{aligned} F_{a,b}(X) &:= \int_a^b e^{iBt}Xe^{-iBt}dt, \\ Y(t,s) &:= -i\left(e^{itB}J^*e^{-i(t-s)A}Ce^{-isB} - e^{itB}C^*e^{-i(t-s)A}Je^{isB}\right), \\ Q(b) &:= e^{ibB}W(t)^*W(s)e^{-bB}. \end{aligned}$$

Then

$$\frac{dQ(b)}{db} = -e^{ibB}Y(t,s)e^{-ibB}$$

shows by integration

$$F_{0,a}(Y(t,s)) = W(t)^*W(s) - e^{iaB}W(t)^*W(s)e^{-iaB}. \tag{7.4}$$

For fixed t and s we have that

$$W(t) - W(s) = i\int_s^t e^{iuA}Ce^{-iuB}du$$

is compact and therefore $W(t)^*(W(t) - W(s))$ is compact. So for $f \in \mathcal{D}$ we have by the laws of the Fourier Transformation that

$$\lim_{a\to\infty} e^{iaB}W(t)^*(W(t) - W(s))e^{-iaB}f = 0,$$

thus with (7.4) we gain for $f \in \mathcal{D}$

$$\langle f, W(t)^*(W(t) - W(s))f\rangle = \lim_{a\to\infty} \langle f, F_{0,a}(Y(t,t) - Y(t,s))f\rangle \,. \tag{7.5}$$

By [RS] Volume I, Section VI.6 there are for the trace class C the orthonormal systems $(f_n)_{n\in\mathbb{N}}$, $(g_n)_{n\in\mathbb{N}}$ and $\lambda_n > 0$ such that $\sum \lambda_n \leqslant \infty$ and

$$C = \sum_n \lambda_n \langle f_n, \cdot\rangle\, g_n.$$

We can estimate

$$\left|\left\langle f, F_{0,a} e^{iuB} X C e^{iuB} f\right\rangle\right| \leqslant c_1 \|X\| \cdot \|f\|_{\mathcal{D}} \sqrt{\sum_n \lambda_n \int_u^\infty |\langle f_n, e^{-ixB} f\rangle|^2 dx}.$$

Hence with (7.5) we get

$$\|(W(t) - W(s))f\|^2 \leqslant c_2 \|J\| \cdot \|f\|_{\mathcal{D}} \sqrt{\sum_n \lambda_n \int_{\min\{s,t\}}^\infty |\langle f_n, e^{-ixB} f\rangle|^2 dx}.$$

By the definition of $\mathcal{D}$ and for $f \in \mathcal{D}$ we obtain (7.3). □

Theorem 7.10 (Kato-Rosenblum) Let A and B be self-adjoint operators with $A - B \in \mathcal{T}_1$, then $\Omega^\pm(A, B)$ exist and are complete.

Proof: As $C := A - B$ is of trace class, we use Theorem 7.9 with $J := 1$ to see that $\Omega^\pm(A, B)$ exists. With C is $-C$ of trace class, so $\Omega^\pm(B, A)$ exist accordingly. Proposition 7.5 gives the desired completeness. □

8 Application of the Scattering Theory

For resembling the physical world, Schrödinger operators and hence the Laplace operator are the main attractions for scattering theory, so we open the chest of $\mathcal{H} = \ell^2(\mathbb{Z})$, again. Again, we investigate anisotropic potentials where Proposition 8.1 returns existence and completeness of the generalized wave operators, completing the proof Theorem 1.1.

Looking back to Theorem 6.5, we want to cover the trace class potentials $V \in o(1/|n|^{1+\varepsilon})$, leaving us in a perfect position to use the scattering theory:

Proposition 8.1 Remember Definition 5.13. Let $\varepsilon > 0$ and take a potential $V \in o(1/|n|^{1+\varepsilon})$, then $\Omega^\pm(H + V(Q), H)$ exist and are complete.

Proof: As $V \in o(\frac{1}{|n|^{1+\varepsilon}})$, we have $\lim_{n\to\infty} V(n)|n|^{1+\varepsilon}=0$; so there exists $N \in \mathbb{N}$ and $c > 0$ such that

$$\sum_{|n|>N} V(n) \leqslant c \sum_{n} \frac{1}{|n|^{1+\varepsilon}} < \infty.$$

Therefore we have that $V \in L^1(\mathbb{Z})$ and consequently $V \in \mathcal{T}_1(\mathbb{Z})$.

We set $A := H + V(Q)$ and $B := H$ to get $A - B = V(Q) \in \mathcal{T}_1(\mathbb{Z})$ enabling us to use the Kato-Rosenblum Theorem 7.10, so $\Omega^{\pm}(A, B)$ exist and are complete. □

Example 8.2 In Proposition 8.1 completeness does not let us expect that $\mathcal{H}_{ac}(H)$ for $H := \Delta + V(Q)$ equals $\mathcal{H} = \mathcal{H}_{ac}(\Delta)$. But suppose that were so, it would solve many questions we answered with Mourre Theory in one stroke, as that would imply $\mathcal{H}_{sc}(H) = \{0\}$; the projections to the absolutely continuous subspaces of Definition 7.1 are dispelling that hope, but are needed to get completeness for our potentials.

Actually, we neither get $\mathcal{H} = \mathcal{H}_{cont}(H)$, for Riesz's Min/Max Principle lets us see $\mathcal{H}_{pp} \neq \{0\}$. So the best we can expect is $\mathcal{H} = \mathcal{H}_{ac}(H) \oplus \mathcal{H}_{pp}(H)$. The pure point spectrum is not empty: Assume a potential $V < 0$. We claim for all $\lambda > 0$ that the operator $H_\lambda = \Delta + \lambda V$ got an eigenvalue.

Proof: Take $f \in \ell^2(\mathbb{Z})$ with $\|f\| = 1$. Moreover for $n \in \mathbb{N}$ and $\varepsilon := n^{-1}$ define the average mapping $y : \mathbb{Z} \to \mathbb{C}$ and the corresponding bounded and selfadjoint operator Y

$$y(k) := (Yf)(k) := \frac{1}{4}\left(f(k-1) + 2f(k) + f(k+1)\right).$$

We note that every $x \in \mathbb{Z}$ can be uniquely disassembled into $x = nk + m$, where $k \in \mathbb{Z}$ and $0 \leqslant m < n$, to construct a linearly interpolated dilation f_ε of f

$$\begin{aligned} f_\varepsilon(x) := f_\varepsilon(nk+m) &:= \sqrt{\varepsilon}\left(y(k) + \frac{m}{n}(y(k+1) - y(k))\right) \\ &= \frac{\sqrt{\varepsilon}}{n}\left((n-m)y(k) + my(k+1)\right). \end{aligned}$$

We claim that $\|f_\varepsilon\|^2 = c + o(\varepsilon)$ for some constant $c > 0$, which is a consequence of the following calculation

$$\begin{aligned}\langle f_\varepsilon, f_\varepsilon\rangle &= \frac{\varepsilon}{n^2}\sum_{k\in\mathbb{Z}}\sum_{0\leqslant m<n} |(n-m)y(k)+my(k+1)|^2\\ &= \frac{1}{n^3}\sum_{k\in\mathbb{Z}}\sum_{0\leqslant m<n} (n-m)^2|y(k)|^2+(n-m)my(k)\overline{y(k+1)}\\ &\qquad + (n-m)my(k+1)\overline{y(k)}+m^2|y(k+1)|^2.\end{aligned}$$

The y are independent of m so we can easily get rid of the sums over m using Gauss' Formulas

$$\begin{aligned}c_1(n) &:= \sum_{0\leqslant m<n} m^2 = \frac{1}{6}n(n+1)(2n+1)-n^2 = \frac{1}{6}(2n^3-3n^2+n),\\ c_2(n) &:= \sum_{0\leqslant m<n} (n-m)^2 = \sum_m n^2-2nm+m^2 = \frac{1}{6}(2n^3-3n^2+n),\\ c_3(n) &:= \sum_{0\leqslant m<n} (n-m)m = \sum_m nm-m^2 = \frac{1}{6}n(n^2-1).\end{aligned}$$

We put this back into $\|f_\varepsilon\|^2$

$$\begin{aligned}\langle f_\varepsilon, f_\varepsilon\rangle = n^{-3}(&c_2(n)\langle f,f\rangle + c_3(n)\langle Yf, YU^*f\rangle\\ &+ c_3(n)\langle YU^*f, Yf\rangle + c_1(n)\langle Yf, Yf\rangle)\end{aligned}$$

and cancel the n^{-3} to see $\|\varphi_\varepsilon\|^2 = c + o(\varepsilon)$.

We have to do some more arithmetic. First, we remember from the introduction of the Laplacian, that

$$\langle f_\varepsilon, \Delta f_\varepsilon\rangle = \langle\nabla f_\varepsilon, \nabla f_\varepsilon\rangle = \sum_k\sum_{0\leqslant m<n} |(\nabla f_\varepsilon)(kn+m)|^2. \tag{8.1}$$

We scrutinize the inner sum over m by unpacking the Nabla

$$\nabla f_\varepsilon(kn+m) = \sqrt{2}^{\,-1}\left(f_\varepsilon(kn+(m+1)) - f_\varepsilon(kn+m)\right).$$

Considering the case $0\leqslant m<n-1$ we can further expand the above expression

$$\begin{aligned}\nabla f_\varepsilon(kn+m) &= \frac{\sqrt{\varepsilon}}{\sqrt{2}n}((n-m-1)y(k)+(m+1)y(k+1)\\ &\quad -(n-m)y(k)-my(k+1))\\ &= \frac{\sqrt{\varepsilon}}{\sqrt{2}n}(y(k+1)-y(k))\end{aligned}$$

and in case of $m = n - 1$ we get

$$\begin{aligned}\nabla f_\varepsilon(kn + n - 1) &= \frac{\sqrt{\varepsilon}}{\sqrt{2}n}(ny(k+1) - y(k) - (n-1)y(k+1)) \\ &= \frac{\sqrt{\varepsilon}}{\sqrt{2}n}(y(k+1) - y(k)).\end{aligned}$$

We are thus very happy as we have removed all the m and equation (8.1) advances to

$$\begin{aligned}\langle f_\varepsilon, \Delta f_\varepsilon\rangle &= \sum_{k\in\mathbb{Z}} \frac{\varepsilon n}{2n^2}\left[(y(k+1) - y(k))\overline{(y(k+1) - y(k)))}\right] \\ &= \frac{\varepsilon^2}{2}\sum_{k\in\mathbb{Z}} |y(k+1) - y(k)|^2.\end{aligned}$$

This implies that for small $\varepsilon > 0$ the product $\langle \varphi_\varepsilon, H_\lambda \varphi_\varepsilon\rangle$ is smaller than 0 and, due to Riesz's Min/Max Principle, we gain an eigenvalue for H_λ. □

9 Appendix: Interpolation

This section prepares an interpolation theorem for unbounded, positive multiplication operators, used only once in Lemma 6.2 in Chapter 5, Application of the Mourre Theory. Its proof is taken from a course which was lectured by V. Georgescu. Let M be a borelian measure space, μ a positive, σ-finite measure. Take a measurable function $A : M \to (0, \infty)$. Fix the Hilbert space $\mathcal{H} := L^2(M)$ and $\mathcal{K} := \{h \in \mathcal{H} \mid \|Ah\| < \infty\}$ the domain of A.

Theorem 9.1 Let M,N be borelian spaces with positive, σ-finite measure and let the functions

$$\begin{aligned}A : M &\to (0, \infty), \\ B : N &\to (0, \infty)\end{aligned}$$

be measurable. Take an operator $T : L^2(M) \to L^2(N)$ with $\|T\| = m_0 < \infty$ and suppose there is a constant m_1 such that for all $k \in L^2(\mathcal{K})$

$$\|BTk\| \leqslant m_1\|Ak\|.$$

Then for all $\theta \in [0, 1]$ and all $k \in L^2(M)$ we have

$$\left\|B^\theta Tk\right\| \leqslant m_0^{1-\theta} m_1^\theta \left\|A^\theta k\right\|.$$

To prove this statement we find for the involved norms a different notation. Lemma 9.2 creates an integrand that will, by Remark 9.3, become integrated and thus a tool to record the $\|B^\theta Tk\|$ and $\|A^\theta k\|$ norms.

Lemma 9.2 Let $z > 0$ and $h \in \mathcal{H}$. Define

$$K_A(z,h) := \inf_{k\in\mathcal{K}} \sqrt{z^2\|Ak\|^2 + \|h-k\|^2}.$$

Then

$$K_A(z,h) = \left\| \frac{zA}{\sqrt{1+z^2A^2}} h \right\|.$$

Proof: Without loss of generality assume $z = 1$, otherwise replace A with zA. Define

$$Q(k) := \|Ak\|^2 + \|k\|^2 - 2\mathrm{Re}\,\langle h, k\rangle$$

for $k \in \mathcal{K}$. Then we have by the Binomial Theorem

$$Q(k) = \left\| \sqrt{A^2+1}k - \sqrt{A^2+1}^{\,-1} h \right\|^2 - \left\| \sqrt{A^2+1} h \right\|^2,$$

which attains its unique minimum at

$$k_0 := \left(A^2+1\right)^{-1} h.$$

Since $K_A(1,h)^2 = Q(k_0) + \|h\|^2$, we have

$$K_A(1,h) = \sqrt{\left\langle h, (1 - \frac{1}{A^2+1})h \right\rangle} = \left\| \frac{A}{\sqrt{A^2+1}} h \right\|,$$

which resembles the result of the lemma. □

Remark 9.3 Let $0 < \theta < 1$. Then

$$\begin{aligned}
\int_0^\infty \left[\frac{K_A(z,h)}{z^\theta}\right]^2 \frac{dz}{z} &= \int_0^\infty \left\langle h, \frac{z^2A^2}{1+z^2A^2} h \right\rangle \frac{dz}{z^{1+2\theta}} \\
&= \int_M |h(x)|^2 \int_0^\infty \frac{((zA(x))^{2(1-\theta)}(A(x))^{2\theta}}{1+z^2A(x)^2} \frac{dz}{z} dx \\
&= \int_M |h(x)|^2 \int_0^\infty \frac{r^{2(1-\theta)}}{1+r^2} \frac{dr}{r} A(x)^{2\theta} dx = C(\theta)\left\|A^\theta h\right\|^2
\end{aligned}$$

We put everything together:

Proof of Theorem 9.1: We estimate

$$K_B(z,Tk)^2 = \inf_{f\in\mathcal{K}_B}\left[z^2\|Bf\|^2 + \|Tk-f\|^2\right] \leqslant \inf_{g\in\mathcal{K}_B}\left[z^2\|BTg\|^2 + \|T(k-g)\|^2\right]$$
$$\leqslant \inf_{g\in\mathcal{K}_B}\left[z^2 m_1^2\|Ag\|^2 + m_0^2\|k-g\|^2\right] = m_0^2\left[K_A\left(z\frac{m_1}{m_0},h\right)\right]^2,$$

so

$$\left\|B^\theta Tk\right\|^2 C(\theta) = \int_0^\infty \left[\frac{K_B(z,Tk)}{z^\theta}\right]^2 \frac{dz}{z}$$
$$\leqslant m_0^2\int_0^\infty \left[\frac{K_A\left(z\frac{m_1}{m_0},h\right)}{z^\theta}\right]^2 \frac{dz}{z} = (m_0^{1-\theta}m_1^\theta)^2 C(\theta)\left\|A^\theta k\right\|^2,$$

is, cancelling $C(\theta)$, just what we wanted to show. □

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Nomenclature

$\mathcal{C}^n(A)$ Class $\mathcal{C}^n$ of A; see Definitions 4.4 and 4.6

C_0^∞ Space of smooth functions, tending to 0 at infinity

C_c^∞ Space of compactly supported, smooth functions

$C_\infty(\mathbb{Z})$ Space of discrete, anisotropic potentials; see Definition 3.9

$\mathcal{H}$ Complex Hilbert space. In the application chapters most often $\mathcal{H} = \ell^2(\mathbb{Z})$ elsewhere mostly $\mathcal{H} = L^2(X)$ for some measure space X

$\mathcal{H}_{ac}$ Absolutely continuous subspace; see Definition 2.22

$\mathcal{H}_{cont}$ Continuous subspace; see Definition 2.22

$\mathcal{H}_{pp}$ Pure point subspace; see Definition 2.22

$\mathcal{H}_{sc}$ Singularly continuous subspace; see Definition 2.22

$\mathcal{H}_\pm$ Incoming respectively outgoing states; see Definition 7.1

ℓ^2 Space of square summable sequences

ℓ_c^2 Space of aborting square summable sequences

L^2 Space of square integrable functions

$[A, B]_\circ$ Closure of the commutator of A and B; see Definition 4.6

$\mathcal{F}$ Fourier Transformation; see Definition 3.3

Δ Laplace operator; see Definition 3.1

$\Delta_\pm$ Perturbed Laplacians on $\ell^2(\mathbb{Z}_\pm)$; see Definition 5.2

Δ_{jt} Glued perturbed Laplacians; see Definition 5.13

$A_\pm$ Conjugates for $\Delta_\pm$; see Definition 5.6

A_{jt} Conjugate for Δ_{jt}; see Definition 5.13

E Spectral projection

L_{jt} Barrier potential; see Definition 5.13

P_{ac} Projection onto the absolutely continuous subspace

Q See Definition 2.14

$Q_\pm$ See Definition 5.2

U Shift operator on $\ell^2(\mathbb{Z})$; see Definition 3.1

$U_\pm$ Shift operators on $\ell^2(\mathbb{Z}_\pm)$; see Definition 5.2

V	Potential
$[A, B]$	Commutator of A and B, i.e. $[A, B] := AB - BA$ for bounded A,B; otherwise see Definition 4.6
σ_{ac}	Absolutely continuous spectrum; see Definition 2.25
σ_{cont}	Continuous spectrum; see Definition 2.25
σ_{disc}	Discrete spectrum; see Definition 2.6
σ_{ess}	Essential spectrum; see Definition 2.6
σ_{pp}	Pure point spectrum; see Definition 2.25
σ_{sc}	Singularly continuous spectrum; see Definition 2.25
σ	Spectrum
$\mathbb{N}_0$	Positive integers and 0
$\mathbb{Z}_\pm$	Splinters of $\mathbb{Z}$; see Definition 5.2
χ	Characteristic function
$\mathcal{T}_n$	n-th Schatten class; see Definition 7.7
$\Omega^\pm$	Generalized wave operator; see Definition 7.1
$\subset\subset$	Compactly embedded
$\varphi(H)$	φ applied on H, defined through the Spectral Theorem
s-lim	Strong limit; see Definition 2.1
w-lim	Weak limit; see Definition 2.1
$\langle\cdot,\cdot\rangle$	Scalar product for $\mathcal{H}$
$\langle A\rangle$	$\sqrt{1+\lvert A\rvert^2}$; see Equation (4.18)
$B(\lambda, \zeta)$	Open metric ball around λ with radius ζ
$D(A)$	Domain of A
F_1	See Definition 5.13
F_2	See Definition 5.20
$f_n \to f$	Convergence or strong convergence; see Definition 2.1
$f_n \rightharpoonup f$	Weak convergence; see Definition 2.1
$\lVert A\rVert$	Operator norm in $\mathcal{H}$
$\lVert f\rVert$	Norm in $\mathcal{H}$

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