Course Spring Term 2015: Scattering Theory

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Contents

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1 Weyl's theorem on the essential spectrum

In quantum mechanical one-particle scattering theory, one is typically interested in the following situation. There is a self-adjoint Hamiltonian $H_0 = H_0^*$ on a separable Hilbert space $\mathcal{H}$ describing the free of a particle. This operator often has purely absolutely continuous spectrum and can be analyzed explicitly (*e.g.* the Laplacian). The perturbed Hamiltonian is then $H = H_0 + V$ with a perturbation $V = V^*$ that is in some sense small. In this section, it will be supposed that V is a compact operator and then the spectral properties of H will be compared to those of H_0. Recall that the discrete spectrum $\sigma_{\text{dis}}(A) \subset \mathbb{C}$ of a closed operator A on $\mathcal{H}$ is defined the union of all isolated eigenvalues of A with finite multiplicity (namely, all $\lambda \in \sigma(A)$ such that there exists an $r > 0$ with $B_r(\lambda) \cap \sigma(A) = \{\lambda\}$ and λ has finite multiplicity). The essential spectrum is then by definition $\sigma_{\text{ess}}(A) = \sigma(A) \setminus \sigma_{\text{dis}}(A)$. Let us remark that there are various other notions of essential spectrum, in particular the set $\sigma'_{\text{ess}}(A) = \{z \in \mathbb{C} \,|\, z\mathbf{1} - A \text{ is Fredholm}\}$ is often called the essential spectrum and it is clearly stable under compact perturbations. For self-adjoint operators these sets coincide (a non-trivial fact), but for non-normal operators they do not.

1.1 Theorem (Weyl's theorem on the essential spectrum) *If V is compact, then*

$$\sigma_{\text{ess}}(H_0 + V) \;=\; \sigma_{\text{ess}}(H_0) \;,$$

namely the essential spectrum is stable under compact perturbations.

Of course, the perturbation V may produce eigenvalues which may accumulate on $\sigma_{\text{ess}}(H_0)$. The arguments in proof are quite robust and apply also to not necessarily self-adjoint operator pairs of operators A and B such that $A - B$ is compact. Let us begin with the following preparatory result [RS, Theorem VI.14].

1.2 Theorem (Analytic Fredholm theorem) *Let $\Omega \subset \mathbb{C}$ be an opend connected set and $f : \Omega \to \mathcal{B}(\mathcal{H})$ an analytic operator-valued function such that $f(z)$ is a compact operator for every $z \in \Omega$. Then one of the following two claims holds true:*

(i) *There is a discrete set $S \subset \Omega$ (without limit points in Ω) such that $\mathbf{1} - f(z)$ is invertible for no $z \in \Omega \setminus S$.*

(ii) *$\mathbf{1} - f(z)$ is invertible for no $z \in \Omega$.*

In the case (i), *$(\mathbf{1} - f(z))^{-1}$ is meromorphis in Ω with poles in S having residues that are finite rank operators. Moreover, for $z \in S$, the equation $f(z)\psi = \psi$ has a non-zero solution $\psi \in \mathcal{H}$.*

Proof. By connectedness, it is sufficient to prove the result locally at every point $z_0 \in \Omega$. Choose an $r > 0$ such that

$$\|f(z) - f(z_0)\| \;<\; \frac{1}{2} \;, \qquad \forall \;\; z \in B_r(z_0) \;.$$

By density of the finite rank operators on the compact operators, choose a finite rank operator F such that

$$\|F - f(z_0)\| \;<\; \frac{1}{2} \;.$$

Then a Neumann series shows that $\mathbf{1} - f(z) + F$ is invertible for all $z \in B_r(z_0)$. Let us write

$$\begin{aligned} \mathbf{1} - f(z) \;&=\; \big(\mathbf{1} - F(\mathbf{1} - f(z) + F)^{-1}\big)(\mathbf{1} - f(z) + F) \\ &=\; (\mathbf{1} - g(z))(\mathbf{1} - f(z) + F) \;, \end{aligned}$$

where we set $g(z) = F(\mathbf{1} - f(z) + F)^{-1}$ which is obviously a finite rank operator. This shows that $\mathbf{1} - f(z)$ is invertible if and only if $\mathbf{1} - g(z)$ is invertible. But the invertibility of $\mathbf{1} - g(z)$ can be tested with a finite dimensional determinant which depends analytically on z so that it is either identical to 0 in $B_r(z_0)$ or has a discrete set of zeros there. With more details, let us write

$$F \;=\; \sum_{n=1}^{N} |\psi_n\rangle\langle\phi_n| \;,$$

with linearly independent vector $\psi_1,\ldots,\psi_N \in \mathcal{H}$, and then

$$g(z) \;=\; \sum_{n=1}^{N} |\psi_n\rangle\langle\phi_n(z)|$$

where $\phi_n(z) = (\mathbf{1}-f(z)^*+F^*)^{-1}\phi_n$. Then $g(z)\psi = \psi$ implies $\psi = \sum_{n=1}^{N}\lambda_n\psi_n$ with coefficients $\lambda_n \in \mathbb{C}$, and $g(z)\psi = \psi$ has a solution if and only if there are coefficients $\lambda_1,\ldots,\lambda_N$ such that

$$\lambda_m \;=\; \sum_{n=1}^{N} \lambda_n\,\langle\phi_m(z)|\psi_n\rangle \;,$$

which in turn is equivalent to having a vanishing determinant

$$d(z) \;=\; \det\left(\mathbf{1}_N - \langle\phi_m(z)|\psi_n\rangle_{n,m=1,\ldots,N}\right) \;.$$

This determinant is analytic so that $S_r = \{z \in B_r(z_0)\,|\,d(z) = 0\}$ is either equal to $B_r(z_0)$ or discrete. If $d(z) = 0$, then clearly $\mathbf{1} - g(z)$ is not invertible. If $d(z) \neq 0$, then we will show that the equation $(\mathbf{1} - g(z))\psi = \phi$ can be solved with $\phi \in \mathcal{H}$ for any $\psi \in \mathcal{H}$, which implies that $\mathbf{1} - g(z)$ is invertible. The solution will be sought-after in the form $\psi = \phi + \sum_{n=1}^{N}\mu_n\psi_n$, so one needs

$$(\mathbf{1} - g(z))\sum_{n=1}^{N}\mu_n\psi_n \;=\; g(z)\phi \;,$$

which is now an equation only involving vectors in the span of $\psi_1,\ldots,\psi_N$. For the coefficient of ψ_n, one finds

$$\mu_n \;-\; \sum_{m=1}^{N}\langle\phi_n(z)|\psi_m\rangle\,\mu_m \;=\; \langle\phi_n(z)|\phi\rangle \;,$$

which is solvable for $\mu_1,\ldots,\mu_N$ because $d(z) \neq 0$. In conclusion, $\mathbf{1} - g(z)$ and thus $\mathbf{1} - f(z)$ is invertible if and only if $z \notin S_r$. The additional facts follow from the explicit form of the solution. □

1.3 Remark In the classical Fredholm alternative, one takes $f(z) = zK$ for a compact operator K. Applying the above theorem at $z = 1$ shows that either $\mathbf{1} - K$ is invertible or the equation $K\psi = \psi$ has a solution $\psi \in \mathcal{H}$. ◇

1.4 Theorem *Let A and B be two bounded operators on a separable Hilbert space such that $A - B$ is compact. Let $\Omega \subset \mathbb{C}$ be one connected component of $\mathbb{C}\setminus\sigma(A)$. Then one of the following two claims holds true:*

(i) *Ω contains a point in the resolvent set of B.*

(ii) *All points of Ω are eigenvalues of B.*

In the case (i)*, the spectrum of B in Ω is discrete.*

Proof. Let $K = A - B$. Then $z \in \Omega \mapsto K(A-z)^{-1}$ is analytic and compact-valued. For $z \in \Omega$ one has $B - z = (\mathbf{1} - K(A-z)^{-1})(A-z)$, so the inverse $(B-z)^{-1}$ exists if and only if $(\mathbf{1} - K(A-z)^{-1})^{-1}$ exists (as $A-z$ is invertible). Now one clearly has the dichotomy that either Ω contains some point in the resolvent set of B or it contains none. The first case corresponds to (i). Then there exists some $z_0 \in \Omega$ such that the inverse $(\mathbf{1} - K(A-z_0)^{-1})^{-1}$ exists. But by the analytic Fredholm theorem, the inverse $(\mathbf{1} - K(A-z)^{-1})^{-1}$ then exists for all $z \in \Omega$ except for a discrete set of points. Hence also the spectrum of B lying in Ω only consists of a discrete set of points. In the second possibility, where no point of Ω lies in the resolvent set of B, the operator $1 - K(A-z)^{-1}$ is not invertible for any $z \in \Omega$. By the Fredholm alternative this implies that for each $z \in \Omega$ there is a vector v_z lying in the kernel of $\mathbf{1} - K(A-z)^{-1}$. Setting $w_z = (A-z)^{-1} v_z$, one then has $(A-z)w_z = K w_z$, that is $B w_z = z w_z$. Therefore in the second possibility all points $z \in \Omega$ are eigenvalues of B. □

Proof of Theorem 1.1 for the case of bounded H_0. Then $A = H_0$ and $B = H_0 + V$ have spectrum on the real line and their resolvent sets are connected in $\mathbb{C}$. As z with $|z| > \|H_0\| + \|V\|$ lies in the resolvent set, only option (i) in Theorem 1.4 applies. Thus $\sigma(H) \setminus \sigma(H_0)$ is discrete and $\sigma_{\text{ess}}(H) \subset \sigma_{\text{ess}}(H_0)$. By symmetry, also $\sigma_{\text{ess}}(H_0) \subset \sigma_{\text{ess}}(H)$. If the operators are only self-adjoint (and not necessarily bounded, then one has to work with resolvents and use the fact that there is a mapping property connecting the essential spectra of the Hamiltonian to that of the resolvents, see [RS]. □

1.5 Remark Here is an example that also possibility (ii) in Theorem 1.4 can happen once one leaves the world of normal operators. Let $S = \sum_{n \in \mathbb{Z}} |n\rangle\langle n-1|$ be the bilateral right shift on $\ell^2(\mathbb{Z})$. It is unitary and its spectrum is $\sigma(S) = \sigma_{\text{ess}}(S) = \mathbb{S}^1$. Now consider the rank one perturbation $V = -|1\rangle\langle 0|$. Then $S + V$ is the sum of two unilateral shifts and the spectrum of $S+V$ is the fill unit disc so that $\sigma_{\text{ess}}(S+V) = \overline{\mathbb{D}^1}$. On the other hand, $\sigma'_{\text{ess}}(S+V) = \mathbb{S}^1$. ◇

2 RAGE theorem and extensions

In this chapter, we begin by discussing basic approaches to the phenomena of quantum transport: escape probabilities and diffusion exponents. In particular, their connections to spectral properties are analyzed.

2.1 The time-averaged transition and return probabilities

Let H be a selfadjoint Hamiltonian on a separable Hilbert space. Suppose the system is initially in a normalized state ψ, *e.g.* the state $|0\rangle$ localized at the origin. Then the probability to be in a normalized state ϕ at time t is $|\langle\phi|e^{-\imath tH}|\psi\rangle|^2$. Unfortunately it is difficult to analyze this quantity directly and one therefore usually considers the time-averaged probability to reach ϕ when starting from ψ:

$$p_T(\phi,\psi) \;=\; \int_0^T \frac{dt}{T}\; |\langle\phi|e^{-\imath tH}|\psi\rangle|^2 \;.$$

Then $p_T(\phi,\psi)$ is called the time-averaged transition probability from ψ to ϕ (under the dynamics generated by H) and $p_T(\psi,\psi)$ is often also called the time-averaged return probability to ψ. Clearly, if ψ is an eigenstate of H with energy E so that $e^{-\imath tH}\psi = e^{-\imath tE}\psi$, then $p_T(\psi,\psi) = 1$. On the other hand, if initial state ψ lies in the continuous spectral subspace of H, that is, its spectral measure contains no atom, then the return probability $p_T(\psi,\psi)$ converges to 0 in the long time limit. This follows from the so-called RAGE theorem which can be tracked back to contributions by Ruelle, Amrein, Georgescu and Enss in 1970's.

2.1 Theorem (RAGE theorem) *Let H be a self-adjoint operator and K a compact operator on a separable Hilbert space $\mathcal{H}$. Then for any ψ in the continuous subspace $\mathcal{H}_c \subset \mathcal{H}$ associated to H, one has*

$$\lim_{T\to\infty} \int_0^T \frac{dt}{T} \, \|K\, e^{-\imath Ht}\, \psi\|^2 \;=\; 0\;.$$

The main ingredient of the proof is following classical result of Wiener on the Fourier transform of a measure.

2.2 Theorem (Wiener) *Let ν be a complex measure on $\mathbb{R}$. Then*

$$\lim_{T\to\infty} \int_0^T \frac{dt}{T} \left| \int \nu(dE)\, e^{\imath tE}\right|^2 \;=\; \sum_{E\in\mathbb{R}} |\nu(\{E\})|^2\;.$$

Proof. Let us begin by evaluating the l.h.s. before the limit:

$$\begin{aligned}\int_0^T \frac{dt}{T} \left| \int \nu(dE)\, e^{\imath tE}\right|^2 \;&=\; \int_0^T \frac{dt}{T} \int \nu(dE) \int \overline{\nu(dE')}\; e^{\imath t(E-E')} \\ &=\; \int \nu(dE) \int \overline{\nu(dE')} \left(\frac{e^{\imath T(E-E')}-1}{\imath(E-E')T}\, \delta_{E\neq E'} + \delta_{E=E'}\right)\;,\end{aligned}$$

where the δ is of Kronecker and not Dirac type. Now the integrand is bounded by 1 and therefore the dominated convergence theorem allows to move the limit inside of the integral. Thus

$$\lim_{T\to\infty} \int_0^T \frac{dt}{T} \left| \int \nu(dE)\, e^{\imath tE}\right|^2 \;=\; \int \nu(dE) \int \overline{\nu(dE')}\, \delta_{E=E'} \;=\; \int \nu(dE)\, \overline{\nu(\{E\})}\;,$$

which implies the result. □

2.3 Lemma *Let H be a self-adjoint operator and ψ,ϕ normalized vectors in Hilbert space. Further let μ be the spectral (probability) measure of ψ and ν the spectral (complex) measure of ψ,ϕ correspondingly, namely*

$$\langle\psi|f(H)|\psi\rangle = \int \mu(dE)\, f(E)\;, \qquad \langle\phi|f(H)|\psi\rangle = \int \nu(dE)\, f(E)\;, \qquad f\in C_0(\mathbb{R})\;. \tag{2.1}$$

Then ν is absolutely continuous w.r.t. μ and the (complex) Radon-Nykodym derivative in $\nu(dE) = g(E)\mu(dE)$ satisfies $g\in L^2(\mu)\cap L^1(\mu)$.

Proof. If P_ψ denotes the orthogonal projection on the cyclic subspace of ψ which by the spectral theorem is isomorphic to $L^2(\mu)$, then $P_\psi|\phi\rangle$ is also in the cyclic subspace and isomorphic to an element $\overline{g}\in L^2(\mu)$. But as by the Cauchy-Schwarz inequality $L^2(\mu)\subset L^1(\mu)$ for any finite measure space, the result follows. Alternatively, for any Borel set $B\subset\mathbb{R}$, the Cauchy-Schwarz inequality implies

$$|\nu(B)| \;=\; |\langle\phi|\chi_B(H)|\psi\rangle| \;\leq\; |\langle\phi|\phi\rangle|^{\frac{1}{2}} |\langle\psi|\chi_B(H)|\psi\rangle|^{\frac{1}{2}} \;=\; \mu(B)^{\frac{1}{2}}\;,$$

where it was used that $\chi_B(H)$ is a projection. Thus ν (more precisely, its real and imaginary parts separately) is absolutely continuous w.r.t. μ and there exists a density $g\in L^1(\mu)$. To prove that g is also in $L^2(\mu)$ requires again the above argument. □

Proof of Theorem 2.1. As the compact operators are norm limits of finite rank operator, it is sufficient to prove the result for finite rank operators. Furthermore, by the triangle inequality one then shows that it is even sufficient to prove the result for a rank one operator $K = |\phi\rangle\langle\phi|$ (it is an exercise to fill in the details). Thus we need to show

$$\lim_{T\to\infty} \int_0^T \frac{dt}{T} \, \left|\langle\phi|e^{-\imath Ht}|\psi\rangle\right|^2 = 0 .$$

But using the spectral measure ν as in (2.1) this becomes

$$\lim_{T\to\infty} \int_0^T \frac{dt}{T} \, \left|\int \nu(dE)\, e^{-\imath Et}\right|^2 = 0 .$$

As ν has no atoms, the Wiener theorem concludes the proof. □

There are two other ways to take time averages which are technically convenient later on. One uses a gaussian cut-off, the other is obtained by averaging with an exponential weight which effectively cuts of the integral at $\frac{1}{2}T$:

$$p^{\mathrm{g}}_T(\phi,\psi) = \frac{1}{(2\pi)^{\frac{1}{2}}T} \int_{\mathbb{R}} dt\; e^{-\frac{t^2}{T^2}}\, |\langle\phi|e^{-\imath tH}|\psi\rangle|^2 , \qquad p^{\mathrm{e}}_T(\phi,\psi) = \frac{2}{T}\int_0^\infty dt\; e^{-\frac{2t}{T}}\, |\langle\phi|e^{-\imath tH}|\psi\rangle|^2 .$$

Using the upper bound $\chi_{[0,T]}(t) \le e\, e^{-\frac{t^2}{T^2}}$ and $(2\pi)^{-\frac{1}{2}}\, e^{-\frac{t^2}{T^2}} \le 2e^{-\frac{t}{T}}$ for $t \ge 0$, one gets

$$p_T(\phi,\psi) \;\le\; e\,(2\pi)^{\frac{1}{2}}\, p^{\mathrm{g}}_T(\phi,\psi) \;\le\; 2\,e\,(2\pi)^{\frac{1}{2}}\, p^{\mathrm{e}}_T(\phi,\psi) .$$

We will see further below that so-called scaling exponent are independent of the choice of time-averaging. The following formula explains why it is convenient to introduce the factor $\frac{1}{2}$ in the exponential average and also why this variant is of the interest in the first place (it is possible to calculated $p^{\mathrm{e}}_T(\phi,\psi)$ from the resolvent of H):

2.4 Lemma *Let H be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$. Then*

$$p^{\mathrm{e}}_T(\phi,\psi) = \frac{1}{\pi\, T}\int_{\mathbb{R}} dE\; \left|\langle\phi|(E+\imath T^{-1}-H)^{-1}|\psi\rangle\right|^2 .$$

Proof. Let ν be the complex spectral measure of H associated to ϕ and ψ. Then

$$\begin{aligned}
p^{\mathrm{e}}_T(\phi,\psi) &= \frac{2}{T}\int_0^\infty dt\; e^{-\frac{2t}{T}} \int \overline{\nu(dE')}\int \nu(dE'')\; e^{\imath t(E'-E'')} \\
&= \frac{2}{T}\int \overline{\nu(dE')}\int \nu(dE'')\; \frac{-1}{2\,T^{-1}-\imath(E'-E'')} \\
&= \frac{2\,\imath}{T}\int \overline{\nu(dE')}\int \nu(dE'')\; \frac{1}{(E''-\imath T^{-1})-(E'+\imath T^{-1})} \\
&= \frac{2\,\imath}{T}\int \overline{\nu(dE')}\int \nu(dE'')\int \frac{dE}{2\pi\imath}\; \frac{1}{E'+\imath T^{-1}-E}\;\frac{1}{E''-\imath T^{-1}-E} ,
\end{aligned}$$

where the last equation follows from a contour integration. Now again using Fubini's theorem and replacing the spectral theorem shows the claim. □

Again a RAGE theorem can be formulated for exponential time averages. Let us directly focus on the return probability in the following proposition.

2.5 Proposition *Let H be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$. If ν denotes the spectral measure of H associated to ϕ and ψ, then one has*

$$\lim_{T\to\infty} p^{\rm e}_T(\phi,\psi) \;=\; \lim_{T\to\infty} p^{\rm g}_T(\phi,\psi) \;=\; \sum_{E\in\mathbb{R}} |\nu(\{E\})|^2 \;.$$

In particular, if ψ is in the continuous subspace $\mathcal{H}_{\rm c} \subset \mathcal{H}$ associated to H, the time-averaged transition probability $p^{\rm e}_T(\phi,\psi)$ vanishes as $T\to\infty$.

Proof. Due to the spectral theorem, one has

$$p^{\rm e}_T(\phi,\psi) \;=\; \frac{2}{T}\int_0^\infty dt\; e^{-\frac{2t}{T}} \int \overline{\nu(dE)} \int \nu(dE')\; e^{\imath t(E-E')} \;=\; \int \overline{\nu(dE)} \int \nu(dE')\; \frac{1}{1+\imath\,\frac{T}{2}\,(E-E')} \;.$$

The integrand is bounded above by 1 and therefore the limit $T\to\infty$ can again be taken into the integral and one can conclude as in the proof of Wiener's theorem. Similarly for the gaussian averages,

$$p^{\rm g}_T(\phi,\psi) \;=\; \frac{1}{(2\pi)^{\frac{1}{2}}T}\int_{\mathbb{R}} dt\; e^{-\frac{t^2}{T^2}} \int \overline{\nu(dE)} \int \nu(dE')\; e^{\imath t(E-E')} \;=\; \int \overline{\nu(dE)} \int \nu(dE')\; e^{-\frac{1}{4}T^2(E-E')^2} \;.$$

Again one can proceed as before. □

The next aim is to get more quantitative information on the decay of transition probabilities. Roughly, one wants to show that continuity properties of the spectral measures implies decay properties of the transition properties. Such continuity properties are typically associated to fractal dimensions of the spectral measure and there is a whole zoology of such dimensions: Hausdorff dimensions, packing dimensions, multifractal dimensions, box-counting dimensions, and so on. A very rough version is the following:

2.6 Definition *Let $\alpha\in\mathbb{R}$. A probability measure μ on $\mathbb{R}$ is said to be uniformly α-continuous if there is a constant C such that for all $E\in\mathbb{R}$ and $\epsilon>0$:*

$$\mu([E-\epsilon,E+\epsilon]) \;\leq\; C\,\epsilon^{\alpha} \;.$$

A measure with Dirac peaks has the minimal regularity $\alpha=0$, which an absolutely continuous measure with a smooth density has $\alpha=1$. In between are the fractal measures. However, if one considers $\mu(dE)=(E^2-1)^{-\frac{1}{2}}\chi_{|E|\leq 1}dE$ (as van Hove singularities at the band edges in dimension 1), then the regularity is only $\alpha=\frac{1}{2}$ even though this results only from the two points $E=\pm1$. Here is a more refined definition:

2.7 Definition *The local spectral exponents of a probability measure μ on $\mathbb{R}$ are defined by*

$$\alpha_\mu(E) \;=\; \liminf_{\epsilon\to 0}\; \frac{\log(\mu([E-\epsilon,E+\epsilon]))}{\log(\epsilon)} \;.$$

The Hausdorff dimension of μ is then

$$\dim_{\rm H}(\mu) \;=\; \mu\text{-}\operatorname*{essinf}_{E\in\mathbb{R}}\; \alpha_\mu(E) \;.$$

Then one can show that to every absolutely continuous measure with an integrable density has Hausdorff dimension 1. In general, for every uniformly α-continuous measure μ one has $\dim_{\rm H}(\mu)\geq\alpha$. Actually the notion of uniform α-continuity is of limit practical use because typically fractal measures have a much larger Hausdorff dimension, but it does allow to derive simple quantitative decay estimates of the transition probability based on the following result from harmonic analysis.

2.8 Theorem (Strichartz 1990) *Let μ be a uniform α-continuous probability measure on $\mathbb{R}$ and let $f \in L^2(\mu)$. Then there is a constant C such that*

$$\int_0^T \frac{dt}{T} \left| \int \mu(dE)\; f(E)\, e^{\imath tE} \right|^2 \;\leq\; C\, T^{-\alpha}\;.$$

The same holds for a gaussian time average.

Proof. Let us begin from

$$\begin{aligned}
\frac{e}{T} \int_{\mathbb{R}} dt\; e^{-\frac{t^2}{T^2}} \left| \int \mu(dE)\; f(E)\, e^{\imath tE} \right|^2 &= \frac{e}{T} \int_{\mathbb{R}} dt\; e^{-\frac{t^2}{T^2}} \int \mu(dE) \int \mu(dE')\; \overline{f(E)}\, f(E')\, e^{\imath t(E-E')} \\
&= e\,(2\pi)^{\frac{1}{2}} \int \mu(dE) \int \mu(dE')\; \overline{f(E)}\, f(E')\, e^{-\frac{1}{4}T^2(E-E')^2} \\
&\leq e\,(2\pi)^{\frac{1}{2}} \int \mu(dE)\, |f(E)|^2 \int \mu(dE')\; e^{-\frac{1}{4}T^2(E-E')^2}\;,
\end{aligned}$$

where in the last step the Cauchy-Schwarz inequality was used. Now using the hypothesis

$$\begin{aligned}
\int \mu(dE')\; e^{-\frac{1}{4}T^2(E-E')^2} &= \sum_{n\geq 0} \int_{\frac{n}{T}\leq|E-E'|<\frac{n+1}{T}} \mu(dE')\; e^{-\frac{1}{4}T^2(E-E')^2} \\
&\leq \sum_{n\geq 0} \int_{\frac{n}{T}\leq|E-E'|<\frac{n+1}{T}} \mu(dE')\; e^{-\frac{1}{4}n^2} \\
&\leq \sum_{n\geq 0} 2\,C\,T^{-\alpha}\; e^{-\frac{1}{4}n^2} \\
&= C'\,T^{-\alpha}\;,
\end{aligned}$$

for some constant C'. Replacing this bound completes the proof. □

Now follows the quantitative version of the RAGE theorem.

2.9 Proposition *Let H be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$. Suppose that the spectral measure μ of H associated to ψ is uniformly α-continuous. Then there is a constant C such that for any ϕ*

$$p^{\rm g}_T(\phi,\psi) \;\leq\; C\,T^{-\alpha}\;.$$

Proof. By Lemma 2.3,

$$p^{\rm g}_T(\phi,\psi) \;=\; \frac{1}{(2\pi)^{\frac{1}{2}}T} \int_{\mathbb{R}} dt\; e^{-\frac{t^2}{T^2}} \left| \int \mu(dE)\; g(E)\, e^{\imath tE} \right|^2\;,$$

with $g \in L^2(\mu)$. Thus the result follows immediately from Strichartz theorem. □

2.2 The diffusion exponents and their basic properties

The RAGE theorem tells us that the particle leaves its initial state when the spectrum is continuous, but it does not tell us where it goes or how far it gets. Of course, in order to address such issues one needs to use the spatial structure of the Hilbert space which is supposed to be $\ell^2(\mathbb{Z}^d)$ in this section. Let us introduce the notations

$$p_T(n,m) \;=\; p_T(|n\rangle, |m\rangle)\;,$$

for the time-averaged probability to pass from site m to n. Note that $(p_T(n,m))_{n\in\mathbb{Z}^d}$ is for each time T and initial site $m\in\mathbb{Z}^d$ a classical probability distribution:

$$\sum_{n\in\mathbb{Z}^d} p_T(n,m) \;=\; \frac{1}{T}\int_0^T dt \sum_{n\in\mathbb{Z}^d} \langle m|e^{\imath Ht}|n\rangle\langle n|e^{-\imath Ht}|m\rangle \;=\; 1\;.$$

As for every classical probability distribution, one can now calcuate the moments of these distributions. For sake of concreteness, let the initial state be localized at the origin:

$$M_q(T) \;=\; \sum_{n\in\mathbb{Z}^d} |n|^q\, p_T(n,0)\;, \qquad q>0\;, \tag{2.2}$$

Now $M_q(T)$ measures the spread of the distribution and it typically grows with a powerlaw in time and the exponent of the powerlaw behavior is then by definition the diffusion exponent. For larger q, the growth is faster so that one should extract a factor q, namely one defines the diffusion exponents β_q roughly by

$$M_q(T) \;\approx\; C_q\, T^{q\beta_q} \qquad \text{as } T\to\infty\;.$$

Some mathematical care is needed to give a precise meaning to the diffusion exponents. Most used in the literature are the upper and lower exponents defined by

$$\beta_{q,+} \;=\; \limsup_{T\to\infty} \frac{\log(M_q(T))}{\log(T^q)}\;, \qquad \beta_{q,-} \;=\; \liminf_{T\to\infty} \frac{\log(M_q(T))}{\log(T^q)}\;,$$

but sometimes it is also technically convenient to work with exponents defined via Mellin transform:

$$\beta_q \;=\; \frac{1}{q}\,\inf\left\{\gamma>0 \;\middle|\; \int_1^\infty dT\, T^{-1-\gamma}\, M_q(T)<\infty\right\}\;,$$

and in this latter case we also write $M_q(T)\sim T^{q\beta_q}$. We shall shortly show that $\beta_q\in[0,1]$, which is why the factor $\frac{1}{q}$ is taken out. Then the following terminology is used:

- If $\beta_q=1$, say for all q, one speaks of ballistic motion.
- If $\beta_q=\frac{1}{2}$, say again for all q, one speaks of diffusive motion.
- If $\beta_q<\frac{1}{2}$ one speaks of subdiffusive motion, for $\beta_q>\frac{1}{2}$ of superdiffusive motion.
- For $\beta_q=0$, the system or Hamiltonian is called localized. As a vanishing diffusion exponent does allow for logarithmically divergent terms (in time), the term dynamical localization is reserved for the situation where

  $$\sup_{T>0} M_q(T) \;\leq\; C \;<\; \infty\;, \qquad q>0\;.$$

  One then speaks of Anderson localization, namely localization of quantum wave packets due to destructive quantum interferences.
- For any other value of the diffusion exponents one speaks of anomalous diffusion (in the framework of classical mechanics also of Levy flights), and if there is, moreover a non-trivial dependence of β_q on q of quantum intermittency.

It is also possible to define local (in energy) diffusion exponents $\beta_q(\Delta)$ by inserting spectral projections $P_\Delta = \chi_\Delta(H)$ on intervals $\Delta \subset \mathbb{R}$:

$$\sum_{n\in\mathbb{Z}^d} \int_0^T \frac{dt}{T}\, |\langle n|e^{-\imath tH} P_\Delta|0\rangle|^2 \;\sim\; T^{q\beta_q(\Delta)} \;.$$

This will not be developed in detail below. We will now first prove a series of general results on diffusion exponents and then come to examples towards the end of this section.

2.10 Proposition *Suppose that $|0\rangle$ is not an eigenvector of H and the matrix elements of H satisfy*

$$|\langle n|H|m\rangle| \;\leq\; C\, e^{-\eta|n-m|} \;,$$

for some positive constants η and C. Then the diffusion exponents satisfy

$$0 \;\leq\; \beta_{q,-} \;\leq\; \beta_q \;\leq\; \beta_{q,+} \;\leq\; 1 \;.$$

The functions $q \in (0,\infty) \mapsto \beta_{q,*}$ are increasing.

Proof. First let us prove $0 \leq \beta_{q,-}$. Using $n^q \geq 1$ for $n \neq 0$, one obtains

$$M_q(T) \;\geq\; \sum_{n\neq 0} p_T(n,0) \;=\; 1 - p_T(0,0) \;.$$

But $p_T(0)$ converges to some number strictly less than 1 by Proposition 2.5 and the hypothesis that $|0\rangle$ is not an eigenvector (note that this does not exclude other point spectrum). Thus $M_q(T)$ is larger than some positive constant and thus $\beta_{q,-} \geq 0$. The proofs for the inequalities $\beta_{q,-} \leq \beta_q \leq \beta_{q,+}$ are elementary and left as an exercise, so let us now focus on the bound $\beta_{q,+} \leq 1$ (this is called a ballistic upper bound). For each $\alpha > 0$ let us define $B_\alpha \subset \ell^2(\mathbb{Z}^d)$ as the set of vectors having finite norm $\|\psi\|_\alpha = \sup_{k\in\mathbb{Z}^d} e^{\alpha|k|}|\langle k|\psi\rangle| < \infty$. Furnished with this norm B_α is actually a Banach space. Let us next show that H is a bounded operator on B_α as long as $\alpha \leq \frac{\eta}{2}$:

$$\begin{aligned}
\|H\psi\|_\alpha &= \sup_{k\in\mathbb{Z}^d} e^{\alpha|k|}|\langle k|H|\psi\rangle| \\
&\leq \sup_{k\in\mathbb{Z}^d} e^{\alpha|k|} \sum_{n\in\mathbb{Z}^d} |\langle k|H|n\rangle|\; |\langle n|\psi\rangle| \\
&\leq \sup_{k\in\mathbb{Z}^d} e^{\alpha|k|} \sum_{n\in\mathbb{Z}^d} C\, e^{-\eta|k-n|}\, \|\psi\|_\alpha\, e^{-\alpha|n|} \\
&\leq \|\psi\|_\alpha\, C \sup_{k\in\mathbb{Z}^d} e^{\alpha|k|} \sum_{n\in\mathbb{Z}^d} e^{-2\alpha|k-n|}\, e^{-\alpha|n|} \\
&\leq \|\psi\|_\alpha\, C \sup_{k\in\mathbb{Z}^d} \sum_{n\in\mathbb{Z}^d} e^{-\alpha|k-n|}
\end{aligned}$$

where in the last step the triangle inequality $|k-n| - |n| + |k| \geq 0$ was used. The sum over n is now finite and thus $\|H\|_\alpha < \infty$. This implies that

$$|\langle n|e^{-\imath Ht}|0\rangle| \;\leq\; e^{-|n|\,\alpha}\, \|e^{-\imath Ht}|0\rangle\|_\alpha \;\leq\; e^{-|n|\,\alpha + t\,\|H\|_\alpha} \;.$$

Thus, for any $\epsilon > 0$,

$$\begin{aligned}\sum_{n\in\mathbb{Z}^d} |n|^q\,|\langle n|e^{-\imath Ht}|0\rangle|^2 \;&\leq\; t^{q(1+\epsilon)} \sum_{|n|\leq t^{1+\epsilon}} |\langle n|e^{-\imath Ht}|0\rangle|^2 \;+\; \sum_{|n|>t^{1+\epsilon}} |n|^q\, e^{-2\,|n|\,\alpha+2\,t\,\|H\|_\alpha} \\ &\leq\; t^{q(1+\epsilon)} \;+\; \sum_{|n|>t^{1+\epsilon}} |n|^q\, e^{-2\,|n|\,\alpha+2\,t\,\|H\|_\alpha}\,.\end{aligned}$$

Now the second summand vanishes in the limit $t \to \infty$. Furthermore, the inequality remains true with exponential time average so that $M_q(T) \leq T^{q(1+\epsilon)} + o(1)$ which implies $\beta_q \leq 1+\epsilon$. As ϵ is arbitrary, the inequality follows.

Now let us come to the fact that the diffusion exponents are increasing in q. Actually, the moments $M_q(T)^{\frac{1}{q}}$ are increasing in q. Indeed, as already pointed out, $p_T = (p_T(n,0))_{n\in\mathbb{Z}^d}$ is a probability measure on $\mathbb{Z}^d$ and $M_q(T) = \mathbf{E}_{p_T}(X^q)$ where X is the position operator on $\mathbb{Z}^d$. Therefore the Hölder inequality implies

$$M_q(T) \;=\; \mathbf{E}_{p_T}(X^q\,1) \;\leq\; \mathbf{E}_{p_T}(X^p)^{\frac{q}{p}}\,\mathbf{E}_{p_T}(1)^{1-\frac{q}{p}} \;=\; M_p(T)^{\frac{q}{p}}\;,$$

so that the claim follows. □

The a priori ballistic upper bound proved above combined with the following lemma shows that one can also use the exponential and gaussian averaged transition probabilities in (2.2) if one is only interested in calculating the diffusion exponents.

2.11 Lemma *Let f be a non-negative measurable function satisfying $f(t) \leq Ct^n$ for some $C > 0$ and $n \geq 0$. Then*

$$\liminf_{T\to\infty} \frac{\log\left(\int_0^T dt\, f(t)\right)}{\log(T)} \;=\; \liminf_{T\to\infty} \frac{\log\left(\int_0^\infty dt\, e^{-t^2/4T^2} f(t)\right)}{\log(T)}\;.$$

Similar equalities hold for $\limsup$ *and other growth exponents, as well as an exponential mean instead of gaussian mean.*

Proof: Let α and β denote the exponents on the left and right hand side respectively. The inequality

$$\int_0^T dt\, f(t) \;\leq\; e^4 \int_0^\infty dt\, e^{-\frac{t^2}{4T^2}} f(t)$$

implies that $\alpha \leq \beta$. On the other hand, we have

$$\begin{aligned}\int_0^\infty dt\, e^{-\frac{t^2}{4T^2}} f(t) \;&\leq\; \int_0^{T^{1+\epsilon}} dt f(t) \,+\, C\int_{T^{1+\epsilon}}^\infty dt\, e^{-\frac{t^2}{4T^2}}\, t^n \\ &\leq\; \int_0^{T^{1+\epsilon}} dt f(t) \,+\, C' e^{-\frac{T^\epsilon}{4}} T^n\,.\end{aligned}$$

This implies that $\beta \leq (1+\epsilon)\alpha$ for any $\epsilon > 0$. The other claims are left as an exercise. □

The following so-called Guarneri bound is the main general (in the sense of model independent) connection there is between diffusion exponents and spectral properties of the Hamiltonian.

2.12 Theorem (Guarneri 1989) *Let H be a Hamiltonian on $\ell^2(\mathbb{Z}^d)$. Suppose that the spectral measure of $|0\rangle$ is uniformly α-continuous. Then*

$$\beta_{q,-} \;\geq\; \frac{\alpha}{d}\;.$$

Proof. Let us work with the gaussian time averages. Then the basic estimates are, for arbitrary N,

$$M_q^{\mathrm{g}}(T) \;\geq\; N^q \sum_{|n|>N} p_T^{\mathrm{g}}(n,0) \;\geq\; N^q \left(1-\sum_{|n|\leq N} p_T^{\mathrm{g}}(n,0)\right) \;\geq\; N^q \left(1-(2N+1)^d \sup_{|n|\leq N} p_T^{\mathrm{g}}(n,0)\right)\;.$$

Now using the hypothesis and Proposition 2.9 one finds

$$M_q^{\mathrm{g}}(T) \;\geq\; N^q \left(1-C\,N^d\,T^{-\alpha}\right) \;=\; \frac{1}{2}\,(2C)^{-\frac{q}{d}}\,T^{q\,\frac{\alpha}{d}}\;,$$

where in the second inequality we chose $N=(\frac{1}{2C}\,T^{\alpha})^{\frac{1}{d}}$. This completes the proof. □

2.13 Remark Theorem 2.12 can be significantly improved to

$$\beta_{q,-} \;\geq \frac{1}{d}\;\dim_{\mathrm{H}}(\mu)\;.$$

Actually this is the bound proved by Guarneri. If furthermore the so-called multifractal dimensions D_q of the spectral measure μ of H associated to $|0\rangle$ are used, another generalization is:

$$\beta_{q,-} \;\geq \frac{1}{d}\,D_{\frac{1}{1+q}}\;, \qquad q>0\;.$$

Also lower bounds on the upper diffusion exponents $\beta_{q,+}$ can be given in terms of packing dimensions. ◇

2.14 Remark The main message of all variants of the Guarneri bound is that continuity properties of the spectral measures (namely, α-continuity) imply diffusion properties of the wave packet spreading, and this in a quantitative way. The bounds imply, in particular:

- In dimension $d=1$ absolutely continuous spectral measures imply ballistic transport.
- In dimension $d=2$ it is possible to have absolutely continuous measures and nevertheless a diffusion motion.
- In dimension $d\geq 3$ one can have a (slow) subdiffusive motion even though the spectral measures are absolutely continuous.
- The Guarneri bound does not exclude non-trivial transport (positive β_q) if the spectral measures are pure point so that the Hausdorff dimension vanishes.

Now let us cite some examples. Each of them needs quite extensive analysis which can be found in the literature, except for the first one which will be studied below:

- For periodic systems (Bloch electrons) the transport is always ballistic.
- There are numerous one-dimensional quasi-periodic and almost periodic models for which one can prove that the transport is anomalous (by proving lower bounds on the Hausdorff dimension of the spectral measures and corresponding upper bounds on the transport).

- There are examples of models with $\lim_{q\to 0}\beta_q = \frac{1}{d}$ and absolutely continuous spectral measures. This means that the Guarneri bound cannot be improved (except with supplementary assumptions).
- There are several models with pure-point spectrum (so that the Hausdorff dimension of the spectral measures vanishes), but $\lim_{q\to\infty}\beta_q = 1$. In these models the Hilbert space is spanned by eigenfunctions of H, but many of these eigenfunctions are very extended.

Finally let us conclude with one of most prominent conjectures in the field Schrödinger operators: in dimension $d \geq 3$ the motion in the Anderson model (Laplacian plus random potential) is expected to be diffusion, namely $\beta_q = \frac{1}{2}$. $\diamond$

3 Existence and basic properties of the wave operators

Let $\mathcal{H}$ be a separable Hilbert space and H_0, V and $H = H_0 + V$ self-adjoint operators on $\mathcal{H}$. We will mainly be interested in two situations:

(i) $\mathcal{H} = L^2(\mathbb{R}^d)$ and $H_0 = -\Delta$, with V a potential, namely a multiplication operator which has a common domain with H_0 given by the Sobolev space. The potential is supposed to fall off at infinity.

(ii) $\mathcal{H} = \ell^2(\mathbb{Z}^d)$ and H_0 is a periodic background operator and V is a local perturbation, *e.g.* a multiplication operator with finite support.

(iii) $\mathcal{H} = \ell^2(\mathbb{Z}^d)$ and H_0 is a periodic background operator and V is a concentrated on a hypersurface and, say, again given by a multiplication operator. This set-up is called surface scattering.

Because V is local, one can expect that for long times (and far away from the support of V) the dynamics of the particle is rather described by H_0 than by H. Hence it is reasonable to assume the following. Suppose that $\psi = \psi(0) \in \mathcal{H}$ is an initial condition which evolves acccoring to the Schrödinger equation as

$$\psi(t) \;=\; e^{-\imath tH}\,\psi\;, \qquad t \in \mathbb{R}\;.$$

Then there exist two initial condition $\phi_\pm \in \mathcal{H}$ such that

$$\lim_{t\to\pm\infty}\; \psi(t) - e^{-\imath tH_0}\phi_\pm \;=\; 0\;,$$

namely using unitary invariance of the norm

$$\lim_{t\to\pm\infty}\; \|\psi(t) - e^{-\imath tH_0}\phi_\pm\| \;=\; \lim_{t\to\pm\infty}\; \|\psi(0) - e^{\imath tH}e^{-\imath tH_0}\phi_\pm\| \;=\; 0\;.$$

Of course, the limit may not exist, but if it does, it defines the wave operator. If ϕ_+ is an eigenvector of H_0, then the limit can only exist if ϕ_+ is also an eigenvector of H with same eigenvalue. Therefore in the definition of the wave operator, one introduces a supplementary projection on the absolutely continuous spectrum of H_0 (which typically is the identity anyway). Again it is possibile and useful to consider general operator pairs $A = H$ and $B = H_0$. For sake of simplicity, we will always assume that A and B are bounded.

3.1 Definition *Let A and B be two self-adjoint operators. Then the generalized wave operators $\Omega_\pm(A,B)$ exist if the strong limits*

$$\Omega_\pm(A,B) \;=\; \operatorname*{s-lim}_{t\to\pm\infty}\; e^{\imath tA}e^{-\imath tB}\,P_{\mathrm{ac}}(B)\;.$$

In many application, $B = H_0$ has purely absolutely continuous spectrum so that $P_{\mathrm{ac}}(B) = \mathbf{1}$.

3.2 Theorem (Cook's method 1957) *Suppose suppose that there are dense subsets $\mathcal{D}_\pm \subset P_{\mathrm{ac}}(B)\mathcal{H}$ such that for $\phi \in \mathcal{D}_\pm$ there is some $T_0 > 0$ with*

$$\int_{T_0}^{\infty} dt \; \|(B - A)e^{\mp\imath tB}\phi\| \; < \; \infty \; .$$

Then $\Omega_\pm(A, B)$ exists.

Proof. Let us introduce the unitary $W(t) = e^{\imath tA}e^{-\imath tB}$. Note that in general this is not a one-parameter group. Then

$$\partial_t W(t) \;=\; \imath \, e^{\imath tA}(A - B)e^{-\imath tB} \; ,$$

and thus for $t \geq s$

$$W(t) - W(s) \;=\; \int_s^t du \; \partial_u W(u) \;=\; \int_s^t du \; \imath \, e^{\imath uA}(A - B)e^{-\imath uB} \; . \tag{3.1}$$

Therefore, for $\phi \in \mathcal{D}_+$,

$$\begin{aligned} \|(W(t) - W(s))\phi\| \;&\leq\; \int_s^t du \; \|e^{\imath uA}(A - B)e^{-\imath uB}\phi\| \\ &=\; \int_s^t du \; \|(A - B)e^{-\imath uB}\phi\| \; . \end{aligned}$$

By the integrability assumption this goes to 0 as $s \to \infty$. Consequently $t \mapsto W(t)\phi$ has the Cauchy property for $t \to \infty$ and therefore the limit

$$\lim_{t\to\infty} e^{\imath tA}e^{-\imath tB} \, P_{\mathrm{ac}}(B)\phi$$

exists. By a 3ϵ-argument it exists for all $\phi \in P_{\mathrm{ac}}(B)\mathcal{H}$ (because $e^{\imath tA}e^{-\imath tB} \, P_{\mathrm{ac}}(B)$ is uniformly bounded in t). For $\phi \in (P_{\mathrm{ac}}(B)\mathcal{H})^\perp$ it exists trivially. Hence the existence of $\Omega_+(A, B)$ is shown. □

3.3 Theorem (Kato 1957, Rosenblum 1957) *Let A and B be two bounded self-adjoint operators such that $A - B$ is traceclass. Then $\Omega_\pm(A, B)$ exist.*

The result also holds for unbounded self-adjoint operators, basically with the same proof. The argument presented here [RS] goes back to Pearson (1978). Let us focus on $\Omega_+(A, B)$ as obviously $\Omega_-(A, B) = \Omega_+(-A, -B)$. By Cook's method it is sufficient to show

$$\lim_{t\to\infty} \; \sup_{s>t} \; \|(W(t) - W(s))\phi\| \;=\; 0 \tag{3.2}$$

for a dense set $\mathcal{D}$ of ϕ's where again $W(t) = e^{\imath tA}e^{-\imath tB}$. Here we choose

$$\mathcal{D} \;=\; \left\{\phi \in P_{\mathrm{ac}}(B) \mid \mu_\phi(dE) = |f(E)|^2 dE \;\text{ with } f \in L^\infty(\mathbb{R})\right\} \; ,$$

where μ_ϕ denotes the spectral measure of B w.r.t. ϕ, satisfying

$$\langle\phi|g(B)\phi\rangle \;=\; \int \mu_\phi(dE) \; g(E) \; , \qquad g \in C_0(\mathbb{R}) \; .$$

For $\phi \in \mathcal{D}$ let us set $|\!|\!|\phi|\!|\!| = \|f\|_\infty$. Then the following estimate holds.

3.4 Lemma *For $\phi \in \mathcal{D}$ and any $\psi \in \mathcal{H}$,*

$$\int_{\mathbb{R}} dt \; |\langle \psi | e^{-\imath t B} \phi \rangle|^2 \;\leq\; 2\pi \, \|\psi\|^2 \, \|\!|\phi|\!\|^2 \; .$$

Proof. Let Q be the projection on the cyclic subspace of ϕ w.r.t. B. By the spectral theorem

$$\langle \psi | e^{-\imath t B} \phi \rangle \;=\; \langle Q\psi | e^{-\imath t B} \phi \rangle \;=\; \int dE \, |f(E)|^2 \, \eta(E) \, e^{-\imath t E} \; , \tag{3.3}$$

where η is a function representing $Q\psi$. It satisfies

$$\int dE \; |\eta(E)|^2 \; |f(E)|^2 \;=\; \langle Q\psi | Q\psi \rangle \;=\; \|Q\psi\|^2 \;\leq\; \|\psi\|^2 \; .$$

Thus $|f(E)|^2 \, \eta(E)$ is in $L^2(\mathbb{R})$ and therefore $\langle \psi | e^{-\imath t B} \phi \rangle$ is its Fourier transform. By the Plancharel theorem, it follows that

$$\int_{\mathbb{R}} dt \; |\langle \psi | e^{-\imath t B} \phi \rangle|^2 \;=\; 2\pi \int dE \; |\eta(E)|^2 \; |f(E)|^4 \; .$$

Using $|f(E)|^4 \leq \|\!|\phi|\!\|^2 |f(E)|^2$ and the above, the bound follows. □

3.5 Lemma *For $\phi \in P_{\mathrm{ac}}(B)\mathcal{H}$ and any $\psi \in \mathcal{H}$,*

$$\lim_{t\to\infty} \langle \psi | e^{-\imath t B} \phi \rangle \;=\; 0 \; ,$$

and for any compact operator K

$$\lim_{t\to\infty} \|K e^{-\imath t B} \phi\| \;=\; 0 \; .$$

Proof. Let us look at (3.3). Choosing $t = 0$ one sees that $E \mapsto |f(E)|^2 \, \eta(E)$ is in $L^1(\mathbb{R})$ and therefore the Riemann-Lebesgue lemma shows the first claim. The second follows by a 3ϵ-argument using that every compact operator can be approximated in norm by a finite rank operator. □

Proof of Theroem 3.3. Let us start from

$$\begin{aligned} \|(W(t) - W(s))\phi\|^2 \;&=\; \langle \phi | W(t)^*(W(t) - W(s))\phi \rangle \;-\; \langle \phi | W(s)^*(W(t) - W(s))\phi \rangle \\ &=\; \langle \phi | (\mathbf{1} - W(t)^* W(s))\phi \rangle \;+\; \langle \phi | (\mathbf{1} - W(s)^* W(t))\phi \rangle \; . \end{aligned} \tag{3.4}$$

Let us focus on the first summand on the r.h.s.. The hypothesis and (3.1) imply that $W(t) - W(s)$ is compact. Therefore by Lemma 3.5

$$\lim_{a\to\infty} e^{\imath a B} W(t)^*(W(t) - W(s)) e^{-\imath a B} \phi \;=\; 0 \; ,$$

that is

$$\phi \;=\; \lim_{a\to\infty} e^{\imath a B} W(t)^* W(s) e^{-\imath a B} \phi \; .$$

Hence

$$\begin{aligned} \langle \phi | (\mathbf{1} - W(t)^* W(s))\phi \rangle \;&=\; \lim_{a\to\infty} \langle \phi | \big(e^{\imath a B} W(t)^* W(s) e^{-\imath a B} - W(t)^* W(s) \big) \phi \rangle \\ &=\; \lim_{a\to\infty} \int_0^a db \; \langle \phi | \partial_b (e^{\imath b B} W(t)^* W(s) e^{-\imath b B}) \phi \rangle \; . \end{aligned}$$

With $K = A - B$ one now finds

$$\begin{aligned}\partial_b(e^{\imath bB}W(t)^*W(s)e^{-\imath bB}) &= \imath\, Be^{\imath bB}e^{\imath tB}e^{-\imath tA}e^{\imath sA}e^{-\imath sB}e^{-\imath bB} - \imath\, e^{\imath bB}e^{\imath tB}e^{-\imath tA}e^{\imath sA}e^{-\imath sB}e^{-\imath bB}B \\ &= \imath\, e^{\imath(b+t)B}[B, e^{\imath(s-t)A}]e^{-\imath(s+b)B} \\ &= -\imath\, e^{\imath(b+t)B}[K, e^{\imath(s-t)A}]e^{-\imath(s+b)B} \;.\end{aligned}$$

It follows that

$$\begin{aligned}\langle\phi|(\mathbf{1} - W(t)^*W(s))\phi\rangle &= \lim_{a\to\infty} -\imath \int_0^a db\; \langle\phi|e^{\imath(b+t)B}[K, e^{\imath(s-t)A}]e^{-\imath(s+b)B}\phi\rangle \\ &= \lim_{a\to\infty} -\imath \int_t^{t+a} db\; \langle\phi|e^{\imath bB}Ke^{\imath(s-t)A}e^{\imath(t-s)B}e^{-\imath bB}\phi\rangle \\ &\quad + \lim_{a\to\infty} \imath \int_s^{s+a} db\; \langle\phi|e^{\imath bB}e^{-\imath(s-t)B}e^{\imath(s-t)A}Ke^{-\imath bB}\phi\rangle \\ &= \lim_{a\to\infty} -\imath \int_t^{t+a} db\; \langle\phi|e^{\imath bB}KW(s-t)e^{-\imath bB}\phi\rangle \\ &\quad + \lim_{a\to\infty} \imath \int_s^{s+a} db\; \langle\phi|e^{\imath bB}W(s-t)^*Ke^{-\imath bB}\phi\rangle \;.\end{aligned}$$

Next let us write out the trace class operator using two orthonormal basis $(\phi_n)_{n\geq 1}$ and $(\psi_n)_{n\geq 1}$

$$K \;=\; \sum_{n\geq 1} \lambda_n\, |\phi_n\rangle\langle\psi_n| \;,$$

where $(\lambda_n)_{n\geq 1}$ are the (positive) singular values and $\sum_{n\geq 1}\lambda_n < \infty$. Now we can bound one of the terms above using the Cauchy-Schwarz inequality:

$$\begin{aligned}\left|\int_t^{t+a} db\; \langle\phi|e^{\imath bB}KW(s-t)e^{-\imath bB}\phi\rangle\right| &= \left|\sum_{n\geq 1}\lambda_n \int_t^{t+a} db\; \langle\phi|e^{\imath bB}\phi_n\rangle\langle\psi_n|W(s-t)e^{-\imath bB}\phi\rangle\right| \\ &\leq \left|\sum_{n\geq 1}\lambda_n \int_t^{t+a} db\; |\langle\phi|e^{\imath bB}\phi_n\rangle|^2\right|^{\frac{1}{2}} \cdot \\ &\qquad \left|\sum_{n\geq 1}\lambda_n \int_t^{t+a} db\; |\langle\psi_n|W(s-t)e^{-\imath bB}\phi\rangle|^2\right|^{\frac{1}{2}} \\ &\leq \left|\int_t^{\infty} db\; \sum_{n\geq 1}\lambda_n\, |\langle\phi_n|e^{-\imath bB}\phi\rangle|^2\right|^{\frac{1}{2}} \cdot \left(2\pi\, \|K\|_1 \|\phi\|^2\right)^{\frac{1}{2}} \\ &\leq 2\pi\, \|K\|_1 \|\phi\|^2 \;,\end{aligned}$$

where in the last two steps Lemma 3.4 was used. Thus the integral over b is bounded uniformly in t and hence has to converge to 0 as $t \to \infty$. All this applies to both contributions in $\langle\phi|(\mathbf{1} - W(t)^*W(s))\phi\rangle$ and, using the first identity (3.4) of the proof, also to

$$\|(W(t) - W(s))\phi\|^2 \;\leq\; 4\, \left(2\pi\, \|K\|_1 \|\phi\|^2\right)^{\frac{1}{2}} \left|\int_{\min\{s,t\}}^{\infty} db\; \sum_{n\geq 1}\lambda_n\, |\langle\phi_n|e^{-\imath bB}\phi\rangle|^2\right|^{\frac{1}{2}} \;. \qquad (3.5)$$

In particular, $\|(W(t) - W(s))\phi\|^2$ converges to 0 as $t \to \infty$ and $s \to \infty$, namely the Cook criterium (3.2) is satisfied. □

3.6 Proposition *Let A and B be bounded operators such that the wave operators exist. Then the intertwining property*

$$f(A)\,\Omega_\pm(A,B) \;=\; \Omega_\pm(A,B)\,f(B)\;,$$

holds for every measurable function f.

Proof. From the definition, one has for all $s\in\mathbb{R}$

$$\begin{aligned}\Omega_\pm(A,B) &= \operatorname*{s-lim}_{t\to\pm\infty} e^{\imath tA}e^{-\imath tB}\,P_{\rm ac}(B)\\ &= \operatorname*{s-lim}_{t\to\pm\infty} e^{\imath(t+s)A}e^{-\imath(t+s)B}\,P_{\rm ac}(B)\\ &= e^{\imath sA}\,\Omega_\pm(A,B)\,e^{-\imath sB}\;,\end{aligned}$$

namely

$$e^{-\imath sA}\,\Omega_\pm(A,B) \;=\; \Omega_\pm(A,B)\,e^{-\imath sB}\;.$$

Now taking a Fourier transform or arguing by density shows the intertwining property. □

3.7 Definition *Let A and B be self-adjoint operators such that the generalized wave operators $\Omega_\pm(A,B)$ exist. Then*

(i) $\mathcal{H}_-=\Omega_-(A,B)\,\mathcal{H}$ is called the set of incoming asymptotic states.

(ii) $\mathcal{H}_+=\Omega_+(A,B)\,\mathcal{H}$ is called the set of outgoing asymptotic states.

3.8 Proposition *Let A and B be bounded operators such that the wave operators $\Omega_\pm(A,B)$ exist.*

(i) $\Omega_\pm(A,B)$ are partial isometries from $P_{\rm ac}(B)\mathcal{H}$ to $\mathcal{H}_\pm$.

(ii) $\mathcal{H}_\pm\subset P_{\rm ac}(A)\mathcal{H}$

(iii) $\sigma_{\rm ac}(B)\subset\sigma_{\rm ac}(A)$

(iv) If C is another operator such that $\Omega_\pm(B,C)$ exist, then $\Omega_\pm(A,C)$ exist and the concatenation property holds:

$$\Omega_\pm(A,C) \;=\; \Omega_\pm(A,B)\,\Omega_\pm(B,C)\;.$$

Proof. (i) For $\psi\in P_{\rm ac}(B)\mathcal{H}$, one has

$$\|\Omega_\pm(A,B)\psi\| \;=\; \lim_{t\to\pm\infty}\|W(t)\psi\| \;=\; \|\psi\|\;,$$

which is already claim (i). For (ii), let us note that the intertwining property shows that $A|_{\mathcal{H}_\pm}$ is unitarily equivalent to $B|_{P_{\rm ac}(B)\mathcal{H}}$ with unitary equivalence given by $\Omega_\pm(A,B)\,:\,P_{\rm ac}(B)\mathcal{H}\to\mathcal{H}_\pm$. As $B|_{P_{\rm ac}(B)\mathcal{H}}$ has only absolutely continuous spectrum by definition, so does $A|_{\mathcal{H}_\pm}$. This also implies (iii). (iv) By (ii) $\Omega_\pm(B,C)\mathcal{H}\subset P_{\rm ac}(B)\mathcal{H}$ so that for all $\psi\in\mathcal{H}$

$$\lim_{t\to\pm\infty}\|(\mathbf{1}-P_{\rm ac}(B))e^{\imath tB}e^{-\imath tC}P_{\rm ac}(C)\psi\| \;=\; 0\;.$$

Thus taking the strong limits of

$$e^{\imath tA}e^{-\imath tC}P_{\rm ac}(C) \;=\; e^{\imath tA}e^{-\imath tB}P_{\rm ac}(B)e^{\imath tB}e^{-\imath tC}P_{\rm ac}(C) \;+\; e^{\imath tA}e^{-\imath tB}(\mathbf{1}-P_{\rm ac}(B))e^{\imath tB}e^{-\imath tC}P_{\rm ac}(C)$$

and using the fact that the strong limit of a product is the product of the strong limits shows the claim. □

3.9 Definition *Let A and B be self-adjoint operators such that the generalized wave operators $\Omega_\pm(A,B)$ exist. Then*

(i) The wave operators are said to be complete if

$$\mathcal{H}_+ \;=\; \mathcal{H}_- \;=\; P_{\text{ac}}(A)\mathcal{H}\;.$$

(ii) The wave operators are said to be asymptotically complete if

$$\mathcal{H}_+ \;=\; \mathcal{H}_- \;=\; (P_{\text{pp}}(A)\mathcal{H})^\perp\;,$$

or, equivalently, if the wave operators are complete and $\sigma_{\text{sc}}(A)=\emptyset$.

(iii) The scattering operator $S=S(A,B)$ is defined as

$$S \;=\; \Omega_+(A,B)^*\,\Omega_-(A,B)\;.$$

3.10 Proposition *Let A and B be bounded operators such that the wave operators $\Omega_\pm(A,B)$ exist. Then they are complete if and only if $\Omega_\pm(B,A)$ exists. Moreover, completess implies $\sigma_{\text{ac}}(B)=\sigma_{\text{ac}}(A)$.*

Proof. "$\Rightarrow$" Let $\phi\in P_{\text{ac}}(A)\mathcal{H}$. There there exist $\psi_\pm\in P_{\text{ac}}(B)\mathcal{H}$ with $\phi=\Omega_\pm(A,B)\psi_\pm$. Hence

$$\begin{aligned} 0 \;&=\; \|\Omega_\pm(A,B)\psi_\pm-\phi\| \\ &=\; \lim_{t\to\pm\infty}\|e^{\imath tA}e^{-\imath tB}\psi_\pm - P_{\text{ac}}(A)\phi\| \\ &=\; \lim_{t\to\pm\infty}\|\psi_\pm - e^{\imath tB}e^{-\imath tA}P_{\text{ac}}(A)\phi\| \end{aligned}$$

namely $\Omega_\pm(B,A)\phi$ exists. On the orthogonal complement of $P_{\text{ac}}\mathcal{H}$ nothing has to be shown. "$\Leftarrow$" By hypothesis and the concatenation property,

$$\Omega_\pm(A,B)\,\Omega_\pm(B,A) \;=\; \Omega_\pm(A,A) \;=\; P_{\text{ac}}(A)\;.$$

In particular, $P_{\text{ac}}(A)\mathcal{H}\subset\Omega_\pm(A,B)\mathcal{H}$. The other inclusion was already proved in Proposition 3.8(ii). The last claim now follows from Proposition 3.8(iii). □

3.11 Proposition *The scattering operator $S=S(A,B)$ satisfies*

$$f(B)\,S \;=\; S\,f(B)\;.$$

If the wave operators $\Omega_\pm(A,B)$ exist and are complete and $\sigma(B)=\sigma_{\text{ac}}(B)$, then S is a unitary operator.

Proof. The first fact follows from the interlacing property, applied twice. The second claim from Proposition 3.8(i). □

4 Invariance principle

4.1 Definition *Let $T\subset\mathbb{R}$ be open and decomposed into a finite union $T=\bigcup_{n=1}^N I_n$ of open intervals. A twice differentiable function $\varphi:T\to\mathbb{R}$ is called admissable if*

(i) on each I_n is φ' either strictly positive or strictly negative and

(ii) the second derivative φ'' is integrable on each compact I_n.

4.2 Theorem (Birman's invariance principle 1962) *Let A and B be self-adjoint operators such that $A-B$ is trace class. Suppose that $\varphi : T = \bigcup_{n=1}^N I_n \to \mathbb{R}$ is an admissable function such that $\sigma(A) \subset \overline{T}$ and $\sigma(B) \subset \overline{T}$ and that each boundary point $E_c \in \partial T$ either φ has a finite limit or A and B have no eigenvalue at E_c. Then $\Omega_\pm(\varphi(A), \varphi(B))$ exists and is complete, and is given by*

$$\Omega_\pm(\varphi(A), \varphi(B)) \;=\; \Omega_\pm(A,B)\, P_B(T_+) \;-\; \Omega_\mp(A,B)\, P_B(T_-)\;,$$

where $(P_B(\Omega))_{\Omega\in\mathcal{B}(\mathbb{R})}$ is the projection valued spectral measure of B, and T_+ and T_- are the sets where $\varphi' > 0$ and $\varphi' < 0$ respectively.

4.3 Lemma *Let $\varphi : T = \bigcup_{n=1}^N I_n \to \mathbb{R}$ be admissable and $\sigma_n \in \{-1, 1\}$ be the sign of φ' on I_n. Then for $w \in L^2(I_n)$*

$$\lim_{s\to\sigma_n\infty} \int_0^\infty dt \left| \int dE\; e^{-\imath(tE+s\varphi(E))}\, w(E)\right|^2 \;=\; 0\;. \tag{4.1}$$

Proof. The function $E \in \mathbb{R} \mapsto e^{-\imath s\varphi(E)}\, w(E)$ is in $L^2(\mathbb{R})$ and $\int dE\;\; e^{-\imath(tE+s\varphi(E))}\, w(E)$ is its Fourier transform. Thus by the Plancharel theorem

$$\int_{\mathbb{R}} dt \left| \int dE\; e^{-\imath(tE+s\varphi(E))}\, w(E)\right|^2 \;=\; 2\pi \int dE\; |e^{-\imath s\varphi(E)}\, w(E)|^2 \;=\; 2\pi\, \|w\|_2^2\;.$$

In particular, the l.h.s. (4.1) is bounded by $2\pi\,\|w\|_2^2$ and therefore it is possible to approximate w by a dense set of functions (in the L^2-norm). This set is chosen to be the span of the indicator functions. Hence it is sufficient to show (4.1) for $w = \chi_{[a,b]}$ with $[a,b] \subset I$. Suppose that

$$\lambda \;=\; \inf_{E\in[a,b]} \;\varphi'(E) \;>\; 0\;.$$

Let us now use the identity

$$e^{-\imath(tE+s\varphi(E))} \;=\; \frac{\imath}{t + s\varphi'(E)}\; \partial_E e^{-\imath(tE+s\varphi(E))}\;.$$

Then for $t > 0$ and $s > 0$, an integration by parts shows

$$\begin{aligned}
\left| \int_a^b dE\; e^{-\imath(tE+s\varphi(E))}\right| \;&=\; \left| \int_a^b dE\; \frac{\imath}{t+s\varphi'(E)}\; \partial_E e^{-\imath(tE+s\varphi(E))}\right| \\
&\leq\; \frac{1}{t+s\varphi'(b)} \;+\; \frac{1}{t+s\varphi'(a)} \;+\; \left| \int_a^b dE\; \frac{s\varphi''(E)}{(t+s\varphi'(E))^2}\; e^{-\imath(tE+s\varphi(E))}\right| \\
&\leq\; \frac{1}{t+s\varphi'(b)} \;+\; \frac{1}{t+s\varphi'(a)} \;+\; \frac{s}{(t+s\lambda)^2} \int_a^b dE\; |\varphi''(E)|\;.
\end{aligned}$$

The last integral is uniformly bounded by hypothesis. Therefore all three summands are in $L^2(\mathbb{R}_{\geq 0})$ in the variable t, with an L^2-norm that converges to 0 as $s \to \infty$. □

Proof of Theorem 4.2. The notations and results of Theorem 3.3 will be used. Let us set $\mathcal{D}' = \mathcal{D}\cap P_B(I_n)\mathcal{H}$. This is a dense subset in $P_B(I_n)\mathcal{H}$, and recall that all vectors have absolutely continuous spectral measure. For $\psi \in \mathcal{D}'$ let us write out (3.5) with $s = 0$ for the vector $\phi = e^{-\imath\varphi(B)s}\psi$ (with a different new s):

$$\|(W(t) - \mathbf{1})e^{-\imath\varphi(B)s}\psi\|^2 \;\leq\; C \left| \int_0^\infty db\; \sum_{n\geq 1} \lambda_n\, |\langle \phi_n | e^{-\imath(bB+\varphi(B)s)}\psi\rangle|^2 \right|^{\frac{1}{2}}\;.$$

As $W(t)$ converges strongly to the wave operator $\Omega_+(A,B)$ as $t\to\infty$, one gets

$$\|(\Omega_+(A,B)-\mathbf{1})e^{-\imath\varphi(B)s}\psi\|^2 \;\leq\; C\;\left|\sum_{n\geq 1}\lambda_n\int_0^\infty db\;|\langle\phi_n|e^{-\imath(bB+\varphi(B)s)}\psi\rangle|^2\right|^{\frac{1}{2}}\;.$$

Each integral on the r.h.s. converges to 0 in the limit $s\to\sigma_n\infty$ by Lemma 4.3. Moreover, by Lemma 3.4 each summand on the r.h.s. can be bounded uniformly in s showing

$$\|(\Omega_+(A,B)-\mathbf{1})e^{-\imath\varphi(B)s}\psi\|^2 \;\leq\; C\;\left|\sum_{n\geq 1}\lambda_n\,2\pi\,\|e^{\imath\varphi(B)s}\phi_n\|^2\,|\!|\!|\psi|\!|\!|^2\right|^{\frac{1}{2}}\;\leq\;C'\;.$$

Consequently

$$\lim_{s\to\sigma_n\infty}\;\|(\Omega_+(A,B)-\mathbf{1})e^{-\imath\varphi(B)s}\psi\|\;=\;0\;.$$

By the intertwining property

$$e^{\imath\varphi(A)s}\,\Omega_\pm(A,B)\;=\;\Omega_\pm(A,B)\,e^{\imath\varphi(B)s}\;,$$

one concludes

$$\lim_{s\to\sigma_n\infty}\;\|(\Omega_+(A,B)\;-\;e^{\imath\varphi(A)s}\,e^{-\imath\varphi(B)s})\psi\|\;=\;0\;,$$

namely

$$\Omega_+(A,B)\;=\;\Omega_{\sigma_n}(\varphi(A),\varphi(B))\;,\qquad\text{on }P_B(I_n)\mathcal{H}\;.$$

This leads to the formula stated in the theorem. The proof of completeness is left as an exercise. □

5 Lattice scattering by a perturbation of finite support

The purpose of this section is to develop the full arsenal of scattering theory for a quantum particle described by a tight-binding Hamiltonian

$$H\;=\;H_0+V\;\;:\ell^2(\mathbb{Z}^d)\to\ell^2(\mathbb{Z}^d)\;,$$

where H_0 is a translation invariant operator with a single band and V is a finite rank perturbation supported by a finite subset $\Lambda\subset\mathbb{Z}^d$. A typical example for a local perturbation is a potential with support Λ, namely $V=\sum_{n\in\Lambda}v_n\,|n\rangle\langle n|$ with $v_n\in\mathbb{R}\backslash\{0\}$. The presentation follows [BS], but leaves out the technicalities linked to threshold eigenvalues.

5.1 Analysis of the free operator

The translation invariance of the free operator H_0 implies that it is of the form

$$H_0\;=\;\sum_{n,m\in\mathbb{Z}^d}\mathcal{E}_{n-m}\,|n\rangle\langle m|\;.$$

Self-adjointness of H_0 implies $\mathcal{E}_{-n}=\overline{\mathcal{E}_n}$. It is supposed that the coefficients $\mathcal{E}_n$ decay rapidly in $\mathcal{E}$ such that

$$\mathcal{E}(k)\;=\;\sum_{n\in\mathbb{Z}^d}e^{\imath kn}\mathcal{E}_n$$

is a real analytic function on the d-dimensional torus $\mathbb{T}^d = \mathbb{R}^d/(2\pi\mathbb{Z}^d)$. This function is the spectral representation of H_0. More precisely, H_0 is diagonalized by the discrete Fourier transform $\mathcal{F} : \ell^2(\mathbb{Z}^d) \to L^2(\mathbb{T}^d)$, where $L^2(\mathbb{T}^d)$ is the Hilbert space of square integrable functions on $\mathbb{T}^d$. It is densely defined by

$$(\mathcal{F}\phi)(k) \;=\; \frac{1}{(2\pi)^{\frac{d}{2}}} \sum_{n\in\mathbb{Z}^d} e^{\imath kn} \,\langle n|\phi\rangle \;.$$

and is unitary. Now $\mathcal{F}H_0\mathcal{F}^*$ =mult$(k \mapsto \mathcal{E}(k)$ is a multiplication operator on $L^2(\mathbb{T}^d)$. Hence we restrict ourselves to a free operator with a single band.

Hypothesis: $\mathcal{E}$ is a real analytic Morse function $\mathcal{E}(k)$ having only one maximum $\mathcal{E}_+$ and one minimum $\mathcal{E}_-$.

A Morse function has by definition only a finite number of critical points $\mathcal{S}^* \subset \mathbb{T}^d$ which are non-degenerate in the sense that the Hessian $\mathcal{E}''(k^*)$ for each $k^* \in \mathcal{S}^*$ is a real symmetric invertible $d \times d$ matrix. The two critical points k^*_- and k^*_+ corresponding to the minimal and maximal values $E_- = \mathcal{E}(k^*_-)$ and $E_+ = \mathcal{E}(k^*_+)$ of $\mathcal{E}$ are the only ones of definite signature. Due to the hypothesis all other critical points $k^* \in \mathcal{S}^*$ have critical values $\mathcal{E}(k^*)$ in (E_-, E_+) and are of indefinite signature. A typical example is the discrete Laplacian

$$H_0 \;=\; \sum_{n\in\mathbb{Z}^d} \sum_{|e|=1} |n-e\rangle\langle n| \;,$$

for which $\mathcal{E}(k) = \sum_{i=1}^d 2\,\cos(k_i)$, and translation invariant perturbations of it.

Let $F : [E_-, E_+] \to \mathbb{R}_{\geq 0}$ be given by

$$F(E) \;=\; 2\,\frac{(E-E_-)(E_+-E)}{E_+-E_-}\;. \tag{5.1}$$

Then let $\widehat{X}$ be the vector field on $\mathbb{T}^d$ defined by

$$\widehat{X}(k) \;=\; F\big(\mathcal{E}(k)\big)\,\frac{\nabla\mathcal{E}(k)}{|\nabla\mathcal{E}(k)|^2}\;, \qquad k \in \mathbb{T}^d\;. \tag{5.2}$$

Apart from the factor $F \circ \mathcal{E}$, the vector field $\widehat{X}$ is precisely the one used in the standard argument of Morse theory [Nic] as well as in the proof of the coarea formula [Sak]. As $\mathcal{E}$ and F are smooth, this vector field is smooth away from the set $\mathcal{S}^*$ of critical points. At the critical points $k^*_\pm$ with extremal energy $\mathcal{E}(k^*_\pm) = E_\pm$, the function $k \mapsto F(\mathcal{E}(k^*_\pm + k))$ vanishes linearly and hence the vector field has a source or a sink there. At all other critical points with critical values lying inside the band $[E_-, E_+]$, the vector field $\widehat{X}$ has a singularity which has to be dealt with below. Let $\theta_b : \mathbb{T}^d \setminus \mathcal{S}^* \to \mathbb{T}^d$ be the flow of $\widehat{X}$, that is,

$$\partial_b\theta_b \;=\; \widehat{X}\circ\theta_b\;, \qquad \theta_0 \;=\; \text{id}\;. \tag{5.3}$$

The flow θ_b is not complete because an orbit can reach one of the critical points with indefinite signature in a finite time. Choosing orbits which stay away from these critical points or times which are sufficiently small, one can calculate the flow of energy along the orbits. By the definition of the vector field $\widehat{X}$,

$$\partial_b\,\mathcal{E}(\theta_b(k)) \;=\; F(\mathcal{E}(\theta_b(k)))\;.$$

This equation shows that the flow θ_b maps constant energy surfaces to constant energy surfaces. Moreover, the energy flow is governed by a simple ordinary differential equation of first order which can be integrated. Choosing some reference energy $E_r \in (E_-, E_+)$, it leads to the following invertible function

$$f(E) \;=\; \int_{E_r}^{E} \frac{de}{F(e)}\,. \tag{5.4}$$

Then $b = f(\mathcal{E}(\theta_b(k))) - f(\mathcal{E}(k))$ and

$$\mathcal{E}(\theta_b(k)) \;=\; f^{-1}\big(b + f(\mathcal{E}(k))\big)\,. \tag{5.5}$$

If $E_r = (E_+ + E_-)/2$, integration gives

$$f(E) \;=\; \frac{1}{2}\ln\left(\frac{E-E_-}{E_+-E}\right)\,, \qquad f^{-1}(b) \;=\; E_r + \Delta\,\tanh(b)\,, \qquad F(f^{-1}(b)) \;=\; \frac{\Delta}{\cosh^2(b)}\,, \tag{5.6}$$

where $\Delta = (E_+ - E_-)/2$. By restricting θ_b to an adequate subset of $\mathbb{T}^d$, a complete flow can be constructed. Let $\mathcal{S}$ be the union of $\mathcal{S}^*$ and of the set of points reaching one of the critical points $k^* \in \mathcal{S}^*$ in finite time (either positive or negative). It is important to remark that, under this flow, almost all points reach the maximum and the minimum eventually, but it takes an infinite time to do so. Therefore the finite time condition is a strong constraint. In fact, $\mathcal{S}$ is the union of $\mathcal{S}^*$ and the stable and unstable manifolds of all critical points of indefinite signature.

5.1 Proposition *The set $\mathcal{S}$ is compact and has zero Lebesgue measure. The flow $\theta_b : \mathbb{T}^d \setminus \mathcal{S} \to \mathbb{T}^d \setminus \mathcal{S}$ is defined for all $b \in \mathbb{R}$, that is, $\widehat{X}$ is complete on $\mathbb{T}^d \setminus \mathcal{S}$. In addition, $\lim_{b\to\pm\infty} \theta_b(k) = k^*_\pm$ for all $k \in \mathbb{T}^d \setminus \mathcal{S}$. Furthermore, for any open neighborhood U of $\mathcal{S}$ there exists an open subset $V \subset U$ which contains $\mathcal{S} \setminus \{k^*_-, k^*_+\}$ and is invariant under the flow θ.*

Sketch of a proof. The vector field $\widehat{X}$ is gradient-like in the terminology of [Nic] (it is actually a gradient vector field). Hence [Nic, Section 2.4] shows that $\lim_{b\to\pm\infty} \theta_b(k) \in \mathcal{S}^*$ and that the stable and unstable manifolds of all critical points of indefinite signature are locally smooth submanifolds of $\mathbb{T}^d$. For each critical point, the sum of the dimensions of the stable and unstable manifolds is equal to d. Along the flow on these submanifolds the energy increases with a finite speed, except in neighborhoods of $k^*_\pm$. Hence either the submanifolds reach another critical point in a finite time (non-generic) or the points $k^*_\pm$ in infinite time. Consequently, the points $k^*_\pm$ compactify the stable and unstable manifolds. As the number of critical points is finite, the set $\mathcal{S}$ is compact with zero Lebesgue measure. To prove the last statement of the proposition, let k^* be a critical point of indefinite signature. Then let $V(k^*)$ be an open neighborhood of k^* contained in U. Then $V = \bigcup_{k^*} \bigcup_{b\in\mathbb{R}} \theta_b(V(k^*))$ is an open set that is invariant by the flow. A compactness argument can be used to show that $V \subset U$ by choosing $V(k^*)$ sufficiently small. □

The level set of $\mathcal{E}$ corresponding to an energy $E \in (E_-, E_+)$ is defined by

$$\Sigma_E \;=\; \Big\{ k \in \mathbb{T}^d \setminus \mathcal{S} \;\Big|\; \mathcal{E}(k) \;=\; E \Big\}\,.$$

These level sets will be called the *quasi-Fermi surfaces*. This terminology is introduced to stress that Σ_E is a strict subset of Fermi surface $\mathcal{E}^{-1}(E)$ because the points on the stable and unstable manifolds of all critical points with indefinite signature are excluded. However, the difference is only of measure zero. A reference quasi-Fermi surface will be taken at energy E_r and denoted by $\Sigma = \Sigma_{E_r}$. Because the singularities are excluded, the sets Σ_E are smooth open submanifolds of $\mathbb{T}^d$ of codimension 1 which, for $d \geq 2$, have several connected components. Now the flow θ_b maps these connected components diffeomorphically into each other. By the above arguments, for each energy E, there is a time $b = f(E)$ such that the flow θ_b maps the reference quasi-Fermi surface Σ diffeomorphically into Σ_E. Consequently we have:

5.2 Proposition *For $E \in (E_-, E_+)$, the map $\theta_{f(E)} : \Sigma \to \Sigma_E$ is a diffeomorphism.*

The next aim is the construction of an unbounded conjugate (or dilation) operator A such that $\imath[A, H_0] = F(H_0)$ where F is as above. The basic idea is to implement the flow θ_b of $\widehat{X}$ in $L^2(\mathbb{T}^d)$ as a strongly continuous group of unitaries. Let $\mathcal{D}$ denote the set of smooth functions on $\mathbb{T}^d$ vanishing in some neighborhood of $\mathcal{S}$. Since $\mathcal{S}$ has zero Lebesgue measure and is compact, $\mathcal{D}$ is dense in $L^2(\mathbb{T}^d)$. Furthermore, Proposition 5.1 implies that every function in $\mathcal{D}$ vanishes on a flow invariant open subset containing $\mathcal{S} \setminus \{k^*_-, k^*_+\}$. Hence for $\phi \in \mathcal{D}$, the following operator can be defined

$$(\mathcal{W}_b\,\phi)(k) \;=\; \exp\left(\frac{1}{2}\int_0^b du\, \mathrm{div}(\widehat{X})(\theta_u(k))\right)\;\phi(\theta_b(k))\,, \tag{5.7}$$

because the singularities of $\widehat{X}$ are not reached, due to the restriction on the support of ϕ. The unitarity of $\mathcal{W}_b$ follows from the change of variables $k \mapsto \theta_b(k)$ and from the Jacobian formula

$$\det(\theta_b'(k)) \;=\; \exp\left(\int_0^b du\, \mathrm{div}(\widehat{X})(\theta_u(k))\right)\,. \tag{5.8}$$

This latter relation follows from integrating $\partial_b \ln\det(\theta_b'(k)) = \mathrm{div}(\widehat{X})(\theta_b(k))$ with the initial condition $\det(\theta_0') = 1$. Furthermore, the group property $\theta_b \circ \theta_u = \theta_{b+u}$ immediately implies $\mathcal{W}_b\mathcal{W}_u = \mathcal{W}_{b+u}$. It can be checked, by a direct calculation, that $\|\mathcal{W}_b\phi\| = \|\phi\|$ for $\phi \in \mathcal{D}$. In addition, using the Lebesgue dominated convergence theorem, $\lim_{b\to 0}\mathcal{W}_b\phi = \phi$ for $\phi \in \mathcal{D}$. It follows, from a 3ϵ argument, that $\mathcal{W}_b$ can be extended as a one-parameter, strongly continuous group of unitary operators on $L^2(\mathbb{T}^d)$. By Stone's theorem the generator $\widehat{A} = \frac{1}{\imath}\partial_b\mathcal{W}_b|_{b=0}$ is self-adjoint and $\mathcal{W}_b = \exp(\imath b\widehat{A})$. Also [BR, Corollary 3.1.7] implies that $\mathcal{D}$ is a core for $\widehat{A}$ because $\mathcal{D}$ is left invariant under $\mathcal{W}_b$. The derivation of equation (5.7) leads to

$$\widehat{A}\,\phi \;=\; \frac{1}{\imath}\left(\widehat{X}(\phi) + \frac{1}{2}\,\mathrm{div}(\widehat{X})\,\phi\right)\,, \tag{5.9}$$

where $\widehat{X}(\phi) = \langle \widehat{X}|\nabla\rangle\phi$ is the action of the vector field on the function $\phi \in \mathcal{D}$. Note that the multiplicative (zero order) operator $\frac{1}{2}\,\mathrm{div}(\widehat{X})$ is needed to make the r.h.s. of (5.9) symmetric w.r.t. the scalar product in $L^2(\mathbb{T}^d)$. The desired commutator property $\imath[A, H_0] = F(H_0)$ now follows directly from (5.9) because $\imath[\widehat{A}, \widehat{H}_0] = \widehat{X}(\mathcal{E}) = F(\widehat{H}_0)$. This can be summarized as follows:

5.3 Theorem *Let $\mathcal{E}$ be a Morse function with only one maximum and one local minimum. Let $\mathcal{W}_b$ be defined by* (5.7) *for $\phi \in \mathcal{D}$ and with $\widehat{X}$ and θ_b given by* (5.2) *and its flow. Then $\mathcal{W}_b$ is a strongly continuous one-parameter group of unitary operators on $L^2(\mathbb{T}^d)$. Its generator $\widehat{A} = \frac{1}{\imath}\partial_b\mathcal{W}_b|_{b=0}$ is self-adjoint with core $\mathcal{D}$ and satisfies*

$$\imath[\widehat{A}, \widehat{H}_0] \;=\; F(\widehat{H}_0)\,, \qquad \imath[\widehat{A}, f(\widehat{H}_0)] \;=\; \mathbf{1}\,.$$

Let us write out another formula for A. Let $X_j = \mathcal{F}^*\widehat{X}_j\mathcal{F}$ be the operator on $\ell^2(\mathbb{Z}^d)$ associated with the jth component $\widehat{X}_j$ of $\widehat{X}$. Also let $Q = (Q_1, \ldots, Q_d)$ be the position operator defined by $Q_j\,\phi(n) = n_j\,\phi(n)$, for $n \in \mathbb{Z}^d$ and ϕ decreasing sufficiently fast. Then the Fourier transform of the r.h.s. of (5.9) leads to

$$A \;=\; \frac{1}{2}\sum_{j=1}^{d}\left(X_j\,Q_j + Q_j\,X_j\right)\,. \tag{5.10}$$

In the remainder of this section, the boundary values of the Green's function will be studied. That these boundary values actually exist is often referred to as the *limit absorption principle*. Recall that $\Lambda \subset \mathbb{Z}^d$ is finite. Associated with Λ is the subspace $\ell^2(\Lambda) = \mathbb{C}^{|\Lambda|}$. Let $\Pi^* : \mathbb{C}^{|\Lambda|} \to \ell^2(\mathbb{Z}^d)$ be the canonical injection obtained by extending elements of $\ell^2(\mathbb{Z}^d)$ by zero outside Λ. It is a partial isometry such that $\Pi^*\Pi$ is the $|\Lambda|$-dimensional projection in $\ell^2(\mathbb{Z}^d)$ onto the subspace of elements supported by Λ, while $\Pi\,\Pi^* = \mathbf{1}_{\mathbb{C}^{|\Lambda|}}$. The finite volume Green matrix is defined by:

$$G_0^\Pi(z) \;=\; \Pi\,(z - H_0)^{-1}\,\Pi^* \;.$$

This is a matrix of size $|\Lambda| \times |\Lambda|$. An important basic fact about the Green matrix is its Herglotz property, that is, $G_0^\Pi(z)$ is analytic in the upper half-plane and

$$-\Im m\, G_0^\Pi(z) \;=\; \frac{\imath}{2}(G_0^\Pi(z) - G_0^\Pi(z)^*) \;>\; 0\;, \qquad \Im m(z) > 0\;.$$

This implies, in particular, that $G_0^\Pi(z)$ is invertible for $\Im m(z) \neq 0$. Indeed, suppose that $v \neq 0$ lies in the kernel. Then

$$0 \;=\; \langle v|G_0^\Pi(z)|v\rangle \;=\; \langle v|\Re e\, G_0^\Pi(z)|v\rangle + \imath\,\langle v|\Im m\, G_0^\Pi(z)|v\rangle \in \mathbb{R} + \imath\mathbb{R}\;,$$

in contradiction to the positivity of $\Im m\, G_0^\Pi(z)$. The boundary values of $G_0^\Pi(z)$ on the real axis will be analyzed next in high dimension.

5.4 Proposition *Let $d \geq 3$ and let $\mathcal{E}$ be analytic. The weak limits $G_0^\Pi(E \pm \imath 0) = \lim_{\epsilon\downarrow 0} G_0^\Pi(E \pm \imath\epsilon)$ exist. Furthermore:*

(i) *Away from the critical values of $\mathcal{E}$, the map $E \in \mathbb{R} \mapsto G_0^\Pi(E \pm \imath 0)$ is real analytic. At the critical points it is Hölder continuous.*

(ii) *$\Im m\, G_0^\Pi(E - \imath 0) = -\Im m\, G_0^\Pi(E + \imath 0)$ vanishes on $(-\infty, E_-] \cup [E_+, \infty)$. It is a positive matrix with nonzero diagonal entries on (E_-, E_+).*

(iii) *The map $E \in \mathbb{R} \mapsto \Re e\, G_0^\Pi(E)$ is negative and decreasing on $(-\infty, E_-]$ and positive and decreasing on $[E_+, \infty)$. Furthermore, $G_0^\Pi(\pm\infty) = 0$.*

The proofs below are taken from [BS], but are merely detailed extensions of the work of van Hove [VH]. Let us also note that [BS] also provides detailed information about the asymptotics of the Green matrix at the band edges by dwelling slightly more into the arguments below.

Proof: For $m, n \in \Lambda$, the matrix elements of $G_0^\Pi(z)$ are given by

$$\langle m|G_0^\Pi(z)|n\rangle \;=\; \langle m|(z - H_0)^{-1}|n\rangle \;=\; \int_{\mathbb{T}^d} \frac{d^d k}{(2\pi)^d}\, \frac{e^{\imath(n-m)\cdot k}}{z - \mathcal{E}(k)}\;.$$

(i) Outside the critical values: By construction the matrix $G_0^\Pi(z)$ is holomorphic for $z \notin \sigma(H_0)$. In particular, since the spectrum of H_0 is the interval $\sigma(H_0) = [E_-, E_+]$, it follows that the map $E \in \mathbb{R} \setminus [E_-, E_+] \mapsto G_0^\Pi(E)$ is real analytic and converges to zero at $\pm\infty$. Moreover, its derivative is negative. In particular, if the limit of this matrix exists at $E_\pm$, this limit is a negative matrix at E_- and a positive matrix at E_+. Now, since $\mathcal{E}$ is analytic, it follows that it has only a finite number of critical points and it admits a holomorphic continuation in $(\mathbb{T} + \imath\mathbb{R})^d$ in a small neighborhood of the form $B_\eta = \{k + \imath\kappa \in (\mathbb{T} + \imath\mathbb{R})^d \,|\, \max_{1\leq i\leq d} |\kappa_i| < \eta\}$. It follows that, for $\epsilon > 0$ small enough, the manifold defined as the set $\mathbb{T}^d_\epsilon = \{k + \imath\epsilon\nabla\mathcal{E}(k) \,|\, k \in \mathbb{T}^d\}$ is entirely contained in B_η. Using the Cauchy formula, it follows that

$$\langle m|G_0^{\Pi}(z)|n\rangle \;=\; \int_{\mathbb{T}_\epsilon^d} \frac{d^dk'}{(2\pi)^d}\,\frac{e^{\imath(n-m)\cdot k'}}{z-\mathcal{E}(k')}\,.$$

Since $k'\in\mathbb{T}_\epsilon^d$, it follows that $k'=k+\imath\epsilon\nabla\mathcal{E}(k)$ for some $k\in\mathbb{T}^d$, so that, using a Taylor expansion,

$$\Im m\,\mathcal{E}(k') \;=\; \epsilon\,|\nabla\mathcal{E}(k)|^2 \;+\; \mathcal{O}(\epsilon^2)\,.$$

Consequently, if $E\in[E_-,E_+]\setminus\mathcal{E}(\mathcal{S}^*)$ is not a critical value, there is $\rho>0$ such that, if $|z-E|<\rho$, the distance of $\mathrm{dist}\{z,\mathcal{E}(\mathbb{T}_\epsilon^d)\}>0$ does not vanish. In particular, $G_0^{\Pi}(z)$ extends as a holomorphic function of z from $\Im m(z)<0$ to a neighborhood of E. In particular, the boundary value $G_0^{\Pi}(E-\imath 0)$ is analytic in E in $[E_-,E_+]\setminus\mathcal{E}(\mathcal{S}^*)$. A similar argument applies to $G_0^{\Pi}(E+\imath 0)$.

(ii) Partitioning: For any $k^*\in\mathcal{S}^*$, let $B_\delta(k^*)$ be the open ball centered at k^* of radius $\delta>0$. Let also $\overline{B}_{\delta/2}(k^*)$ be the closed ball also centered at k^* of radius $\delta/2$. Let U_{reg} be the open set obtained by removing from $\mathbb{T}^d$ the union of the balls $\overline{B}_{\delta/2}(k^*)$, $k^*\in\mathcal{S}^*$. It follows that the family $\{U_{\text{reg}}\}\cup\{B_\delta(k^*)\,|\,k^*\in\mathcal{S}^*\}$ is a finite open cover of $\mathbb{T}^d$. Let then $\{\chi_{\text{reg}}\}\cup\{\chi_{k^*}\,|\,k^*\in\mathcal{S}^*\}$ be a smooth partition of unity associated with this open cover. The previous integral can be decomposed into a sum

$$\langle m|(z-H_0)^{-1}|n\rangle \;=\; G_{\text{reg}}(z)+\sum_{k^*\in\mathcal{S}^*}G_{k^*}(z)\,,\qquad G_{k^*}(z)\;=\;\int_{B_\delta(k^*)}\frac{d^dk}{(2\pi)^d}\,\chi_{k^*}(k)\,\frac{e^{\imath(n-m)\cdot k}}{z-\mathcal{E}(k)}\,. \tag{5.11}$$

The contribution G_{reg} is regular because the integral vanishes around all critical points. Using the coarea formula and the results of Appendix C, it follows that G_{reg} is holomorphic in the complement of the spectrum of H_0 and its boundary values are smooth everywhere on the real line.

(iii) Non extremal critical points: The boundary values of the G_{k^*}'s, however, may not be smooth because of the contribution of the critical point. Let k^* be one of the critical points of signature $d=(d_+,d_-)$ with $d_\pm\neq 0$ and in the following $G_*=G_{k^*}$ will denote its contribution to the previous decomposition. If δ is small enough, the Morse lemma [Nic] implies that there exists a neighborhood U of k^* containing $B_\delta(k_*)$ and a diffeomorphism $\varphi:B_\delta(0)\to U$ such that $\varphi(0)=k^*$ and $\mathcal{E}_\varphi=\mathcal{E}\circ\varphi$ is quadratic:

$$\mathcal{E}_\varphi(k)\;=\;E_*+\frac{1}{2}\sum_{i=1}^{d_+}k_i^2-\frac{1}{2}\sum_{j=d_++1}^{d}k_j^2\,,$$

for $\|k\|<\delta$ and where $E_*=\mathcal{E}(k^*)$. This diffeomorphism has a Jacobian matrix $J=\varphi'(0)$ satisfying $J\mathrm{diag}(\mathbf{1}_{d_+},-\mathbf{1}_{d_-})J^*=\mathcal{E}''(k^*)^{-1}$. Thus the Jacobi determinant of φ stays close to $|\det(\mathcal{E}''(k^*))|^{-1/2}$ over the neighborhood U and is a smooth function. It follows that the integral defining G_* is given by

$$G_*(z)\;=\;\int_{\|k\|<\delta}\frac{d^dk}{(2\pi)^d}\,\left|\det(\varphi'(k))\right|\chi_{k^*}(\varphi(k))\,\frac{e^{\imath(n-m)\cdot\varphi(k)}}{z-\mathcal{E}_\varphi(k)}\,.$$

It will be convenient to use the following polar variables

$$k_i\;=\;r_+\omega_+\quad\text{if }\;1\le i\le d_+\,,\qquad\qquad k_j\;=\;r_-\omega_-\quad\text{if }\;d_+<j\le d\,,$$

were $r_\pm\ge 0$ are the radial variables and $\omega_\pm\in\mathbb{S}^{d_\pm-1}$ the angular ones. It follows that

$$G_*(z)\;=\;\int_{r_+^2+r_-^2<\delta^2}\frac{r_+^{d_+-1}dr_+\,r_-^{d_--1}dr_-}{(2\pi)^d}\;\frac{F(r_+,r_-)}{z-E_*-\frac{1}{2}(r_+^2-r_-^2)}\,,$$

where F is a smooth function with support inside the disk $r_+^2+r_-^2<\delta^2$ given by

$$F(r_+,r_-) \;=\; \int_{\mathbb{S}^{d_+-1}\times\mathbb{S}^{d_--1}} d\omega_+\, d\omega_- \; \left|\det(\varphi'(k))\right| \chi_{k^*}(\varphi(k))\; e^{\imath(n-m)\cdot\varphi(k)}\,.$$

Equivalently G_* can be expressed as

$$G_*(z) \;=\; \int_{\mathbb{R}} \frac{\rho(e)de}{z-E_*-e}\,,$$

where ρ is defined by

$$\rho(e) \;=\; \int_{r_+^2+r_-^2<\delta^2} \frac{r_+^{d_+-1}dr_+\, r_-^{d_--1}dr_-}{(2\pi)^d}\; F(r_+,r_-)\,\delta\left(\frac{r_+^2-r_-^2}{2}-e\right)\,.$$

If $e>0$, the usual rule followed by the Dirac distribution δ leads to

$$\rho(e) \;=\; \int_0^\delta \frac{dr}{(2\pi)^d}\; r^{d_--1}(e+r^2)^{(d_+-2)/2}\; F(\sqrt{r^2+e},r) \tag{5.12}$$

For $e<0$, a similar formula holds by exchanging d_+ with d_- and $F(r,r')$ with $F_s(r,r')=F(r',r)$. The previous expression shows that, if $d_-\geq 2$, the Lebesgue dominated convergence theorem implies that the limits $\rho(\pm 0)$ exist and are equal. In particular, ρ is continuous at $e=0$. Moreover, since $d\geq 3$, if $d_+=1$, then $d_-=d-1\geq 2$. Then $r^{d_--1}(e+r^2)^{(d_+-2)/2}=r^{d-2}(e+r^2)^{-1/2}\leq r^{d-5/2}$ showing that, again, ρ is continuous at $e=0$.

Equation (5.12) also shows that ρ is differentiable for $e\neq 0$. Moreover, its derivative is given by the sum of two terms $\rho_1'+\rho_2'$ with

$$\rho_1'(e) \;=\; \frac{d_+-2}{2}\int_0^\delta \frac{dr}{(2\pi)^d}\; r^{d_--1}(e+r^2)^{d_+/2-2}\; F(\sqrt{r^2+e},r)\,,$$

$$\rho_2'(e) \;=\; \frac{1}{2}\int_0^\delta \frac{dr}{(2\pi)^d}\; r^{d_--1}(e+r^2)^{d_+/2-3/2}\; \partial_1 F(\sqrt{r^2+e},r)\,.$$

The same argument as before shows that, if $d\geq 3$, ρ_2' admits a finite limit as $\pm e\downarrow 0$. However, these two limits may not be equal, if $F\neq F_s$. On the other hand, if $d\geq 5$, ρ_1' also admits limits and the two limits coincide. For $d=3,4$, however, it follows that $d_+<4$ so that ρ_1' may diverge at $e\to 0$. Nevertheless, the integrand can be bounded by

$$r^{d_--1}(e+r^2)^{d_+/2-2} \;\leq\; e^{-\alpha}\, r^{d-5+2\alpha}\,,$$

which is integrable if $\alpha>1/2$ for $d=3$ and $\alpha>0$ for $d=4$. Hence in both cases, there is $K>0$ such that

$$|\partial_e\rho| \;\leq\; \frac{K}{e^\alpha} \qquad\Longrightarrow\qquad |\rho(e)| \;\leq\; \frac{K}{1-\alpha}\, e^{1-\alpha}\,,$$

showing that ρ is Hölder continuous at the critical points. Using the Plemelj-Privalov theorem (Lemma C.1 of Appendix C), it follows that the same is true for the boundary values of G_*.

(iv) Near the extrema: The behavior near the maximum or the minimum can be treated similarly so that it is enough to consider only the minimum at k_-^*. Again by the Morse lemma, there is a neighborhood U of k_-^* containing $B_\delta(k_-^*)$ and a diffeomorphism $\varphi: B_\delta(0)\to U$ with $\varphi(0)=k_-^*$ and such that $\mathcal{E}\circ\varphi(k)=E_-+\frac{1}{2}\sum_{i=1}^d k_i^2$. Introducing the polar coordinates $r=\|k\|$ and $\omega\in\mathbb{S}^{d-1}$ so that $k=r\omega$, the contribution $G_-(z)=G_{k_-^*}(z)$ is given by the integral

$$G_-(z) \;=\; \int_0^\delta \frac{r^{d-1}dr}{(2\pi)^d}\,\frac{e^{\imath(n-m)\cdot k_-^*}\,F(r)}{z-E_- - \frac{1}{2}r^2}\,, \quad F(r) \;=\; \int_{\mathbb{S}^{d-1}} d\omega\,|\det(\varphi'(r\omega))|\,\chi_-(\varphi(r\omega))\,e^{\imath(n-m)\cdot(\varphi(r\omega)-k_-^*)}\,.$$

with χ_- a smooth function with support in $U(k_-^*)$ which is equal to 1 on the ball $\|k-k_-^*\| \le \delta/2$. In particular, F is smooth and bounded in $0<r<\delta$, it vanishes in a neighborhood of $r=\delta$ and all its derivatives have a limit at $r=0$. Consequently, the integration domain can be extended to $[0,\infty)$ without change. Let us note that $F(0)=|\det(\varphi'(0))|\,|\mathbb{S}^{d-1}|>0$ and the Morse lemma shows that $|\det(\varphi'(0))| = \det(\mathcal{E}''(k_-^*))^{1/2}$. Next the change of variable $e=r^2/2$ yields

$$G_-(z) \;=\; \frac{e^{\imath(n-m)\cdot k_-^*}}{(2\pi)^d}\int_0^\infty de\,\frac{(2e)^{\frac{d}{2}-1}F(\sqrt{2e})}{z-E_- - e}\,. \tag{5.13}$$

Since $d\ge 3$, the function $e\in[0,\infty)\mapsto e^{\frac{d}{2}-1}F(\sqrt{2e})$ is continuous and vanishes at $e=0$ like $e^{d/2-1}$. Hence it can be continued as a Hölder continuous function on the entire real line with support in $[0,\frac{\delta^2}{2})$. Consequently, thanks to the Lemma C.1, $G_-(E\pm\imath 0)$ is also continuous w.r.t. E. In particular, it has a finite value at $E=E_-$. Since the other contributions to G_0^Π are regular near E_-, $G_0^\Pi(E\pm\imath 0)$ is also a Hölder continuous function of E near $E=E_-$. □

5.2 Resolvent and spectral analysis of perturbed problem

Now the coupled Hamiltonian $H=H_0+V$ with a perturbation V supported by a finite set $\Lambda\subset\mathbb{Z}^d$ is considered. This implies

$$V \;=\; \Pi^*\,V^\Pi\,\Pi\,, \qquad \text{with } V^\Pi \;=\; \Pi\,V\,\Pi^*\,.$$

For sake of simplicity, we will suppose that V^Π is invertible. Let

$$G^\Pi(z) \;=\; \Pi(z-H)^{-1}\Pi^*$$

be the Green matrix of the perturbed Hamiltonian. As for the unperturbed case, it is also a Herglotz matrix which is invertible for $\Im m(z)\neq 0$. Let us first write out widely used formulas for the resolvent.

5.5 Lemma *For $z\in\mathbb{C}\setminus\mathbb{R}$,*

$$G^\Pi(z) \;=\; \big(G_0^\Pi(z)^{-1}-V^\Pi\big)^{-1} \;=\; \big(\mathbf{1}-G_0^\Pi(z)V^\Pi\big)^{-1}G_0^\Pi(z)\,, \tag{5.14}$$

Let the T-matrix be defined by

$$T(z) \;=\; \Pi^*\,T^\Pi(z)\,\Pi\,, \qquad T^\Pi(z) \;=\; \big(\mathbf{1}-V^\Pi G_0^\Pi(z)\big)^{-1}V^\Pi\,. \tag{5.15}$$

Then

$$\frac{1}{z-H} \;=\; \frac{1}{z-H_0}+\frac{1}{z-H_0}\,T(z)\,\frac{1}{z-H_0}\,, \tag{5.16}$$

Proof: The resolvent identity yields

$$\frac{1}{z-H_0} \;=\; \frac{1}{z-H}+\frac{1}{z-H_0}\,V\,\frac{1}{z-H} \;=\; \left(\mathbf{1}+\frac{1}{z-H_0}\,V\right)\frac{1}{z-H}\,.$$

Applying Π and Π^* from the left and right respectively gives

$$G_0^{\Pi}(z) \;=\; \big(\mathbf{1} - G_0^{\Pi}(z)V^{\Pi}\big)G^{\Pi}(z)\,.$$

Now $G_0^{\Pi}(z)$ is Herglotz and thus invertible since $z \notin \mathbb{R}$. Hence, $G_0^{\Pi}(z)^{-1} - V^{\Pi}$ is also Herglotz and invertible, leading to the invertibility of $\mathbf{1} - G_0^{\Pi}(z)V^{\Pi} = G_0^{\Pi}(z)(G_0^{\Pi}(z)^{-1} - V^{\Pi})$. To prove (5.16), the resolvent identity gives the factor $\mathbf{1} - \frac{1}{z-H_0}V$. This operator is invertible, because it is a finite rank perturbation of $\mathbf{1}$ and any element in its kernel is an eigenvector of $H = H_0 + V$ with eigenvalue $z \notin \mathbb{R}$, namely the kernel is trivial. Using the identity $(\mathbf{1} - A)^{-1}A = (\mathbf{1} - A)^{-1}(A - \mathbf{1} + \mathbf{1}) = (\mathbf{1} - A)^{-1} - \mathbf{1}$, the inverse can be written as

$$\left(\mathbf{1} - \frac{1}{z - H_0}\,V\right)^{-1} \;=\; \mathbf{1} + \frac{1}{z - H_0}\,\Pi^*\,V^{\Pi}\,\Pi\,\left(\mathbf{1} - \frac{1}{z - H_0}\,V\right)^{-1}\,.$$

Since

$$\Pi\left(\mathbf{1} - \frac{1}{z - H_0}\,V\right) \;=\; \big(\mathbf{1} - G_0^{\Pi}(z)\,V^{\Pi}\big)\,\Pi\,,$$

it follows that

$$\Pi\,\left(\mathbf{1} - \frac{1}{z - H_0}\,V\right)^{-1} \;=\; \big(\mathbf{1} - G_0^{\Pi}(z)\,V^{\Pi}\big)^{-1}\,\Pi\,,$$

When combined with the resolvent identity this completes the proof. □

Because the perturbation has finite range, the essential spectrum of H is given by the essential spectrum of H_0 by Weyl's theorem. However, H may have some discrete spectrum, which, since H is selfadjoint, is given by the simple poles of the resolvent on the real axis. Thanks to Proposition 5.4, it follows from equation (5.14) that the only way to get a polar singularity in the Green matrix of H is for $\mathbf{1} - G_0^{\Pi}(z)\,V^{\Pi} = \big((V^{\Pi})^{-1} - G_0^{\Pi}(z)\big)\,V^{\Pi}$ to have a nontrivial kernel (recall that we restrict ourselves to the case of invertible V^{Π}). This can be analyzed using the determinant of $\mathbf{1} - G_0^{\Pi}(z)\,V^{\Pi}$ which is also called the *perturbation determinant* [Yaf]. Furthermore, if E is an eigenvalue of H,

$$\text{multiplicity of } E \;=\; \dim \operatorname{Ker}\big((V^{\Pi})^{-1} - G_0^{\Pi}(E \pm \imath 0)\big)\,. \tag{5.17}$$

If $E \notin [E_-, E_+]$, it is called an *isolated eigenvalue* while, if $E \in (E_-, E_+)$, it is called an *embedded eigenvalue*. For $E = E_\pm$, a non-trivial kernel of $(V^{\Pi})^{-1} - G_0^{\Pi}(E_\pm)$ leads to a so-called *threshold singularity*. Both of these latter singularities are of positive co-dimension and will not be further considered here. See again [BS] for a detailed analysis.

5.3 The wave operator as an integral operator

The perturbation being finite rank, the Kato-Rosenblum theorem for trace class scattering theory implies that the wave operators

$$\Omega_\pm \;=\; \operatorname*{s-lim}_{t \to \pm\infty}\; e^{\imath H t}\, e^{-\imath H_0 t}\,,$$

exist and are complete, that is, $\mathrm{Ran}(\Omega_+) = \mathrm{Ran}(\Omega_-) = P_{\mathrm{ac}}(H)$ where $P_{\mathrm{ac}}(H)$ is the projection on the absolutely continuous subspace of H. Then the wave operators are partial isometries satisfying

$$\Omega_\pm^*\,\Omega_\pm \;=\; \mathbf{1}\,, \qquad \Omega_\pm\,\Omega_\pm^* \;=\; P_{\mathrm{ac}}(H) \;=\; \mathbf{1} \;-\; P_{\mathrm{pp}}(H)\,, \tag{5.18}$$

where $P_{\rm pp}(H)$ is the projection on the pure-point spectrum of H and the last equality holds because there is no singular continuous spectrum. Now we will derive an explicit formula for $\widehat{\Omega}_\pm = \mathcal{F}\Omega_\pm\mathcal{F}^*$ which will serve as a tool to calculate the wave operator and the scattering operator.

5.6 Proposition *The following formula holds*

$$\big((\widehat{\Omega}_\pm - \mathbf{1})\phi\big)(k) \;=\; \lim_{\epsilon\downarrow 0} \int_{\mathbb{T}^d} \frac{dk'}{(2\pi)^d} \sum_{n,m\in\Lambda} \langle n|\, T(\mathcal{E}(k')\mp \imath\epsilon)\,|m\rangle \; \frac{e^{\imath(k\cdot n - k'\cdot m)}}{\mathcal{E}(k')\mp\imath\epsilon - \mathcal{E}(k)}\;\phi(k')\,.$$

5.7 Lemma (Tauberian Lemma) *Let* $f:\mathbb{R}\to\mathbb{R}$ *be a measurable function such that*

$$L \;=\; \lim_{t\to\infty}\int_0^t ds\; f(s)$$

exists. Then

$$L \;=\; \lim_{\epsilon\downarrow 0}\int_0^\infty ds\, e^{-\epsilon s}\, f(s)\,.$$

Proof: It follows from a partial integration that

$$\int_0^T ds\, e^{-\epsilon s}\, f(s) \;=\; e^{-\epsilon T}\int_0^T ds\, f(s) \;+\; \epsilon \int_0^T ds\, e^{-\epsilon s}\int_0^s ds'\; f(s')\,.$$

For $\epsilon>0$, one can now take the limit $T\to\infty$ and the first term on the r.h.s. vanishes. Next the limit $\epsilon\to 0$ can be taken and this yields the claim. □

Proof of Proposition 5.6: It follows from DuHamel's formula (3.1) and the Tauberian lemma that

$$\Omega_\pm \;=\; \mathbf{1} \,\pm\, \imath\,\text{s-}\lim_{t\to\infty}\int_0^t ds\; e^{\pm\imath Hs}\; V\; e^{\mp\imath H_0 s} \;=\; \mathbf{1}\,\pm\,\imath\,\text{s-}\lim_{\epsilon\downarrow 0}\int_0^\infty ds\; e^{-\epsilon s}\; e^{\pm\imath Hs}\; V\; e^{\mp\imath H_0 s}\,.$$

Hence

$$\Big((\widehat{\Omega}_\pm - \mathbf{1})\phi\Big)(k) \;=\; \pm\,\imath\lim_{\epsilon\downarrow 0}\int_0^\infty ds\; e^{-\epsilon s}\;\big(\mathcal{F}\,e^{\pm\imath Hs}\; V\; e^{\mp\imath H_0 s}\,\mathcal{F}^*\,\phi\big)(k)\,.$$

In the following, the notation $V_{l,m} = \langle l|V|m\rangle$ will be used. In addition,

$$\langle m|\,e^{\mp\imath H_0 s}\,\mathcal{F}^*\,|\phi\rangle \;=\; \int_{\mathbb{T}^d}\frac{dk'}{(2\pi)^d}\; e^{-\imath k'\cdot m}\;\; e^{\mp\imath\mathcal{E}(k')s}\,\phi(k')$$

Consequently the previous formula leads to

$$\Big((\widehat{\Omega}_\pm - \mathbf{1})\phi\Big)(k) \;=\; \pm\imath\sum_{l,m\in\Lambda} V_{l,m}\;\lim_{\epsilon\downarrow 0}\int_0^\infty ds\; e^{-\epsilon s}\;\big(\mathcal{F}\,e^{\pm\imath Hs}|l\rangle\big)(k)\int_{\mathbb{T}^d}\frac{dk'}{(2\pi)^d}\; e^{-\imath k'\cdot m}\;\; e^{\mp\imath\mathcal{E}(k')s}\,\phi(k')\,.$$

The integral over s can be performed to give

$$\Big((\widehat{\Omega}_\pm - \mathbf{1})\phi\Big)(k) \;=\; \lim_{\epsilon\downarrow 0}\int_{\mathbb{T}^d}\frac{dk'}{(2\pi)^d}\sum_{l,m\in\Lambda} V_{l,m}\,e^{-\imath k'\cdot m}\;\left(\mathcal{F}\,\frac{1}{\mathcal{E}(k')\mp\imath\epsilon - H}\;|l\rangle\right)(k)\;\phi(k')\,.$$

In the previous expression, it becomes possible to compute the part in the parenthesis. For indeed, using the resolvent identity as in Lemma 5.5 yields

$$\frac{1}{z\mathbf{1}-H}\,\Pi^* \;=\; \frac{1}{z\mathbf{1}-H_0}\,\Pi^*\,\frac{1}{\mathbf{1}-V^\Pi G_0^\Pi(z)}\,,$$

and remarking that $l\in\Lambda$. Hence, passing to the Fourier space leads to

$$\left(\mathcal{F}\,\frac{1}{z-H}\,|l\rangle\right)(k) \;=\; \sum_{n\in\Lambda}\,\frac{1}{z-\mathcal{E}(k)}\,e^{\imath k\cdot n}\,\langle n|\left(\mathbf{1}-V^\Pi G_0^\Pi(z)\right)^{-1}|l\rangle\,.$$

Replacing this in the above expression for $\widehat{\Omega}_\pm-\mathbf{1}$ completes the proof. □

5.4 Change of variables and REF representation

This section is devoted to the definition and the properties of the *rescaled energy and Fermi surface* (REF) representation. The proof of Theorem 5.3 was mainly based on the change of variables $\theta_b:\mathbb{T}^d\to\mathbb{T}^d$ with Jacobian (5.8) where θ_b is the time b flow (5.3) of the vector field $\widehat{X}$ defined in (5.2):

$$\begin{aligned}\int_{\mathbb{T}^d}dk\;\phi(k) \;&=\; \int_{\mathbb{T}^d}dk\;\det(\theta_b'(k))\,\phi(\theta_b(k))\\ &=\;\int_{\mathbb{T}^d}dk\;\exp\left(\int_0^b du\;\mathrm{div}(\widehat{X})(\theta_u(k))\right)\phi(\theta_b(k))\,.\end{aligned}$$

It will be supplemented by the *coarea formula* (see *e.g.* [Sak] for a proof and note that $\mathcal{S}$ is of zero measure). If ν_E denotes the Riemannian volume measure on Σ_E (induced by the euclidean metric on $\mathbb{T}^d$),

$$\int_{\mathbb{T}^d}dk\;\phi(k) \;=\; \int_{E_-}^{E_+}dE\int_{\Sigma_E}\nu_E(d\sigma)\,\frac{1}{|\nabla\mathcal{E}(\sigma)|}\,\phi(\sigma)\,. \tag{5.19}$$

This holds for ϕ in the set $\mathcal{D}=C_K^\infty(\mathbb{T}^d\setminus\mathcal{S})$ of smooth functions vanishing on a neighborhood of the stable and unstable manifolds of the critical points with indefinite signature. For the reference energy surface $\Sigma=\Sigma_{E_r}$, the measure is simply denoted by $\nu=\nu_{E_r}$. The coarea formula leads to the following:

5.8 Lemma *Let $\phi\in\mathcal{D}$. Then its integral can be written in the following three equivalent ways:*

$$\begin{aligned}\int_{\mathbb{T}^d}dk\;\phi(k) \;&=\; \int_{\mathbb{R}}db\int_\Sigma\nu(d\sigma)\left|\det(\theta_b'|_{T_\sigma\Sigma})\right|\left|\widehat{X}(\theta_b(\sigma))\right|\phi\left(\theta_b(\sigma)\right)\,, &(5.20)\\ &=\;\int_{\mathbb{R}}db\int_\Sigma\nu(d\sigma)\;\exp\left(\int_0^b du\;\mathrm{div}(\widehat{X})(\theta_u(\sigma))\right)\left|\widehat{X}(\sigma)\right|\phi\left(\theta_b(\sigma)\right)\,, &(5.21)\\ &=\;\int_{E_-}^{E_+}dE\int_\Sigma\nu(d\sigma)\,\frac{|\det(\theta_{f(E)}'|_{T_\sigma\Sigma})|}{|\nabla\mathcal{E}(\theta_{f(E)}(\sigma))|}\,\phi\left(\theta_{f(E)}(\sigma)\right)\,, &(5.22)\end{aligned}$$

where $\theta_b'|_{T_\sigma\Sigma}$ denotes the derivative of θ_b restricted to the tangent space of Σ at σ (so that this is a $(d-1)\times(d-1)$ matrix).

Proof: Starting from the coarea formula (5.19), the substitution $b=f(E)$ given in (5.4) and the diffeomorphism of Proposition 5.2 will be used in the following change of variables. With $dE=F(f^{-1}(b))db$,

$$\int_{\mathbb{T}^d} dk\, \phi(k) \;=\; \int_{\mathbb{R}} db \int_{\Sigma_{f^{-1}(b)}} \nu_{f^{-1}(b)}(d\sigma)\, \frac{F(f^{-1}(b))}{|\nabla\mathcal{E}(\sigma)|}\, \phi(\sigma)$$
$$\;=\; \int_{\mathbb{R}} db \int_{\Sigma} \nu(d\sigma) \left|\det(\theta'_b|_{T_\sigma\Sigma})\right| \frac{F(\mathcal{E}(\theta_b(\sigma)))}{|\nabla\mathcal{E}(\theta_b(\sigma))|}\, \phi(\theta_b(\sigma))\,.$$

In the second equality, the diffeomorphism $\theta_b : \Sigma \to \Sigma_{f^{-1}(b)}$ as well as the identity $F(f^{-1}(b)) = F(\mathcal{E}(\sigma))$ for $\sigma \in \Sigma_{f^{-1}(b)}$ were used. Replacing the definition of $\widehat{X}$ already shows (5.20) as well as (5.22). Next θ'_b can be decomposed as $\theta'_b|_{T_\sigma\mathbb{T}^d} = \theta'_b|_{T_\sigma\Sigma} \oplus \theta'_b|_{(T_\sigma\Sigma)^\perp}$ implying

$$|\det(\theta'_b|_{T_\sigma\mathbb{T}^d})| \;=\; |\det(\theta'_b|_{T_\sigma\Sigma})|\, |\theta'_b|_{(T_\sigma\Sigma)^\perp}|\,. \tag{5.23}$$

In order to compute $\theta'_b|_{(T_\sigma\Sigma)^\perp}$ it should be remarked that the derivative of the equation $\partial_b\theta_b = \widehat{X}\circ\theta_b$ is $\partial_b\theta'_b = \widehat{X}'\circ\theta_b\,\theta'_b$, leading to $\theta'_b(\widehat{X}(\sigma)) = \widehat{X}(\theta_b(\sigma))$. As the one-dimensional space $(T_\sigma\Sigma)^\perp$ is spanned by $\widehat{X}(\sigma)$, it follows that

$$|\theta'_b|_{(T_\sigma\Sigma)^\perp}| \;=\; \left|\theta'_b\Big(\frac{\widehat{X}(\sigma)}{|\widehat{X}(\sigma)|}\Big)\right| \;=\; \frac{|\widehat{X}(\theta_b(\sigma))|}{|\widehat{X}(\sigma)|}\,.$$

Consequently

$$\left|\det(\theta'_b|_{T_\sigma\Sigma})\right| \left|\widehat{X}(\theta_b(\sigma))\right| \;=\; \exp\left(\int_0^b du\, \mathrm{div}(\widehat{X})(\theta_u(\sigma))\right) \left|\widehat{X}(\sigma)\right|. \tag{5.24}$$

Replacing this in (5.20) proves (5.21). □

The following notation will be useful

$$d_b(\sigma) \;=\; \left|\det(\theta'_b|_{T_\sigma\Sigma})\right|^{\frac{1}{2}} \left|\widehat{X}(\theta_b(\sigma))\right|^{\frac{1}{2}} \;=\; \exp\left(\frac{1}{2}\int_0^b du\, \mathrm{div}(\widehat{X})(\theta_u(\sigma))\right) \left|\widehat{X}(\sigma)\right|^{\frac{1}{2}}. \tag{5.25}$$

From (5.21), it follows that the map $\mathcal{U}$ defined on $\mathcal{D}$ by

$$(\mathcal{U}\phi)_b(\sigma) \;=\; d_b(\sigma)\, \phi(\theta_b(\sigma))\,, \qquad\qquad \phi \in \mathcal{D} \subset L^2(\mathbb{T}^d)\,, \tag{5.26}$$

extends to a unitary from $L^2(\mathbb{T}^d)$ to $L^2(\mathbb{R})\otimes L^2(\Sigma,\nu)$. The variable b is the rescaled energy difference w.r.t. the reference quasi-Fermi surface Σ. Expressing this in terms of $\mathcal{W}_b$ (see equation (5.7)), leads to

$$(\mathcal{U}\phi)_b(\sigma) \;=\; |\widehat{X}(\sigma)|^{\frac{1}{2}}(\mathcal{W}_b\phi)(\sigma)\,.$$

The inverse, acting on $\psi \in L^2(\mathbb{R})\otimes L^2(\Sigma,\nu)$, is given by

$$(\mathcal{U}^*\psi)(k) \;=\; d_b(\theta_{-b}(k))^{-1}\, \psi_b(\theta_{-b}(k))\,, \qquad\qquad b = f(\mathcal{E}(k))\,.$$

The expression $\widetilde{H}_0 = \mathcal{U}\widehat{H}_0\mathcal{U}^* = \mathcal{U}\mathcal{F}H_0\mathcal{F}^*\mathcal{U}^*$ will be called the REF representation of H_0. Any operator in the REF representation will carry a tilde. The operator $(\widetilde{B}\psi)_b = b\psi_b$ is the *rescaled energy*. Its conjugate operator clearly is $\widetilde{A}$ with $(\widetilde{A}\psi)_b = \frac{1}{\imath}\partial_b\psi_b$. Both of these operators are unbounded and have the standard self-adjoint domains. The following result states that these notations are consistent with the above.

5.9 Proposition *The following relations hold*

$$\mathcal{U}\,\widehat{H}_0\,\mathcal{U}^* \;=\; f^{-1}(\widetilde{B})\otimes\mathbf{1}_\Sigma\,, \qquad\qquad \mathcal{U}\,f(\widehat{H}_0)\,\mathcal{U}^* \;=\; \widetilde{B}\,, \qquad\qquad \mathcal{U}\,\widehat{A}\,\mathcal{U}^* \;=\; \widetilde{A}\,.$$

Proof: The only point to be checked is how the commutation relations of H_0 and A, as proved in Theorem 5.3, are implemented under $\mathcal{U}$. The first identity results from (5.26) and

$$f^{-1}(b)\phi(\theta_b(\sigma)) \;=\; \mathcal{E}(\theta_b(\sigma))\phi(\theta_b(\sigma)) \;=\; \Big(\widehat{H}_0\phi\Big)(\theta_b(\sigma))\,.$$

The second formula is obtained from the first one through (unbounded) functional calculus. The third one follows from

$$(\widetilde{A}\otimes \mathbf{1}\mathcal{U}\phi)_b(\sigma) \;=\; \frac{1}{\imath}\,\partial_b\,(|\widehat{X}|^{\frac{1}{2}}\,e^{\imath b\widehat{A}}\phi)(\sigma) \;=\; (\frac{1}{2}\,e^{\imath b\widehat{A}}\,\widehat{A}\,\phi)(\sigma) \;=\; (\mathcal{U}\widehat{A}\,\phi)_b(\sigma)\,,$$

where $\mathcal{U}$ is expressed in terms of the unitary group $\mathcal{W}_b = e^{\imath b\widehat{A}}$ up to the factor $|\widehat{X}(\sigma)|^{\frac{1}{2}}$ which does not depend on b. □

It is worth comparing the previous construction to the usual one used in scattering theory on $\mathbb{R}^d$, where $H_0 = -\Delta$ is the Laplacian acting on $L^2(\mathbb{R}^d)$. Then, the (unitary) Fourier transform $\mathcal{F} : L^2(\mathbb{R}^d) \mapsto L^2(\mathbb{R}^d)$ diagonalizes H_0, that is, $\mathcal{F}H_0\mathcal{F}^*$ is the operator of multiplication by $\mathcal{E}(k) = k^2$. This function has only one critical point at $k^*_- = 0$ corresponding to the minimum of energy $E_- = 0$. The vector field $\widehat{X}$ is defined as in (5.2), now with $k \in \mathbb{R}^d$. Let the reference energy be $E_r = 1$ so that the (quasi-) Fermi surface Σ is the unit sphere $\mathbb{S}^{d-1}$. Furthermore let $F(E) = 2E$, which vanishes at the only critical value. Then $\widehat{X}(k) = k$ and $f(E) = \int_1^E \frac{de}{2e} = \frac{1}{2}\ln(E)$. The flow is $\theta_b(\sigma) = e^b\sigma$. As $\mathrm{div}(\widehat{X}) = d$, it follows that $d_b(\sigma) = e^{\frac{1}{2}db}$. Therefore the unitary transformation $\mathcal{U} : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}) \otimes L^2(\mathbb{S}^{d-1})$ to the REF representation is given by

$$(\mathcal{U}\phi)_b(\sigma) = e^{\frac{1}{2}db}\,\phi(e^b\sigma)\,.$$

This transformation is discussed and used, *e.g.* in [Yaf].

The REF representation of the localized state at site $m \in \mathbb{Z}^d$ is

$$\psi_m \;=\; \mathcal{U}\mathcal{F}\,|m\rangle\,.$$

The states $(\psi_m)_{m\in\mathbb{Z}^d}$ form an orthonormal basis in $L^2(\mathbb{R}) \otimes L^2(\Sigma,\nu)$. More explicitly, they are given by

$$\psi_{m,b}(\sigma) \;=\; \frac{1}{(2\pi)^{\frac{d}{2}}}\,d_b(\sigma)\,e^{\imath m\cdot\theta_b(\sigma)}\,, \tag{5.27}$$

for any $\sigma \in \Sigma$ avoiding $\mathcal{S}$. It will be convenient below to consider $\psi_{m,b}$ as a state in $L^2(\Sigma,\nu)$. These restricted localized states are not normalized, but their norm is independent of m:

$$\|\psi_{m,b}\|^2_{L^2(\Sigma,\nu)} \;=\; \frac{1}{(2\pi)^d}\int_\Sigma \nu(d\sigma)\,|d_b(\sigma)|^2\,.$$

This norm as well as scalar products between these states are linked to the resolvent.

5.10 Lemma *The following holds*

$$\langle\psi_{n,b}|\psi_{m,b}\rangle_{L^2(\Sigma,\nu)} \;=\; \frac{F(f^{-1}(b))}{\pi}\,\langle n|\mp\Im m\Big((f^{-1}(b)\pm\imath 0 - H_0)^{-1}\Big)|m\rangle\,.$$

Proof: Thanks to the coarea formula and the Plemelj-Privalov theorem (see Lemma C.1)

$$\begin{aligned}\langle n|\,\Im m\big((E\pm\imath 0-H_0)^{-1}\big)\,|m\rangle &= \frac{1}{2\imath}\int_{E_-}^{E_+} de\,\left(\frac{1}{E\pm\imath 0-e}-\frac{1}{E\mp\imath 0-e}\right)\int_{\Sigma_e}\frac{\nu_e(d\sigma)}{(2\pi)^d}\,\frac{e^{\imath(m-n)\cdot\sigma}}{|\nabla\mathcal{E}(\sigma)|}\\ &= \mp\pi\int_{\Sigma_E}\frac{\nu_E(d\sigma)}{(2\pi)^d}\,\frac{1}{|\nabla\mathcal{E}(\sigma)|}\,e^{\imath(m-n)\cdot\sigma}\,.\end{aligned}$$

Always using $E=f^{-1}(b)$, the map $\theta_b:\Sigma\to\Sigma_E$ is a diffeomorphism. Thus the associated change of variables gives

$$\begin{aligned}\langle n|\,\Im m\big((E\pm\imath 0-H_0)^{-1}\big)\,|m\rangle &= \mp\,\pi\int_{\Sigma}\frac{\nu(d\sigma)}{(2\pi)^d}\,\big|\det(\theta_b'|_{T_\sigma\Sigma})\big|\,\frac{1}{|\nabla\mathcal{E}(\theta_b(\sigma))|}\,e^{\imath(m-n)\cdot\theta_b(\sigma)}\\ &= \frac{\mp\,\pi}{F(f^{-1}(b))}\int_{\Sigma}\frac{\nu(d\sigma)}{(2\pi)^d}\,\big|\det(\theta_b'|_{T_\sigma\Sigma})\big|\,|\widehat{X}(\theta_b(\sigma))|\,e^{\imath(m-n)\cdot\theta_b(\sigma)}\,.\end{aligned}$$

Now the formula follows from the definition of $\psi_{m,b}$ and (5.25). □

5.11 Corollary *Let us introduce the operator $\mathcal{R}_b=\sum_{m\in\Lambda}|\psi_{m,b}\rangle\langle m|$ mapping $\ell^2(\Lambda)=\mathbb{C}^{|\Lambda|}$ onto the subspace of $L^2(\Sigma,\nu)$ spanned by the $(\psi_{m,b})_{m\in\Lambda}$. The range of its adjoint $\mathcal{R}_b^*=\sum_{m\in\Lambda}|m\rangle\langle\psi_{m,b}|$ is denoted by*

$$\mathcal{F}_b\;=\;\mathrm{Ran}(\mathcal{R}_b^*)\;\subset\;\mathbb{C}^{|\Lambda|}\,.$$

Further let Π_b be a partial isometry from $\mathcal{F}_b$ onto the subspace of $L^2(\Sigma,\nu)$ spanned by the $(\psi_{m,b})_{m\in\Lambda}$.
(i) *The following holds*

$$\mathcal{R}_b^*\mathcal{R}_b\;=\;\frac{F(E)}{\pi}\,\Im m\,G_0^{\Pi}(E-\imath 0)\,,\qquad\qquad b=f(E)\,.$$

(ii) *If P_b denotes the orthogonal projection in $\mathbb{C}^{|\Lambda|}$ onto the subspace $\mathcal{F}_b$, then*

$$\mathcal{R}_b\;=\;\Pi_b\sqrt{\frac{F(E)}{\pi}}\,\big(\Im m\,G_0^{\Pi}(E-\imath 0)\big)^{\frac12}\,P_b\,,\qquad\qquad b=f(E)\,.$$

(iii) *The map $b\in\mathbb{R}\mapsto\mathcal{R}_b\in\mathcal{B}\left(\mathbb{C}^{|\Lambda|},L^2(\Sigma,\nu)\right)$ is norm continuous.*

Proof: (i) is a re-phrasing of Lemma 5.10 and (ii) just the usual polar decomposition. (iii) Since $\mathcal{R}_b$ has finite rank, the norm continuity follows form the strong continuity. In turns the strong continuity follows from the continuity of the inner products $\langle\psi_{n,b}|\psi_{m,b}\rangle_{L^2(\Sigma,\nu)}$. The latter property follows from Lemma 5.10 and from the continuity of F, f^{-1} and the imaginary part of the Green function (see Proposition 5.4), with respect to E or to b. □

It is worth remarking that $P_b=\Pi_b^*\Pi_b$ and $\Pi_b=\Pi_bP_b$. Furthermore, $\Im m\,G_0^{\Pi}(f^{-1}(b)\pm\imath 0)$ commutes with P_b.

5.5 EF representation

Another natural useful representation is the *energy and Fermi surface* (EF) representation. A local version of this representation is used in the paper by Birman and Yafaev [BY]. It is associated with the unitary map $\mathcal{V}:L^2(\mathbb{T}^d)\to L^2([E_-,E_+])\otimes L^2(\Sigma,\nu)$ defined on $\mathcal{D}$ by

$$(\mathcal{V}\phi)_E(\sigma) \;=\; \frac{|\det(\theta'_{f(E)}|_{T_\sigma\Sigma})|^{\frac{1}{2}}}{|\nabla\mathcal{E}(\theta_{f(E)}(\sigma))|^{\frac{1}{2}}}\;\phi(\theta_{f(E)}(\sigma))\,, \qquad\qquad \phi\in\mathcal{D}\,.$$

The unitarity follows directly from (5.22). It is related to the unitary operator $\mathcal{U}$ as follows

$$(\mathcal{V}\phi)_E(\sigma) \;=\; \frac{1}{F(E)^{\frac{1}{2}}}\,\frac{1}{|\widehat{X}(\sigma)|^{\frac{1}{2}}}\;(\mathcal{U}\phi)_{f(E)}(\sigma)\,. \tag{5.28}$$

The EF representation of an operator on $L^2(\mathbb{T}^d)$ is then obtained by conjugation with $\mathcal{V}$. It will carry a circle instead of a tilde, such as $\mathring{H}_0 = \mathcal{V}\widehat{H}_0\mathcal{V}^*$, $\mathring{A} = \mathcal{V}\widehat{A}\,\mathcal{V}^*$ and so on. Any operator that is a direct integral in the REF representation is also a direct integral in the EF representation. The first example of this type is the Hamiltonian H_0 itself:

$$(\mathring{H}_0\phi)_E(\sigma) \;=\; E\,\phi_E(\sigma)\,.$$

More generally, given any fibered operator $\widetilde{O} = \int^{\oplus} db\,\widetilde{O}_b$ in the REF representation, its EF representation is given by $\mathring{O} = \int^{\oplus} dE\,\mathring{O}_E$ with $\mathring{O}_E = \widetilde{O}_{f(E)}$. Another example will be the scattering matrix below. The dilation operator in the EF representation can be easily deduced from (5.28):

$$(\mathring{A}\phi)_E(\sigma) \;=\; F(E)\,\frac{1}{\imath}\,\partial_E\phi_E(\sigma) + \frac{1}{2\imath}\,F'(E)\,\phi_E(\sigma)\,,$$

where ϕ is in the domain of $\mathring{A}$, in particular, its derivative is square integrable and ϕ vanishes at the boundaries of $[E_-, E_+]$.

5.6 The wave operator in the REF representation

In this section, the REF representation will be used to calculate the wave operator $\widetilde{\Omega}_\pm = \mathcal{U}\widehat{\Omega}_\pm\mathcal{U}^*$ in dimension $d\geq 3$. It is an operator on $L^2(\mathbb{R})\otimes L^2(\Sigma,\nu)$. From Proposition 5.6, the definition (5.26), the change of variables formula (5.21) and the definition (5.27) of the states $\psi_{m,b}$, it follows that

$$((\widetilde{\Omega}_\pm - \mathbf{1})\phi)_b \;=\; \lim_{\epsilon\downarrow 0}\int db' \sum_{n,m\in\Lambda} |\psi_{n,b}\rangle\,\frac{\langle n|\,T(f^{-1}(b')\mp\imath\epsilon)\,|m\rangle}{f^{-1}(b')\mp\imath\epsilon - f^{-1}(b)}\,\langle\psi_{m,b'}|\phi_{b'}\rangle\,,$$

where $\langle\psi_{m,b'}|\phi_{b'}\rangle$ stands for the inner product in the Hilbert space $L^2(\Sigma,\nu)$ and the integral of b' carries over $\mathbb{R}$. Thanks to Corollary 5.11, the sums over n and m can be computed to give

$$((\widetilde{\Omega}_\pm - \mathbf{1})\phi)_b \;=\; \lim_{\epsilon\downarrow 0}\int \frac{db'}{\pi}\,\frac{F(f^{-1}(b))^{\frac{1}{2}}\,F(f^{-1}(b'))^{\frac{1}{2}}}{f^{-1}(b')\mp\imath\epsilon - f^{-1}(b)}\,\Pi_b\,\big|\Im m\,G_0^{\Pi}(f^{-1}(b))\big|^{\frac{1}{2}}(\widetilde{O}_\pm\phi)_{b'}\,, \tag{5.29}$$

where $\widetilde{O}_\pm = \int db\,\widetilde{O}_{\pm,b}$ with

$$\widetilde{O}_{\pm,b} \;=\; \lim_{\epsilon\downarrow 0}\,T^{\Pi}(f^{-1}(b)\mp\imath\epsilon)\,\big|\Im m\,G_0^{\Pi}(f^{-1}(b))\big|^{\frac{1}{2}}\,\Pi_b^*\,. \tag{5.30}$$

It is part of the proof of the following result to show that the limit in (5.30) exists and that the expression (5.15) for the T-matrix can be replaced to give

$$\widetilde{O}_{\pm,b} \;=\; \Big((V^{\Pi})^{-1} - \Re e\,G_0^{\Pi}(f^{-1}(b))\,\mp\,\imath\,\big|\Im m\,G_0^{\Pi}(f^{-1}(b))\big|\Big)^{-1}\,\big|\Im m\,G_0^{\Pi}(f^{-1}(b))\big|^{\frac{1}{2}}\,\Pi_b^*\,. \tag{5.31}$$

5.12 Theorem *Let $d \geq 3$ and let V have finite support. In addition, F is chosen as in* (5.1) *and it will be assumed that there are no threshold singularities and no embedded eigenvalues. Then the operators $\widetilde{O}_{\pm,b}$ are well-defined, continuous in b and uniformly bounded. The wave operators are given by*

$$\widetilde{\Omega}_{\pm} \;=\; \mathbf{1} + \imath\, \Pi_{\widetilde{B}} \left|\Im m\, G_0^{\Pi}(f^{-1}(\widetilde{B}))\right|^{\frac{1}{2}} \Big(\pm\,\mathbf{1} \,+\, \tanh(\tfrac{\pi}{2}\widetilde{A})\Big)\, \widetilde{O}_{\pm}\,. \qquad (5.32)$$

Formula (5.32) shows that the wave operator can be calculated in terms of $\widetilde{O}_{\pm}$ and the dilation operator $\widetilde{A}$. In [BS] it is shown that a modified formula also holds in presence of certain threshold singularities and embedded eigenvalues. The formula is similar to those obtained by Kellendonk and Richard for continuous scattering systems [KR].

Proof of Theorem 5.12: It follows from the hypothesis that the operators $\widetilde{O}_{\pm}$ are well-defined and bounded with fibers $\widetilde{O}_{\pm,b}$ depending continuously on b. We now show how (5.32) follows from (5.29). Thanks to the formulas (5.6), $\mathcal{E}(\theta_b(\sigma)) = f^{-1}(b) = E_r + \Delta\tanh(b)$ and $F(f^{-1}(b)) = \Delta\cosh^{-2}(b)$, a bit of algebra now leads to

$$((\widetilde{\Omega}_{\pm} - \mathbf{1})\phi)_b \;=\; \Pi_b \left|\Im m\; G_0^{\Pi}(f^{-1}(b))\right|^{\frac{1}{2}} \int \frac{db'}{\pi}\; \frac{1}{\sinh(b'-b)\mp\imath 0}\; (\widetilde{O}_{\pm}\phi)_{b'}\,.$$

In the previous formula, $\widetilde{O}_{\pm}\phi$ is a vector in the Hilbert space $L^2(\mathbb{R})\otimes\mathbb{C}^{|\Lambda|}$. As previously let $\widetilde{A} = -\imath\partial_b$ be the generator of the translation group in $L^2(\mathbb{R})\otimes L^2(\Sigma,\nu)$ as well as $L^2(\mathbb{R})\otimes\mathbb{C}^{|\Lambda|}$. Changing the integration variable b' to $u = b'-b$ leads to $(\widetilde{O}_{\pm}\phi)_{u+b} = (e^{\imath\widetilde{A}u}\widetilde{O}_{\pm}\phi)_b$. Hence

$$\Big((\widetilde{\Omega}_{\pm} - \mathbf{1})\phi\Big)_b \;=\; \sum_{\kappa=\pm1} \Pi_b \left|\Im m\; G_0^{\Pi}(f^{-1}(b))\right|^{\frac{1}{2}} \int \frac{du}{\pi}\; \frac{1}{\sinh(u)\mp\imath 0}\; \Big(e^{\imath\widetilde{A}u}\widetilde{O}_{\pm}\phi\Big)_b\,.$$

Now (5.32) is obtained from the following identity:

$$\int \frac{du}{\pi\imath}\; \frac{e^{\imath\widetilde{A}u}}{\sinh\big(u\big)\mp\imath 0} \;=\; \pm\mathbf{1} \,+\, \tanh(\tfrac{\pi}{2}\widetilde{A})\,.$$

This concludes the proof. □

5.7 The scattering operator and scattering matrices

Whenever the wave operators are complete, the scattering operator is defined by:

$$S \;=\; \Omega_+^*\Omega_-\,.$$

It is unitary and satisfies $[S, H_0] = 0$. Hence, in the REF representation, $[\widetilde{S},\widetilde{B}] = 0$ and thus $\widetilde{S} = \int db\, \widetilde{S}_b$ with unitary operators $\widetilde{S}_b$ on $L^2(\Sigma,\nu)$. The intertwining relation and the invariance principle (Theorem 4.2) imply that for any admissible function f with $f' > 0$, one has

$$\operatorname*{s-lim}_{t\to\pm\infty}\; e^{\imath t f(H_0)}\,\Omega_{\pm}\, e^{-\imath t f(H_0)} \;=\; \Omega_{\pm}^*\Omega_{\pm} \;=\; \mathbf{1}\,, \qquad\qquad \operatorname*{s-lim}_{t\to\mp\infty}\; e^{\imath t f(H_0)}\,\Omega_{\pm}\, e^{-\imath t f(H_0)} \;=\; \Omega_{\mp}^*\Omega_{\pm}\,.$$

The second expression is either S or S^*. Let now $f : (E_-, E_+) \to \mathbb{R}$ be chosen as in (5.6). It is smooth and has positive derivative and integrable second derivative. It is therefore admissible for Birman's invariance principle. In the REF representation, Proposition 5.9 then leads to

$$\underset{t\to\pm\infty}{\text{s-lim}}\; e^{\imath t\widetilde{B}}\,\widetilde{\Omega}_{\pm}\,e^{-\imath t\widetilde{B}} \;=\; \mathbf{1}\,, \qquad \underset{t\to\infty}{\text{s-lim}}\; e^{\imath t\widetilde{B}}\,\widetilde{\Omega}_{-}\,e^{-\imath t\widetilde{B}} \;=\; \widetilde{S}\,, \qquad \underset{t\to-\infty}{\text{s-lim}}\; e^{\imath t\widetilde{B}}\,\widetilde{\Omega}_{+}\,e^{-\imath t\widetilde{B}} \;=\; \widetilde{S}^*\,. \tag{5.33}$$

Using the explicit formula for $\widetilde{\Omega}_-$ given in Theorem 5.12 now leads to an explicit expression for the on-shell scattering matrix. The structure of such formulas (in particular, the EF representation of the formula (5.35) in the proof below) is well-known and has appeared in various guises (see [Yaf] for a list of references).

5.13 Theorem *Let the assumptions of* Theorem 5.12 *hold. Then the on-shell scattering matrix $\widetilde{S}_b$ is a unitary operator on $L^2(\Sigma,\nu)$ depending continuously on b and given by*

$$\widetilde{S}_b \;=\; (\mathbf{1}-\Pi_b\Pi_b^*) + \Pi_b(C_b-\imath)(C_b+\imath)^{-1}\Pi_b^*\,,$$

where the selfajoint $L\times L$ matrix $C_b : P_b\,\mathbb{C}^{|\Lambda|}\to P_b\,\mathbb{C}^{|\Lambda|}$ is defined by

$$C_b \;=\; P_b\big|\Im m\, G_0^{\Pi}(f^{-1}(b))\big|^{-\frac{1}{2}}\Big((V^{\Pi})^{-1} - \Re e\, G_0^{\Pi}(f^{-1}(b))\Big)\big|\Im m\, G_0^{\Pi}(f^{-1}(b))\big|^{-\frac{1}{2}}\,P_b\,.$$

Proof: For any function g the following formula holds $e^{\imath t\widetilde{B}}g(\widetilde{A})e^{-\imath t\widetilde{B}} = g(\widetilde{A}-t)$. The limits $t\to\pm\infty$ can be taken whenever g has limits at infinity. The function appearing in (5.32) is of that type. The middle formula in equation (5.33) and the expression of $\widetilde{\Omega}_-$ given in Theorem 5.12 leads to the calculation of $\widetilde{S}$, namely

$$\widetilde{S}_b \;=\; \mathbf{1} + \imath\,\Pi_b\,\big|\Im m\, G_0^{\Pi}(f^{-1}(b))\big|^{\frac{1}{2}}\,(-2)\,\widetilde{O}_{\pm,b}\,, \tag{5.34}$$

Because Theorem 5.12 states that $\widetilde{O}_{\pm,b}$ is continuous in b, this formula already shows that $\widetilde{S}_b$ is continuous in b. Using equation (5.31), it now follows that

$$\widetilde{S}_b \;=\; \mathbf{1} - 2\,\imath\,\Pi_b\,\big|\Im m\, G_0^{\Pi}(f^{-1}(b))\big|^{\frac{1}{2}}\Big((V^{\Pi})^{-1} - G_0^{\Pi}(f^{-1}(b)+\imath 0)\Big)^{-1}\big|\Im m\, G_0^{\Pi}(f^{-1}(b))\big|^{\frac{1}{2}}\,\Pi_b^*\,.$$

After simplification, one gets

$$\widetilde{S}_b \;=\; \mathbf{1} - 2\,\imath\,\Pi_b(C_b+\imath)^{-1}\Pi_b^*\,. \tag{5.35}$$

This allows to prove the claim. □

Similar formulas hold for the EF-representation of the scattering matrix. The comments made in Section 5.5 and the results of Theorem 5.13 lead to (with $C_E = C_b$ for $b = f(E)$),

$$\overset{\circ}{S}_E \;=\; \widetilde{S}_{f(E)} \;=\; (\mathbf{1}-\Pi_E\Pi_E^*) + \Pi_E(C_E-\imath)(C_E+\imath)^{-1}\Pi_E^*\,.$$

It is now possible to get results on the asymptotics of the scattering matrix.

5.14 Proposition *Let the assumptions of* Theorem 5.12 *hold. Then* $\lim_{b\to\pm\infty}\,\widetilde{S}_b = \mathbf{1}$.

Proof. If there are no threshold singularities, then $\lim_{b\to\pm\infty}\widetilde{O}_{\pm,b} = 0$ as was shown in Section 5.6. As $\big|\Im m\, G_0^{\Pi}(f^{-1}(b))\big|^{\frac{1}{2}}\,e^{\kappa\frac{b}{2}}$ is bounded, it follows from (5.34) that $\lim_{b\to\pm\infty}\;\widetilde{S}_b = \mathbf{1}$. For $d\geq 5$, it has been shown that $\widetilde{O}_{\pm,b}$ is uniformly bounded even in the presence of threshold singularities. As the factor $\big|\Im m\, G_0^{\Pi}(f^{-1}(b))\big|^{\frac{1}{2}}\,e^{\kappa\frac{b}{2}}$ vanishes in the limits $b\to\pm\infty$, the same conclusion holds thanks to equation (5.34). □

5.8 The time delay operator

The time delay operator T is the derivative of the scattering matrix w.r.t. the energy (the notation T should not be confused the T-matrix). More formally, it is defined by $T = \frac{1}{\imath} S^{-1}[A, S]$ whenever S is differentiable w.r.t. to the dilation A. In the REF it becomes

$$\widetilde{T} \;=\; \int db\, \widetilde{T}_b\,, \qquad\qquad \widetilde{T}_b \;=\; \frac{1}{\imath}\,(\widetilde{S}_b)^{-1}\partial_b\widetilde{S}_b\,,$$

while in the EF representations it is given by

$$\overset{\circ}{T} \;=\; \int_{E_-}^{E_+} dE\, \overset{\circ}{T}_E\,, \qquad\qquad \overset{\circ}{T}_E \;=\; \frac{1}{\imath}\,(\overset{\circ}{S}_E)^{-1}\partial_E\overset{\circ}{S}_E\,.$$

The *total time delay* is the trace of T. The formula given in the following result is sometimes called the *spectral property* of the time-delay [TO, New]

5.15 Theorem *Let the assumptions of* Theorem 5.12. *In addition, suppose that* $\mathcal{F}_E = \mathbb{C}^{|\Lambda|}$ *for almost all* E. *Then, for almost all* $E \in [E_-, E_+]$,

$$\mathrm{Tr}_{L^2(\Sigma,\nu)}(\overset{\circ}{T}_E) \;=\; \lim_{\epsilon\downarrow 0}\; 2\,\Im m\; \mathrm{Tr}_{\ell^2(\mathbb{Z}^d)}\left(\frac{1}{E-\imath\epsilon-H} \;-\; \frac{1}{E-\imath\epsilon-H_0}\right)\,. \qquad (5.36)$$

Proof of Theorem 5.15: The following notation will be used $\Pi_E = \Pi_{f(E)}$, $C_E = C_{f(E)}$ etc. From equation (5.35), it follows that

$$\frac{1}{2\imath}\,\partial_E\overset{\circ}{S}_E \;=\; -\partial_E\Pi_E(C_E+\imath)^{-1}\Pi_E^* + \Pi_E(C_E+\imath)^{-1}\partial_E C_E(C_E+\imath)^{-1}\Pi_E^* - \Pi_E(C_E+\imath)^{-1}\partial_E\Pi_E^*\,.$$

The equation $\Pi_E\Pi_E^* = \mathbf{1}_{\mathbb{C}^{|\Lambda|}}$ implies $\partial_E\Pi_E\Pi_E^* = -\Pi_E\partial_E\Pi_E^*$. Hence,

$$\mathrm{Tr}_{L^2(\Sigma,\nu)}(\overset{\circ}{T}_E) \;=\; \frac{1}{\imath}\,\mathrm{Tr}_{\mathcal{F}_E}\left(\Pi_E^*(\overset{\circ}{S}_E)^*\Pi_E\,\Pi_E^*\partial_E\overset{\circ}{S}_E\Pi_E\right) \;=\; 2\,\mathrm{Tr}_{\mathbb{C}^{|\Lambda|}}\left((C_E^2+1)^{-1}\partial_E C_E\right)\,.$$

This can be rewritten as

$$\mathrm{Tr}_{L^2(\Sigma,\nu)}(\overset{\circ}{T}_E) \;=\; \frac{1}{\imath}\,\partial_E\,\ln\,\det\left(\frac{C_E-\imath}{C_E+\imath}\right)\,.$$

Therefore dividing out the imaginary part of the Green function appearing in the definition of C_E (see Theorem 5.13) gives

$$\begin{aligned}\mathrm{Tr}_{L^2(\Sigma,\nu)}(\overset{\circ}{T}_E) \;&=\; \frac{1}{\imath}\,\partial_E\,\ln\,\det\Big(P_E\big((V^\Pi)^{-1}-G_0^\Pi(E-\imath 0)\big)P_E\big(P_E((V^\Pi)^{-1}-G_0^\Pi(E+\imath 0))P_E\big)^{-1}\Big)\\ &=\; 2\,\Im m\,\partial_E\,\ln\,\det\big(P_E((V^\Pi)^{-1}-G_0^\Pi(E-\imath 0))P_E\big)\,.\end{aligned}$$

On the other hand, using (5.16) and the cyclicity of the trace, leads to

$$\mathrm{Tr}_{\ell^2(\mathbb{Z}^d)}\big((z-H)^{-1}-(z-H_0)^{-1}\big) \;=\; \mathrm{Tr}_{\mathbb{C}^{|\Lambda|}}\Big(\Pi(z-H_0)^{-2}\Pi^*\big((V^\Pi)^{-1}-G_0^\Pi(z)\big)^{-1}\Big)\,.$$

Since $\partial_z G_0^\Pi(z) = -\Pi(z-H_0)^{-2}\Pi^*$, it follows that

$$\mathrm{Tr}_{\ell^2(\mathbb{Z}^d)}\big((z-H)^{-1}-(z-H_0)^{-1}\big) \;=\; \partial_z\,\mathrm{Tr}_{\mathbb{C}^{|\Lambda|}}\Big(\ln((V^\Pi)^{-1}-G_0^\Pi(z))\Big)\,.$$

This leads to the identity. □

5.9 A Levinson-type theorem

5.16 Theorem *Let the assumptions of* Theorem 5.12 *hold. Further let* $N = \mathrm{Tr}(P_{\mathrm{pp}})$ *be the number of bound states of* H*. Then*

$$\frac{1}{2\pi} \int_{E_-}^{E_+} dE \; \mathrm{Tr}_{L^2(\Sigma,\nu)}(\mathring{T}_E) \; + \; N \; = \; 0 \, . \tag{5.37}$$

Proof of Theorem 5.16: The number N of eigenvalues is obtained by counting the poles of the resolvent using the Cauchy formula and a contour integration. The contour is given by two circles, one large counterclockwise oriented circle γ around the spectrum of H and a second small clockwise oriented circle Γ around the spectrum of H_0 (but not touching it). Then

$$N \; = \; \oint_{\Gamma+\gamma} \frac{dz}{2\pi\imath} \, \mathrm{Tr}_{\ell^2(\mathbb{Z}^d)}\big((z-H)^{-1} - (z-H_0)^{-1}\big) \, . \tag{5.38}$$

The resolvent identity implies that the contribution of γ vanishes in the limit where its radius goes to infinity. Then let Γ converge to the concatenation of the two intervals $[E_- + \imath 0, E_+ + \imath 0]$ and $[E_- - \imath 0, E_+ - \imath 0]$. Since it has been assumed that there is no threshold singularity, the regularity of the Green function at the band edges implies that the small circle connecting these contours near the band edges have a vanishing contribution in the contour integral. Thus

$$N \; = \; \int_{E_-}^{E_+} \frac{dE}{2\pi\imath} \, \mathrm{Tr}_{\ell^2(\mathbb{Z}^d)} \left(\frac{1}{E+\imath 0 - H} - \frac{1}{E+\imath 0 - H_0} - \frac{1}{E-\imath 0 - H} + \frac{1}{E-\imath 0 - H_0} \right) \, .$$

The formula for the total time delay, proved in Theorem 5.15, gives

$$N \; = \; -\frac{1}{2\pi} \int_{E_-}^{E_+} dE \; \mathrm{Tr}_{L^2(\Sigma,\nu)}(\mathring{T}_E) \, .$$

This is the result in the situation considered. □

A Spectral decomposition

Recall that the Lebesgue decomposition theorem states every measure μ on the real line can be uniquely decomposed into an absolutely continuous part w.r.t. the Lebesgue measure on $\mathbb{R}$ (this means that sets of zero Lebesgue measure also have zero μ_{ac}-measure, by the theorem of Radon-Nikodym this is equivalent to having a L^1-density f such that $\mu_{\mathrm{ac}}(dE) = f(E)dE$ holds), a pure-point part μ_{pp} (consisting of countable set of Dirac peaks with summable weights) and a remainder called the singular continuous part μ_{sc}:

$$\mu \;=\; \mu_{\mathrm{ac}} + \mu_{\mathrm{pp}} + \mu_{\mathrm{sc}}\;.$$

Moreover, the three measures on the r.h.s. are mutually singular, namely one is supported on a zero measure set of the others. Let us point out that μ_{pp} is readily defined using all atoms of μ. If one then sets $\mu_{\mathrm{c}} = \mu - \mu_{\mathrm{pp}}$, the main claim of the Lebesgue decomposition is that $\mu_{\mathrm{c}} = \mu_{\mathrm{ac}} + \mu_{\mathrm{sc}}$. But μ_{ac} is just obtained as the Radon-Nikodym derivative of μ_{c} w.r.t. $\mu_{\mathrm{c}} + \mu_{\mathrm{Leb}}$ (for details see any book on measure theory), and then μ_{sc} is simply the remainder. Furthermore, the mutual singularity implies

$$L^2(\mu) \;=\; L^2(\mu_{\mathrm{ac}}) \oplus L^2(\mu_{\mathrm{pp}}) \oplus L^2(\mu_{\mathrm{sc}})\;.$$

Now given a self-adjoint operator H on a Hilbert space $\mathcal{H}$, one introduces the pure point subspace $\mathcal{H}_{\mathrm{pp}} \subset \mathcal{H}$ as the closure of the span of all eigenvectors of H. Then $\mathcal{H}_{\mathrm{c}} = (\mathcal{H}_{\mathrm{pp}})^{\perp}$ is the continuous subspace. Then the absolutely continuous subspace is defined as

$$\mathcal{H}_{\mathrm{ac}} \;=\; \{\phi \in \mathcal{H}_{\mathrm{c}} \,|\, \mu_\phi \;\text{ is purely absolutely continuous}\}\;,$$

and finally $\mathcal{H}_{\mathrm{sc}} = \mathcal{H}_{\mathrm{c}} \ominus \mathcal{H}_{\mathrm{ac}}$.

A.1 Proposition *The subspaces $\mathcal{H}_{\mathrm{ac}}$, $\mathcal{H}_{\mathrm{pp}}$ and $\mathcal{H}_{\mathrm{sc}}$ associated to a bounded selfadjoint operator H are closed, mutually orthogonal, invariant under H and*

$$\mathcal{H} \;=\; \mathcal{H}_{\mathrm{ac}} \oplus \mathcal{H}_{\mathrm{pp}} \oplus \mathcal{H}_{\mathrm{sc}}\;. \tag{A.1}$$

Proof. It just remains to show that $\mathcal{H}_{\mathrm{ac}}$ is closed. Let $(\psi_n)_{n\geq 1}$ be a sequence in $\mathcal{H}_{\mathrm{ac}}$ converging to ψ. Then $\mu_{\psi_n} \to \mu_\psi$ weakly. If now $N \subset \mathbb{R}$ is a set of zero Lebesgue measure, then $\mu_\psi(N) = \lim_n \mu_{\psi_n}(N) = 0$ so that $\psi \in \mathcal{H}_{\mathrm{ac}}$. □

Now one sets $H_{\mathrm{ac}} = H|_{\mathcal{H}_{\mathrm{ac}}}$ and $\sigma_{\mathrm{ac}}(H) = \sigma(H_{\mathrm{ac}})$, and similarly $\sigma_{\mathrm{pp}}(H)$ and $\sigma_{\mathrm{sc}}(H)$ are defined. Obviously one has

$$\sigma(H) \;=\; \sigma_{\mathrm{ac}}(H) \cup \sigma_{\mathrm{pp}}(H) \cup \sigma_{\mathrm{sc}}(H)\;,$$

but this decomposition is in general not disjoint. Also note that if $\sigma_{\mathrm{p}}(H)$ denotes the set of eigenvalues of H (which is hence a countable set because $\mathcal{H}$ is separable), then $\sigma_{\mathrm{pp}}(H) = \overline{\sigma_{\mathrm{p}}(H)}$ as the spectrum of an operator such as $H_{\mathrm{pp}} = H|_{\mathcal{H}_{\mathrm{pp}}}$ is always closed.

B Morse lemma

We prove a global Morse lemma providing a change of coordinates on the torus for which each critical point is in the normal form.

B.1 Lemma *Let $\mathcal{E} : \mathbb{T}^d \to \mathbb{R}$ be a smooth Morse function. Then there is a smooth diffeomorphism $\varphi : \mathbb{T}^d \to \mathbb{T}^d$ and a number $\delta > 0$ such that for all critical points $k^* \in \mathcal{S}^*$*

$$\mathcal{E} \circ \varphi(k^* + k) \;=\; \mathcal{E}(k^*) \;+\; \frac{1}{2}\,\langle k|\nabla^2\mathcal{E}(0)|k\rangle\,, \qquad |k| < \delta\,.$$

Moreover, φ leaves the set $\mathcal{S}^*$ invariant and satisfies $\varphi'(k^*) = \mathbf{1}$ for all $k^* \in \mathcal{S}^*$.

Proof. This proof follows a standard procedure [Nic]. The idea is to construct φ using the inverse of the flow φ_t at time $t = 1$ associated to a time-dependent smooth vector field $Y_t : \mathbb{T}^d \to \mathbb{R}^d$. This vector field is first constructed locally at every critical point k^*, which we may choose to be $k^* = 0$. Set

$$\mathcal{E}_t(k) \;=\; (1-t)\mathcal{E}(k) \;+\; t\,Q(k)\,,$$

where $Q(k) = \frac{1}{2}\,\langle k|\mathcal{E}''(0)|k\rangle$ is the quadratic form associated to the critical point. We first search diffeomorphisms φ_t such that $\mathcal{E} = \mathcal{E}_t \circ \varphi_t$ and $\varphi_t(0) = 0$ and attempt to find them locally as flow of a vector fields Y_t defined by $Y_t \circ \varphi_t = \partial_t \varphi_t$. This field then has to satisfy

$$0 \;=\; \partial_t\,\mathcal{E}_t \circ \varphi_t \;=\; Y_t(\mathcal{E}_t) \circ \varphi_t - \mathcal{E} \circ \varphi_t + Q \circ \varphi_t\,,$$

where $Y_t(\mathcal{E}_t) = \langle Y_t|\nabla\rangle\mathcal{E}_t$. Hence one needs to find a local solution to the homology equations

$$Y_t(\mathcal{E}_t) \;=\; \mathcal{E} - Q\,, \qquad Y_t(0) = 0\,.$$

Inversely, once these equations are solved, we find φ_t as the flow of Y_t. The construction of Y_t is now as follows. As $(\mathcal{E} - Q)(0) = 0$ and $\nabla(\mathcal{E} - Q)(0) = 0$, one has

$$(\mathcal{E} - Q)(k) \;=\; \int_0^1 ds' \int_0^{s'} ds\, \partial_s^2(\mathcal{E} - Q)(sk) \;=\; \int_0^1 ds' \int_0^{s'} ds\, \langle k|\nabla^2(\mathcal{E} - Q)(sk)|k\rangle\,.$$

Because the critical point is non-degenerate, the inverse function theorem implies that the map $k \in B_\delta(0) \mapsto \nabla\mathcal{E}_t(k)$ is invertible for some $\delta > 0$. Let this inverse be denoted by $\xi_t(\nabla\mathcal{E}_t(k)) = k$. It satisfies $\xi_t(0) = 0$ so that

$$k \;=\; \int_0^1 dr\; \partial_r \xi_t(r\nabla\mathcal{E}_t(k)) \;=\; \int_0^1 dr\; \nabla\xi_t(r\nabla\mathcal{E}_t(k))\,\nabla\mathcal{E}_t(k)\,.$$

Replacing in the above shows that

$$Y_t(k) \;=\; \int_0^1 dr \int_0^1 ds' \int_0^{s'} ds\, \nabla\xi_t(r\nabla\mathcal{E}_t(k))^t\, \nabla^2(\mathcal{E} - Q)(sk)|k\rangle\,,$$

solves the homology equation. It also satisfies $|Y_t(k)| \leq C\,|k|$ for some constant C. This construction provides a smooth vector field in $B_\delta(k^*)$ for every $k^* \in \mathcal{S}^*$ and an adequate $\delta > 0$. It can be smoothly continued to a vector field Y_t which vanishes except in $B_{2\delta}(k^*)$. Let φ_t be the associated flow. Then

$$\mathcal{E} \circ \varphi_1^{-1}(k^* + k) \;=\; \langle k|\nabla^2\mathcal{E}(k^*)|k\rangle\,, \qquad |k| < \delta\,, \quad k^* \in \mathcal{S}^*\,.$$

Summing such contributions from all critical points one obtains a smooth vector field Y on $\mathbb{T}^d$ and its associated flow φ_1 at time 1 diagonalizes the Hessians at all critical points. Then $\varphi = (\varphi_1)^{-1}$ is the desired diffeomorphism. □

The proof shows that the diffeomorphism φ can, moreover, be constructed such that it is given by the identity on the complement of $\bigcup_{k^* \in \mathcal{S}^*} B_{2\delta}(k^*)$.

C Boundary values of the Borel transform

Here the Plemelj-Privalov theorem on properties of the Borel transform of a function is proved. Ohter arguments can be found in the literature, [Mus] and [Kre, Section 7].

C.1 Lemma *Let $\rho : \mathbb{R} \to \mathbb{C}$ be a Hölder continuous function of exponent $\alpha \in (0, 1]$ with compact support. Then, for any β such that $0 < \beta < \alpha$, its Borel transform*

$$G_\rho(z) \; = \; \int_{\mathbb{R}} \frac{\rho(e)\, de}{z - e} \tag{C.1}$$

is holomorphic in $\mathbb{C} \setminus \mathrm{supp}(\rho)$ and its boundary value on the real axis is Hölder continuous with exponent β. If ρ is real-valued, then

$$G_\rho(E \pm \imath 0) \; = \; \mp \imath \, \pi \, \rho(E) \; + \; ⨍_{\mathbb{R}} \frac{\rho(e)\, de}{E - e}$$

where $⨍$ denotes the Cauchy principal value.

Proof: The holomorphy of G_ρ outside supp(ρ) is a standard result that will not be proved here. By decomposing ρ into its real and imaginary part, if necessary, there is no loss of generality in assuming that ρ is real-valued. For $\epsilon > 0$ and $E \in \mathbb{R}$, $G_\rho(E + \imath\epsilon)$ is given by

$$G_\rho(E \pm \imath\epsilon) \; = \; \int_{\mathbb{R}} de \, \frac{\rho(e)(E - e \mp \imath\epsilon)}{(E - e)^2 + \epsilon^2} \; = \; R_\rho(E, \epsilon) \; \mp \; \imath \, I_\rho(E, \epsilon) \, ,$$

where

$$I_\rho(E, \epsilon) \; = \; \int_{\mathbb{R}} de \, \frac{\rho(e)\epsilon}{(E - e)^2 + \epsilon^2} \, , \qquad\qquad R_\rho(E, \epsilon) \; = \; \int_{\mathbb{R}} de \, \frac{\rho(e)(E - e)}{(E - e)^2 + \epsilon^2} \, . \tag{C.2}$$

The first term admits $\pi\rho(E)$ as a limit as $\epsilon \downarrow 0$. This is because, using the change of variables $e = E + \epsilon x$ and the Lebesgue dominated convergence theorem, gives

$$\lim_{\epsilon \downarrow 0} \; I_\rho(E, \epsilon) \; = \; \lim_{\epsilon \downarrow 0} \int_{\mathbb{R}} \frac{dx}{x^2 + 1} \, \rho(E + \epsilon x) \; = \; \rho(E) \int_{\mathbb{R}} \frac{dx}{x^2 + 1} \; = \; \pi \, \rho(E) \, . \tag{C.3}$$

Similarly, using the change of variable $u = e - E$ and the symmetry $u \mapsto -u$, one obtains

$$R_\rho(E, \epsilon) \; = \; \int_0^\infty \frac{u \, du}{u^2 + \epsilon^2} \, \big(\rho(E - u) - \rho(E + u)\big) \, . \tag{C.4}$$

For all $a > 0$, the part of the integral corresponding to $0 < a \leq u$ is also Hölder continuous of exponent α w.r.t. E, thanks to Lebesgue's dominated convergence theorem. In particular, if E is not in the support of ρ, the integral over u never reaches $u = 0$ so that $R_\rho(E)$ is Hölder continuous outside the support of ρ. However, if ρ is real valued, R_ρ is the restriction to the complement of the support of ρ (in the real line) of the real part of an holomorphic function and is therefore analytic. On the other hand, since ρ is Hölder continuous of exponent α and with compact support, it follows that there is a constant $K > 0$ for which $|\rho(E + \delta \pm u) - \rho(E \pm u)| \leq K\delta^\alpha$ uniformly w.r.t. E and u. In particular, $|\rho(E - u) - \rho(E + u)| \leq K(2u)^\alpha$ and

$$|\rho(E + \delta + u) - \rho(E + u) - \rho(E + \delta - u) + \rho(E - u)| \; \leq \; 2K \min\{\delta^\alpha, (2u)^\alpha\} \; \leq \; 2^{1+\alpha-\beta} K \delta^\beta u^{\alpha-\beta} \, ,$$

for any $0 < \beta < \alpha$. Using this estimate inside the part of the integral for which $u \in [0, 1]$ and thanks to the dominated convergence theorem, it follows that $\lim_{\epsilon \downarrow 0} R_\rho(E, \epsilon)$ exists and is Hölder continuous of exponent β for $E \in \mathrm{supp}(\rho)$. The last formula also follows from the above. $\Box$

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