Introduction to Scattering Theory

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Chapter 1

Classical particle scattering

Scattering occurs in a variety of physical situations. It normally involves a comparison of two different dynamics for the same system: the given dynamics and a "free" dynamics. It is hard to give a precise definition of "free dynamics" but important characteristics of a free dynamical system are that it is simpler than the given dynamics and that it conserves the momentum of the "individual constituents" of the physical system.

The simplest system with which to illustrate the ideas of scattering theory is the classical mechanics of a single particle moving in an external force field $f(x)$, $x \in \mathbb{R}^3$. This theory is equivalent to the scattering of two particles interacting with each other through a force field $f(x_1 - x_2)$ because the center of mass motion of such a two-body system separates from the motion of $x_{12} = x_1 - x_2$. The states of such a single particle system are points in *phase space* $\mathbb{R}^3 \times \mathbb{R}^3$, i.e. pairs $u(t) = (x(t), \dot{x}(t)) \in \mathbb{R}^6$ representing the position and the velocity of the particle. The evolution is given by the equation

$$\frac{\mathrm{d}}{\mathrm{d}t} u(t) = F(u(t)). \tag{1.1}$$

The force field is obtained from a *potential* $V(x)$ and equals $-\mathrm{grad}\ V(x)$. The right-hand side of the evolution equation (1.1) thus reads

$$F(u(t)) = F \begin{pmatrix} x(t) \\ \dot{x}(t) \end{pmatrix} = \begin{pmatrix} \dot{x}(t) \\ -\frac{1}{m}\,\mathrm{grad}\ V(x(t)) \end{pmatrix}.$$

Let us assume for simplicity that V has compact support and that the particle moves outside the support of V (and hence outside of the corresponding force field) for large $|t|$. We can then expect that

$$\begin{aligned} x(t) &= x_- + tv_-, \quad t \to -\infty, \\ x(t) &= x_+ + tv_+, \quad t \to +\infty. \end{aligned}$$

Conservation of the energy E implies that $|v_+| = |v_-|$. Furthermore, integrating the conservation law $\frac{1}{2} m\dot{x}(t)^2 = E - V(x(t))$ with a given initial condition $(x(t_0), \dot{x}(t_0)) =$

$(x_- + t_0 v_-, v_-)$, for t_0 sufficiently near $-\infty$ so that $\{x_- + tv_-, t < t_0\} \cap \operatorname{supp} V = \emptyset$, we observe that x_+ and v_+ are functions of x_- and v_-. This motivates to define the *scattering map*

$$S\colon \mathbb{R}^6 \to \mathbb{R}^6, \quad \begin{pmatrix} x_- \\ v_- \end{pmatrix} \mapsto \begin{pmatrix} x_+ \\ v_+ \end{pmatrix}.$$

Let us consider a particle moving in one spatial direction and assume that V is bounded, $V(x) \leq E_0 = \max V$. For energies $E < E_0$, the particle will be reflected by the potential; its velocity will change sign (and vary temporarily while the particle is moving inside the support of V). The scattering map thus is of the form

$$\begin{pmatrix} x_- \\ v_- \end{pmatrix} \mapsto \begin{pmatrix} x_+(x_-, v_-) \\ -v_- \end{pmatrix}.$$

For $E > E_0$ the particle moves through and we expect a time delay compared with the free dynamics and again a temporary change of the velocity such that finally $v_+ = v_-$. The scattering map now has the form

$$\begin{pmatrix} x_- \\ v_- \end{pmatrix} \mapsto \begin{pmatrix} x_+(x_-, v_-) \\ v_- \end{pmatrix}.$$

In the case $E = E_0$ the particle stops at x_0 with $V(x_0) = E_0$ (if this point is reached in finite time).

Next, let us suppose that $\operatorname{supp} V$ is not compact but that V and $\operatorname{grad} V$ are sufficiently small for $|x| \to \infty$. Then we expect that the position of the particle will not exactly but asymptotically be of the form $x_\pm + tv_\pm$, i.e.

$$\exists (x_\pm, v_\pm) \in \mathbb{R}^6\colon |x(t) - x_\pm - tv_\pm| \to 0, \quad t \to \pm\infty. \tag{1.2}$$

Observe that the potential must indeed be very small at $\pm\infty$; even for the Coulomb potential, the particle will not be asymptotically free.

Let us now consider a one-dimensional particle with positive energy E in a force field with the potential

$$V(x) = C(1 + |x|)^{-\alpha}, \quad \alpha > 0, \quad C \neq 0.$$

We show that the particle moves asymptotically free in the sense of (1.2) if $\alpha > 1$. For simplicity, let $m = 2$. It suffices to consider the case $t \to +\infty$. We can choose an initial condition such that $x(t) \to \infty$, $t \to \infty$. By conservation of energy, $\dot{x}(t)^2 = E - V(x(t))$ so that

$$\dot{x}(t) = \sqrt{E - V(x(t))} \to \sqrt{E}, \quad t \to +\infty. \tag{1.3}$$

In particular, $\dot{x}(t)$ does not change sign for large t and hence $\dot{x}(t) > 0$.

(1) Let $\alpha > 1$; here, it suffices to suppose that $|V(x)| \leq C(1+|x|)^{-\alpha}$. By (1.3), there are constants $t_0 \in \mathbb{R}$, $x_1 \in \mathbb{R}$ and $v_1 > 0$ such that for $t \geq t_0$

$$\begin{aligned} v_1 &\leq \dot{x}(t) \text{ and} \\ x_1 + v_1 t &\leq x(t). \end{aligned}$$

For any $y > 0$, the mean value theorem ensures the existence of $\eta \in (0, y)$ such that

$$\sqrt{E-y} = \sqrt{E-0} + y\left[\frac{\mathrm{d}}{\mathrm{d}s}\sqrt{E-s}\right]_{s=\eta} = \sqrt{E} - \frac{y}{2\sqrt{E-\eta}}.$$

For sufficiently large t, $E - V(x(t))$ is bounded away from zero so that there is a function $\eta(t)$ satisfying $|\eta(t)| \leq c(1+t)^{-\alpha}$ for some constant $c > 0$ and

$$\begin{aligned} \dot{x}(t) &= \sqrt{E - V(x(t))} = \sqrt{E} + \eta(t) \text{ and} \\ x(t) &= x_0 + \sqrt{E}\, t + \int_{t_0}^{t} \eta(\tau)\,\mathrm{d}\tau \\ &= x_0 + \sqrt{E}\, t + \int_{t_0}^{\infty} \eta(\tau)\,\mathrm{d}\tau - \int_{t}^{\infty} \eta(\tau)\,\mathrm{d}\tau \\ &= \tilde{x}_0 + \sqrt{E}\, t + \tilde{\eta}(t) \end{aligned}$$

with $|\tilde{\eta}(t)| \leq \tilde{c}\, t^{1-\alpha}$. This is the desired result with $x_+ = \tilde{x}_0$ and $v_+ = \sqrt{E}$.

(2) Assume that $\alpha \leq 1$. By (1.3) there are $c_1, c_2 > 0$ (for $C > 0$) or $c_1, c_2 < 0$ (for $C < 0$) so that for $\alpha < 1$ and large t

$$\begin{aligned} \dot{x}(t) &= \sqrt{E - V(x(t))} \begin{cases} \leq \sqrt{E} - c_1(1+t)^{-\alpha} \\ \geq \sqrt{E} - c_2(1+t)^{-\alpha} \end{cases} \quad \text{and} \\ x(t) &\begin{cases} \leq \sqrt{E}\, t + c_3 - \frac{c_1}{1-\alpha}(1+t)^{1-\alpha} \\ \geq \sqrt{E}\, t + c_4 - \frac{c_2}{1-\alpha}(1+t)^{1-\alpha}. \end{cases} \end{aligned}$$

For $\alpha = 1$, the term $\frac{1}{1-\alpha}(1+t)^{1-\alpha}$ has to be replaced by $\ln(1+t)$. Let us assume for a contradiction that (1.2) holds true. Let $\alpha < 1$. Then, for sufficiently large t,

$$\sqrt{E}\, t + c_4 - \frac{c_2}{1-\alpha}(1+t)^{1-\alpha} - 1 \leq x_+ + v_+ t \leq \sqrt{E}\, t + c_3 - \frac{c_1}{1-\alpha}(1+t)^{1-\alpha} + 1.$$

Dividing by t and computing the limit $t \to \infty$, this implies that $\sqrt{E} \leq v_+ \leq \sqrt{E}$, i.e. $v_+ = \sqrt{E}$. Hence $c_1 = 0$, a contradiction. Similarly, a contradiction is obtained in the case $\alpha = 1$.

Assume that the particle is asymptotically free in the sense of (1.2). The maps

$$\Omega_\pm \colon (x_\pm, v_\pm) \mapsto (x(t), v(t))$$

have an important analogy in the quantum mechanical setting where they are called the *(Møller)-wave operators.* The scattering map thus satisfies

$$S = \Omega_+^{-1}\Omega_-.$$

It describes the process of scattering without comprising the time-dependent details of the event. One of the most important and most difficult problems in scattering theory yet is the *inverse problem*: given the scattering map S what can we say about the scattering center or the potential respectively?

Concerning *Coulomb scattering*, we will observe a similar phenomenon in the quantum mechanical setting: the wave operators exist in general only for potentials that decay faster than the Coulomb potential.

Finally, to make contact with physical experiments, we comment briefly on the notions *cross section* and *scattering angles*: A beam of constant energy is sent towards a target. The beam has a wide spread and an approximately uniform density ρ of particles per unit area of the plane $\mathbb{R}^2$ orthogonal to the beam. A detector sits at some scattering angle (ϑ, φ) far away from the target and collects (and counts) all particles that leave the target within some angular region of size $\Delta\Omega$ about (ϑ, φ). The measured quantity is

$$\frac{\text{number of particles hitting the detector}}{(\Delta\Omega)\rho}.$$

If $\Delta\Omega$ is very small and the detector and source of particles are very far from the target, this quantity is called the *differential cross section.* The integral of the differential cross section over all spatial directions yields the *total cross section.*

Chapter 2

Basic principles of scattering in Hilbert spaces

We begin with a brief overview about some relevant aspects of spectral theory in Hilbert spaces. For more details, we refer to [K-I, K-II] and of course [RS-I].

Let $(A_n)_{n\in\mathbb{N}}$ be a sequence of bounded operators on the Hilbert space $\mathcal{H}$, $(A_n)_{n\in\mathbb{N}} \subset \mathcal{L}(\mathcal{H})$, and let $A \in \mathcal{L}(\mathcal{H})$ be given. We say:

$$\begin{aligned} A_n \to A \textit{ weakly} \quad &:\Longleftrightarrow \quad \langle A_n f, g\rangle \to \langle Af, g\rangle\,,\ \forall f, g \in \mathcal{H}, \\ A_n \to A \textit{ strongly} \quad &:\Longleftrightarrow \quad A_n f \to Af,\ \forall f \in \mathcal{H}, \\ A_n \to A \textit{ in norm} \quad &:\Longleftrightarrow \quad \|A_n - A\| = \sup\{\|A_n f - Af\|\,;\ \|f\| \le 1\} \to 0. \end{aligned}$$

Clearly, norm convergence $\Longrightarrow$ strong convergence $\Longrightarrow$ weak convergence. For the purposes of scattering theory, we will see that strong convergence is the appropriate notion.

Lemma 2.1. *Assume that* $A_n, B_n, A, B \in \mathcal{L}(\mathcal{H})$, $n \in \mathbb{N}$, *and that* $A_n \to A$ *strongly and* $B_n \to B$ *strongly. Then* $A_nB_n \to AB$ *strongly.*

Proof. By the Uniform Boundedness Principle, there exists a constant $c \ge 0$ with $\|A_n\| \le c$ for all $n \in \mathbb{N}$. Thus

$$\begin{aligned} \|A_nB_nf - ABf\| &\le \|A_nBf - ABf\| + \|A_nB_nf - A_nBf\| \\ &\le \|(A_n - A)Bf\| + \|A_n\|\,\|(B_n - B)f\| \\ &\to 0 \end{aligned}$$

as $n \to \infty$. □

Let $\mathcal{H}$ be a Hilbert space and let $A\colon D(A) \to \mathcal{H}$ be a self-adjoint operator. By the spectral theorem, there exists a unique spectral family $(E(\lambda))_{\lambda\in\mathbb{R}}$ such that $A = \int_{\mathbb{R}} \lambda\, \mathrm{d}E(\lambda)$. The operators $E(\lambda)$ are bounded, $E(\lambda) \in \mathcal{L}(\mathcal{H})$ for any $\lambda \in \mathbb{R}$, and projections, $E(\lambda)^2 = E(\lambda) = E(\lambda)^*$ for any $\lambda \in \mathbb{R}$, and satisfy the following properties:

(i) Monotonicity: $\lambda \leq \mu \implies E(\lambda) \leq E(\mu)$.

(ii) Strong right continuity: $\forall \lambda \in \mathbb{R}\, \forall f \in \mathcal{H}\colon E(\lambda+\varepsilon)f \to E(\lambda)f$, $\varepsilon \downarrow 0$.

(iii) For all $f \in \mathcal{H}$, we have that $E(\lambda)f \to f$, $\lambda \to \infty$, and $E(\lambda)f \to 0$, $\lambda \to -\infty$.

For any $\varphi, \psi \in \mathcal{H}$, the sesquilinear form $\langle A\varphi, \psi\rangle$ is the Riemann-Stieltjes integral

$$\langle A\varphi, \psi\rangle = \int_{\mathbb{R}} \lambda \, \mathrm{d} \langle E(\lambda)\varphi, \psi\rangle . \tag{2.1}$$

The function $\lambda \mapsto \langle E(\lambda)\varphi, \varphi\rangle = \|E(\lambda)\varphi\|^2$ is the spectral measure μ_φ associated with the vector φ. The spectral theorem also says that given a spectral family $(E(\lambda))_{\lambda\in\mathbb{R}}$, there exists a unique self-adjoint operator A such that $A = \int_{\mathbb{R}} \lambda \, \mathrm{d}E(\lambda)$. In fact, the domain of integration in (2.1) is $\sigma(A) \subset \mathbb{R}$, the spectrum of A, as $E(\cdot)$ is locally constant on the resolvent set $\rho(A)$.

The spectral theorem also allows to study functions of operators; we say that there exists a functional calculus in the following sense: For $A \in \mathcal{L}(\mathcal{H})$ there is a unique map $\Phi\colon C(\sigma(A)) \to \mathcal{L}(\mathcal{H})$ such that

(i) Φ is an algebraic $*$-homomorphism, that is

$$\begin{aligned} \Phi(fg) &= \Phi(f)\Phi(g), \\ \Phi(\lambda f) &= \lambda\Phi(f), \\ \Phi(1) &= I, \\ \Phi(\overline{f}) &= \Phi(f)^*. \end{aligned}$$

(ii) Φ is continuous, i.e. $\|\Phi(f)\|_{\mathcal{L}(\mathcal{H})} \leq C \|f\|_\infty$.

(iii) Let f be the function $f(x) = x$. Then $\Phi(f) = A$.

For unbounded operators one has a map $\hat{\Phi}$ from the bounded Borel functions on $\mathbb{R}$ into $\mathcal{L}(\mathcal{H})$ with similar properties. We then write $\Phi(f) = f(A)$ and have that

$$\langle f(A)\varphi, \varphi\rangle = \int_{\sigma(A)} f(\lambda) \, \mathrm{d}\mu_\varphi, \quad \forall \varphi \in \mathcal{H}.$$

We will see that $\mathrm{e}^{-\mathrm{i}tA}$, $t \in \mathbb{R}$, generates a strongly continuous group of unitary operators and that $u(t) := \mathrm{e}^{-\mathrm{i}tA}u_0$ solves the Schrödinger equation with initial value $u_0 \in L_2(\mathbb{R}^d)$, provided $A = -\Delta + V$ is a self-adjoint operator in the Hilbert space $L_2(\mathbb{R}^d)$. On the other hand, e^{-tA}, $t \geq 0$ and $A \geq 0$, is a strongly continuous semi-group of operators and $v(t) := \mathrm{e}^{-tA}v_0$ is a solution to the initial value problem for the heat equation, provided A is a self-adjoint extension of $-\Delta$. Characteristic functions $\chi_{(a,b]}(A) = E((a,b]) = E(b) - E(a)$ yield spectral projections associated with intervals. The operator $\sqrt{A}$ is the square root of A provided $A \geq 0$.

Concerning the spectrum $\sigma(A)$, we comment on three different decompositions:

$$\begin{aligned}\sigma(A) &= \sigma_{\mathrm{p}}(A) \,\dot\cup\, \sigma_{\mathrm{cont}}(A) \,\dot\cup\, \sigma_{\mathrm{res}}(A) &(2.2)\\ &= \sigma_{\mathrm{disc}}(A) \,\dot\cup\, \sigma_{\mathrm{ess}}(A) &(2.3)\\ &= \sigma_{\mathrm{pp}}(A) \cup \sigma_{\mathrm{ac}}(A) \cup \sigma_{\mathrm{sc}}(A). &(2.4)\end{aligned}$$

If $A - \lambda$ is not injective, i.e. $(A-\lambda)u = 0$ for some $u \in D(A)\backslash\{0\}$ or equivalently $N(A-\lambda) \neq \{0\}$, then $\lambda \in \sigma_{\mathrm{p}}(A)$ (point spectrum). If $A - \lambda$ is injective (but not surjective), one distinguishes between $\overline{R(A-\lambda)} = \mathcal{H}$ ($\lambda \in \sigma_{\mathrm{cont}}(A)$, continuous spectrum) and $R(A-\lambda)$ is not dense in $\mathcal{H}$ ($\lambda \in \sigma_{\mathrm{res}}(A)$, residual spectrum). In fact, for a self-adjoint operator, $\sigma_{\mathrm{res}}(A) = \emptyset$. The discontinuities of the spectral family correspond precisely to the point spectrum $\sigma_{\mathrm{p}}(A)$ whereas $E(\lambda)$ is strongly continuous at $\lambda_0 \in \sigma(A)$ if and only if $\lambda_0 \in \sigma_{\mathrm{cont}}(H)$.

In the second decomposition, the discrete spectrum $\sigma_{\mathrm{disc}}(A)$ comprises the eigenvalues of A having finite multiplicity and being isolated points of the spectrum. In other words, $\lambda \in \sigma_{\mathrm{disc}}(A)$ if and only if $0 < \dim N(A-\lambda) < \infty$ and if there is $\varepsilon > 0$ with the property $\sigma(A) \cap (\lambda - \varepsilon, \lambda + \varepsilon) = \{\lambda\}$. The essential spectrum $\sigma_{\mathrm{ess}}(A)$ contains the eigenvalues of infinite multiplicity and the accumulation points of the spectrum.

The third decomposition refers to Lebesgue's decomposition of a monotonic function $f\colon \mathbb{R} \to \mathbb{R}$ into a jump function f_{pp}, an absolutely continuous function f_{ac} and a singularly continuous function f_{sc} in the sense that $f = f_{\mathrm{pp}} + f_{\mathrm{ac}} + f_{\mathrm{sc}}$. For a spectral family $(E(\lambda))_{\lambda\in\mathbb{R}}$, the function $\lambda \mapsto \langle E(\lambda)\varphi, \varphi\rangle$ is monotonic and thus Lebesgue's decomposition applies to the associated spectral measure μ_φ. We define the following subspaces of $\mathcal{H}$:

$$\begin{aligned}\mathcal{H}_{\mathrm{pp}} &\coloneqq \overline{\operatorname{span}\{u \in D(A)\backslash\{0\}; \exists \lambda \in \mathbb{R}\colon Au = \lambda u\}},\\ \mathcal{H}_{\mathrm{ac}} &\coloneqq \{f \in \mathcal{H}; \|E(\cdot)f\|^2 \text{ is absolutely continuous}\},\\ \mathcal{H}_{\mathrm{sc}} &\coloneqq \{f \in \mathcal{H}; \|E(\cdot)f\|^2 \text{ is singularly continuous}\};\end{aligned}$$

here, the abbreviation pp stands for "pure point". These are closed subspaces of $\mathcal{H}$ and

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

Moreover, the subspaces $\mathcal{H}_{\mathrm{pp}}$, $\mathcal{H}_{\mathrm{ac}}$ and $\mathcal{H}_{\mathrm{sc}}$ reduce A, i.e. if P_{pp}, P_{ac} and P_{sc} denote the projections on $\mathcal{H}_{\mathrm{pp}}$, $\mathcal{H}_{\mathrm{ac}}$ and $\mathcal{H}_{\mathrm{sc}}$, then for $P \in \{P_{\mathrm{pp}}, P_{\mathrm{ac}}, P_{\mathrm{sc}}\}$,

$$PA \subset AP$$

i.e. $u \in D(A)$ implies $Pu \in D(A)$ and $APu = PAu$. Furthermore, one defines, for $M \in \{\mathcal{H}_{\rm pp}, \mathcal{H}_{\rm ac}, \mathcal{H}_{\rm sc}\}$, operators

$$D(A_M) := D(A) \cap M, \quad A_M u := Au, \quad \forall u \in D(A_M),$$

in M. Setting $\sigma_{\rm pp}(A) := \overline{\{\lambda \in \mathbb{R}; \exists u \in D(A)\backslash\{0\} \colon Au = \lambda u\}}$, $\sigma_{\rm ac}(A) := \sigma(A_{\mathcal{H}_{\rm ac}})$ and $\sigma_{\rm sc}(A) := \sigma(A_{\mathcal{H}_{\rm sc}})$, we obtain the decomposition (2.4).

Finally, let us recall some elementary results on strongly continuous one-parameter groups: Let $\{U(t); t \in \mathbb{R}\}$ be unitary operators with the properties

(i) $U(t+s) = U(t)U(s)$, for all $s, t \in \mathbb{R}$, and

(ii) for all $f \in \mathcal{H}$ and all sequences $(t_n)_{n\in\mathbb{N}} \subset \mathbb{R}$ with $t_n \to t_0$ one has the strong convergence $U(t_n)f \to U(t_0)f$.

Then we have the following important theorems.

Theorem 2.2. *Let A be a self-adjoint operator in the Hilbert space $\mathcal{H}$ and let $(E(\lambda))_{\lambda\in\mathbb{R}}$ be the associated spectral family.*

(1) *The operator*

$$U(t) := \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\lambda t}\, \mathrm{d}E(\lambda), \quad t \in \mathbb{R},$$

is unitary and $\{U(t); t \in \mathbb{R}\}$ is a strongly continuous unitary group.

(2) *For all $\psi \in D(A)$,*

$$\lim_{t\to 0} \frac{1}{t}(U(t)\psi - \psi) = \mathrm{i}A\psi.$$

(3) *If $\lim_{t\to 0} \frac{1}{t}(U(t)\psi - \psi)$ exists for some $\psi \in \mathcal{H}$, then $\psi \in D(A)$.*

Proof. See [RS-I, Thm. VIII.7]. □

Theorem 2.3 (Stone). *Let $\{U(t); t \in \mathbb{R}\}$ be a strongly continuous unitary group. Then there is a unique self-adjoint operator A satisfying*

$$U(t) = \mathrm{e}^{\mathrm{i}tA}, \quad t \in \mathbb{R}.$$

Proof. See [RS-I, Thm. VIII.8]. □

We will also make use of the following lemma.

Lemma 2.4.

(1) *Let A be a self-adjoint operator in the Hilbert space $\mathcal{H}$ with the spectral family $(E(\lambda))_{\lambda\in\mathbb{R}}$ and let $B \in \mathcal{L}(\mathcal{H})$. Then:*

$$[A, B] = 0, \quad \Longleftrightarrow \quad [B, E(\lambda)] = 0, \forall \lambda \in \mathbb{R}.$$

(2) *Let A be a self-adjoint operator in the Hilbert space $\mathcal{H}$ and let $M \subset \mathcal{H}$ be a closed subspace with the associated orthogonal projection P. Then:*

$$PA \subset AP \quad \Longleftrightarrow \quad \mathrm{e}^{\mathrm{i}tA}P = P\mathrm{e}^{\mathrm{i}tA}, \forall t \in \mathbb{R}.$$

Proof. Exercises 2 (for the case $A \in \mathcal{L}(\mathcal{H})$) and 4. □

The motion of a quantum mechanical particle which is shot towards a fixed target (of infinite mass) is described by the Schrödinger equation

$$\frac{\partial}{\partial t} f(\cdot, t) = \frac{1}{\mathrm{i}} H f(\cdot, t), \tag{2.5}$$

$$f(\cdot, 0) = f_0(\cdot), \tag{2.6}$$

where $H = -\Delta + V$ is a suitable Schrödinger operator in the Hilbert space $L_2(\mathbb{R}^d)$. Here, $f_0 \in L_2(\mathbb{R}^d)$ with

$$\int_{\mathbb{R}^d} |f_0(x)|^2 \, \mathrm{d}x = 1,$$

i.e. we may interpret $|f(\cdot, t)|^2$ as a probability density so that $\int_Q |f(x,t)|^2 \, \mathrm{d}x$ is the probability to localize the quantum mechanical particle at time t in the (measurable) set $Q \subset \mathbb{R}^d$. Hence we also claim that

$$\int_{\mathbb{R}^d} |f(x,t)|^2 \, \mathrm{d}x = 1, \quad \forall t \in \mathbb{R}. \tag{2.7}$$

The solution to the IVP (2.5)–(2.6) is given by

$$f(\cdot, t) = \left[\mathrm{e}^{-\mathrm{i}tH} f_0\right](\cdot), \quad t \in \mathbb{R}.$$

As the operators $\mathrm{e}^{-\mathrm{i}tH}$ are unitary, the claim (2.7) is satisfied.

We now distinguish between three different types of solutions that stem from the decomposition $\mathcal{H} = \mathcal{H}_{\mathrm{pp}} \oplus \mathcal{H}_{\mathrm{ac}} \oplus \mathcal{H}_{\mathrm{sc}}$ of the Hilbert space.

(1) $f_0 \in \mathcal{H}_{\mathrm{pp}}$: *Bound state.* The particle is quasi-localized and moves on some trajectory (not necessarily periodic) within the potential.

(2) $f_0 \in \mathcal{H}_{\mathrm{ac}}$: *Scattering state.* The particle is deflected and emerges (in $\mathbb{R}^2$) under a certain angle of deflection. However, some special phenomena are possible: if the so-called wave operators are not complete, it is possible that the particle is captured or that a particle is emitted.

(3) $f_0 \in \mathcal{H}_{\mathrm{sc}}$: The particle can heuristically speaking not decide to stay in or to leave the scattering center. The physicist hopes that $\mathcal{H}_{\mathrm{sc}} = \{0\}$.

Of particular interest for the issues discussed here is the case (2): Our aim is to describe the asymptotic behavior of the solution $\mathrm{e}^{-\mathrm{i}tH}f_0$ as $t \to \pm\infty$ in terms of the free dynamics given by $\left(\mathrm{e}^{-\mathrm{i}tH_0}\right)_{t\in\mathbb{R}}$ with

$$H_0 \coloneqq \overline{-\Delta \restriction_{C_c^\infty(\mathbb{R}^d)}}.$$

We will see that this will only be successful if $f_0 \perp \mathcal{H}_{\mathrm{pp}}(H)$ and if the potential V has a short range,

$$|V(x)| \leq c(1+|x|)^{-\alpha}, \quad x \in \mathbb{R}^d,$$

with some $\alpha > 1$. If a state f_0 evolves to ∞ according to $\mathrm{e}^{-\mathrm{i}tH}f_0$ as $t \to \pm\infty$, we expect that the influence of the potential V will be negligible. Note that the assumption $f_0 \perp \mathcal{H}_{\mathrm{pp}}(H)$ does not necessarily guarantee that the state $\mathrm{e}^{-\mathrm{i}tH}f_0$ evolves to ∞ in space as $t \to \pm\infty$; indeed we will need the stronger assumption that $f_0 \in \mathcal{H}_{\mathrm{ac}}(H)$.

What does it mean when we say that $\mathrm{e}^{-\mathrm{i}tH}f$ evolves as a free particle for $t \to \infty$? We thereby mean that there exists $f_+ \in \mathcal{H}$ with

$$\lim_{t\to\infty} \left\|\mathrm{e}^{-\mathrm{i}tH}f - \mathrm{e}^{-\mathrm{i}tH_0}f_+\right\| = 0. \tag{2.8}$$

As the $\mathrm{e}^{-\mathrm{i}tH}$ are unitary, (2.8) is equivalent to

$$\lim_{t\to\infty} \left\|f - \mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}f_+\right\| = 0.$$

Thus our first goal is to prove the existence of the strong limit $s-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}$. We will also see that it is necessary to study $f_\pm \in \mathcal{H}_{\mathrm{ac}}(H_0)$. Nevertheless, for $H_0 = -\Delta$ in $\mathbb{R}^d$ this is no restriction, as $\mathcal{H}_{\mathrm{ac}}(H_0) = L_2(\mathbb{R}^d)$, see Exercise 10. Thus, we are interested in the existence of the *wave operators*

$$\Omega_\pm \coloneqq s - \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}P_{\mathrm{ac}}(H_0),$$

which interrelate $f_\pm$ and f_0. The operator $S \coloneqq \Omega_+^*\Omega_-$ is the *scattering operator* which figuratively speaking maps the direction of arrival to the direction of deflection. Apart from existence, completeness of the wave operators ($R(\Omega_-) = R(\Omega_+)$ or more strongly $R(\Omega_\pm) = \mathcal{H}_{\mathrm{ac}}$) is a key issue. These questions are related to aspects of the spectral theory of Schrödinger operators, for instance:

- $\sigma_{\mathrm{ac}}(H) = \sigma_{\mathrm{ac}}(H_0)$?
- $\sigma_{\mathrm{sc}}(H) = \emptyset$?
- How many positive eigenvalues can H have? ...

As an example for an important result in this context, we cite a theorem of Volker Enß.

Theorem 2.5 (Enß, 1978/79). *Let $V : \mathbb{R}^3 \to \mathbb{R}$ with $|V(x)| \leq c\rho^{-\alpha}$ be given, with some $\alpha > 1$ and $\rho(x) := \sqrt{1 + |x|^2}$. Then:*

(1) *The wave operators $\Omega_\pm(H, H_0)$ exist and are complete.*

(2) *The singularly continuous spectrum of H is empty.*

(3) *The eigenvalues of H accumulate at most at zero. The eigenvalues different of zero have finite multiplicity.*

Remark 2.6. As in Chapter 1, the decay property in Theorem 2.5 excludes Coulomb potentials. We have to modify the wave operators in order to discuss potentials that are $\rho(x)^{-1}$-like at ∞. Note that the singularity of the Coulomb potential at $x = 0$ does not lead to substantial difficulties.

Chapter 3

Wave operators

A major difficulty in Scattering Theory is the problem of comparing two different strongly continuous unitary groups. Under which assumptions can one expect that for two self-adjoint operators A and B the strong limits

$$s - \lim_{t \to \pm\infty} \mathrm{e}^{\mathrm{i}tA} \mathrm{e}^{-\mathrm{i}tB}$$

exist? First of all, we motivate why we can exclude eigenfunctions of B for the following considerations:

Assume that $\lambda \in \mathbb{R}$ is an eigenvalue of B with eigenvector $u \in D(B) \backslash \{0\}$, i.e. $Bu = \lambda u$. Let $W(t) := \mathrm{e}^{\mathrm{i}tA} \mathrm{e}^{-\mathrm{i}tB}$. Then

$$W(t)u = \mathrm{e}^{\mathrm{i}tA} \left(\mathrm{e}^{-\mathrm{i}tB} u \right) = \mathrm{e}^{\mathrm{i}tA} \left(\mathrm{e}^{-\mathrm{i}t\lambda} u \right) = \mathrm{e}^{\mathrm{i}t(A-\lambda)} u.$$

We assume that the strong limit $\lim_{t \to \infty} W(t)u$ exists so that

$$\|W(t+a)u - W(t)u\| \to 0, \quad t \to \infty,$$

for all $a \in \mathbb{R}$. As $\mathrm{e}^{\mathrm{i}t(A-\lambda)}$ is unitary,

$$\left\| \mathrm{e}^{\mathrm{i}a(A-\lambda)} u - u \right\| = \left\| \mathrm{e}^{\mathrm{i}(a+t)(A-\lambda)} u - \mathrm{e}^{\mathrm{i}t(A-\lambda)} u \right\| = \|W(t+a)u - W(t)u\| \to 0, \quad t \to \infty,$$

so that

$$\mathrm{e}^{\mathrm{i}a(A-\lambda)} u = u, \quad \forall a \in \mathbb{R},$$

meaning that

$$\lim_{a \to 0} \frac{1}{a} \left(\mathrm{e}^{\mathrm{i}a(A-\lambda)} u - u \right) = 0.$$

In view of Stones Theorem, $u \in D(A - \lambda) = D(A)$ and $(A - \lambda)u = 0$.

We conclude: If u is an eigenvector of B then the strong limit $\lim_{t \to \infty} \mathrm{e}^{\mathrm{i}tA} \mathrm{e}^{-\mathrm{i}tB}$ exists if and only if u is an eigenvector of A (with the same eigenvalue). As such a harmonic relationship between the operators A and B can usually not be expected we therefore define the wave operators by first projecting onto the absolutely continuous subspace of B. When we will discuss completeness, it will be clear that this is a very clever choice.

Definition 3.1. Let A and B be self-adjoint operators in the Hilbert space $\mathcal{H}$ and let $P_{\mathrm{ac}}(B)$ be the projection onto $\mathcal{H}_{\mathrm{ac}}(B)$, the absolutely continuous subspace of $\mathcal{H}$ with respect to B. We say that the *generalized wave operators* $\Omega_\pm(A,B)$ *exist* if the strong limits

$$\Omega_\pm(A,B) \coloneqq s - \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}tB}P_{\mathrm{ac}}(B) \tag{3.1}$$

exist. When $\Omega_\pm(A,B)$ exist, we define

$$\mathcal{H}_{\mathrm{in}} \coloneqq R(\Omega_-), \quad \mathcal{H}_{\mathrm{out}} \coloneqq R(\Omega_+).$$

For notational convenience, we sometimes use $\mathcal{H}_-$ for $\mathcal{H}_{\mathrm{in}}$ and $\mathcal{H}_+$ for $\mathcal{H}_{\mathrm{out}}$.

Remark 3.2.

(1) The existence of $\Omega_-(A,B)$ means that for any $f_- \in \mathcal{H}_{\mathrm{ac}}(B)$ there is $f \in \mathcal{H}$ such that
$$\lim_{t\to-\infty} \left\| \mathrm{e}^{-\mathrm{i}tA}f - \mathrm{e}^{-\mathrm{i}tB}f_- \right\| = 0,$$
precisely $f = \Omega_-(A,B)f_-$, and similarly for Ω_+.

(2) If $P_{\mathrm{ac}}(B) = I$, the *norm* limit in (3.1) exists if and only if $A = B$, see Exercise 8.

(3) If A has purely discrete spectrum, the *weak* limit in (3.1) exists (and is 0) though A and B are very dissimilar. Thus the *strong* limit turns out to be the right one to take.

Definition 3.3. An operator $D \in \mathcal{L}(\mathcal{H})$ is called *partially isometric* or a *partial isometry* if there is a closed subspace $M \subset \mathcal{H}$ with

$$\|Du\| = \|u\|, \forall u \in M, \quad Du = 0, \forall u \in M^\perp.$$

We call M the *initial subspace of* D and $D(M)$ the *final subspace of* D.

Proposition 3.4. *Assume that $\Omega_\pm(A,B)$ exist. Then:*

(1) *$\Omega_\pm(A,B)$ are partial isometries with initial subspace $P_{\mathrm{ac}}(B)\mathcal{H} = \mathcal{H}_{\mathrm{ac}}(B)$ and final subspace $\mathcal{H}_\pm$.*

(2) *The subspaces $\mathcal{H}_\pm$ reduce A and*
$$\Omega_\pm[D(B)] \subset D(A), \quad A\Omega_\pm(A,B) = \Omega_\pm(A,B)B. \tag{3.2}$$

(3) *$\mathcal{H}_\pm \subset R(P_{\mathrm{ac}}(A)) = \mathcal{H}_{\mathrm{ac}}(A)$.*

Proof.

(1) For $u \in \mathcal{H}_{\mathrm{ac}}(B)^{\perp}$ clearly $\Omega_{\pm} u = 0$. For $u \in \mathcal{H}_{\mathrm{ac}}(B)$ we find that

$$\left\| \mathrm{e}^{\mathrm{i}tA} \mathrm{e}^{-\mathrm{i}tB} P_{\mathrm{ac}}(B) u \right\| = \|u\|, \quad t \in \mathbb{R},$$

and hence

$$\|\Omega_{\pm}(A,B)u\| = \|u\|;$$

note that we assume the existence of the strong limits (3.1).

(2) For any fixed $s \in \mathbb{R}$,

$$s - \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tA} \mathrm{e}^{-\mathrm{i}tB} P_{\mathrm{ac}}(B) = s - \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}(t+s)A} \mathrm{e}^{-\mathrm{i}(t+s)B} P_{\mathrm{ac}}(B).$$

As $[\mathrm{e}^{-\mathrm{i}sB}, P_{\mathrm{ac}}(B)] = 0$,

$$\Omega_{\pm}(A,B) = \mathrm{e}^{\mathrm{i}sA} \Omega_{\pm}(A,B) \mathrm{e}^{-\mathrm{i}sB}$$

or equivalently

$$\mathrm{e}^{-\mathrm{i}sA} \Omega_{\pm}(A,B) = \Omega_{\pm}(A,B) \mathrm{e}^{-\mathrm{i}sB}, \quad s \in \mathbb{R}. \tag{3.3}$$

Let $f \in D(B)$. Then

$$-\mathrm{i}Bf = \lim_{s\to 0} \frac{1}{s} \left(\mathrm{e}^{-\mathrm{i}sB} f - f \right)$$

so that

$$\begin{aligned}\lim_{s\to 0} \Omega_{\pm}(A,B) \left(\frac{1}{s} \left(\mathrm{e}^{-\mathrm{i}sB} - I \right) \right) f &= \Omega_{\pm}(A,B) \left[\lim_{s\to\infty} \left(\frac{1}{s} \left(\mathrm{e}^{-\mathrm{i}sB} - I \right) \right) f \right] \\ &= -\mathrm{i}\Omega_{\pm}(A,B) Bf.\end{aligned}$$

By (3.3),

$$\left(\frac{1}{s} \left(\mathrm{e}^{-\mathrm{i}sA} - I \right) \right) \Omega_{\pm}(A,B) f = \Omega_{\pm}(A,B) \left(\frac{1}{s} \left(\mathrm{e}^{-\mathrm{i}sB} - I \right) \right) f.$$

As the limit on the right hand side exists, the limit on the left hand side must also exist and both limits are equal. Furthermore,

$$\Omega_{\pm}(A,B) f \in D(A), \quad \forall f \in D(B),$$

and

$$\begin{aligned}-\mathrm{i}A\Omega_{\pm}(A,B) f &= \lim_{s\to 0} \left(\frac{1}{s} \left(\mathrm{e}^{-\mathrm{i}sA} - I \right) \right) \Omega_{\pm}(A,B) f \\ &= \lim_{s\to 0} \Omega_{\pm}(A,B) \left(\frac{1}{s} \left(\mathrm{e}^{-\mathrm{i}sB} - I \right) \right) f\end{aligned}$$

$$= -\mathrm{i}\Omega_\pm(A,B)Bf.$$

Finally, we show that the subspaces $\mathcal{H}_\pm = R(\Omega_\pm)$ reduce the operator A: By (3.3), $\mathcal{H}_\pm$ are invariant under $\mathrm{e}^{-\mathrm{i}sA}$, for all $s \in \mathbb{R}$,

$$\mathrm{e}^{-\mathrm{i}sA}(\mathcal{H}_\pm) \subset \mathcal{H}_\pm.$$

Applying Lemma 2.4, we are done.

(3) By (2), $A\restriction_{\mathcal{H}_\pm}$ is a self-adjoint operator in the Hilbert space $\mathcal{H}_\pm$; note that $\mathcal{H}_\pm = R(\Omega_\pm)$ is closed as $\Omega_\pm$ is a partial isometry. Furthermore,

$$\Omega_\pm(A,B) \colon P_{\mathrm{ac}}(B)\mathcal{H} = \mathcal{H}_{\mathrm{ac}}(B) \to \mathcal{H}_\pm$$

is unitary. By means of (3.2), we see that $A\restriction_{\mathcal{H}_\pm}$ is unitarily equivalent to $B\restriction_{\mathcal{H}_{\mathrm{ac}}(B)}$ where the unitary equivalence is given by $\Omega_\pm(A,B)$. Hence $A\restriction_{\mathcal{H}_\pm}$ is purely absolutely continuous,

$$\mathcal{H}_\pm \subset \mathcal{H}_{\mathrm{ac}}(A) = P_{\mathrm{ac}}(A)\mathcal{H},$$

which completes our proof. □

Remark 3.5. The second identity in (3.2) is called *intertwining relation.*

Proposition 3.6 (Chain rule for wave operators). *Let A, B, and C be self-adjoint operators. If $\Omega_\pm(A,B)$ and $\Omega_\pm(B,C)$ exist, then $\Omega_\pm(A,C)$ exist and*

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

Proof. By Proposition 3.4, (3),

$$R(\Omega_\pm(B,C)) \subset R(P_{\mathrm{ac}}(B)) = \mathcal{H}_{\mathrm{ac}}(B)$$

and hence for all $\varphi \in \mathcal{H}$

$$(I - P_{\mathrm{ac}}(B))\mathrm{e}^{\mathrm{i}tB}\mathrm{e}^{-\mathrm{i}tC}P_{\mathrm{ac}}(C)\varphi \to 0, \quad t \to \pm\infty.$$

Then

$$\begin{aligned}
\mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}tC}P_{\mathrm{ac}}(C)\varphi &= \mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}tB}\mathrm{e}^{\mathrm{i}tB}\mathrm{e}^{-\mathrm{i}tC}P_{\mathrm{ac}}(C)\varphi \\
&= \mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}tB}P_{\mathrm{ac}}(B)\mathrm{e}^{\mathrm{i}tB}\mathrm{e}^{-\mathrm{i}tC}P_{\mathrm{ac}}(C)\varphi \\
&\quad + \mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}tB}(I - P_{\mathrm{ac}}(B))\mathrm{e}^{\mathrm{i}tB}\mathrm{e}^{-\mathrm{i}tC}P_{\mathrm{ac}}(C)\varphi
\end{aligned}$$

converges to $\Omega_\pm(A,B)\Omega_\pm(B,C)\varphi$ as $t \to \pm\infty$ by Lemma 2.1 as

$$\mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}tB}P_{\mathrm{ac}}(B) \to \Omega_\pm(A,B) \text{ strongly}, \quad \mathrm{e}^{\mathrm{i}tB}\mathrm{e}^{-\mathrm{i}tC}P_{\mathrm{ac}}(C) \to \Omega_\pm(B,C) \text{ strongly}.$$

□

Definition 3.7. Let A and B be self-adjoint operators in the Hilbert space $\mathcal{H}$. Assume that the wave operators $\Omega_\pm(A, B)$ exist.

(1) The wave operators are called *weakly (asymptotically) complete* if

$$\mathcal{H}_{\text{in}} = \mathcal{H}_{\text{out}}.$$

(2) The wave operators are called *asymptotically complete* if

$$\mathcal{H}_{\text{in}} = \mathcal{H}_{\text{out}} = (\mathcal{H}_{\text{pp}}(A))^\perp.$$

(3) The wave operators are called *complete* if

$$\mathcal{H}_{\text{in}} = \mathcal{H}_{\text{out}} = \mathcal{H}_{\text{ac}}(A).$$

Remark 3.8.

(1) Asymptotic completeness is equivalent to the pair of statements: $\Omega_\pm(A, B)$ are complete and $\sigma_{\text{sc}}(A) = \emptyset$.

(2) Asymptotic completeness $\Longrightarrow$ completeness $\Longrightarrow$ weak completeness.

(3) We will only deal with the notion of completeness henceforth.

(4) Asymptotic completeness means that

$$\mathcal{H}_{\text{in}} \oplus \mathcal{H}_{\text{pp}}(A) = \mathcal{H}_{\text{out}} \oplus \mathcal{H}_{\text{pp}}(A),$$

in other words,

$$\text{incoming states} \oplus \text{bound states} = \text{outgoing states} \oplus \text{bound states.}$$

(5) Weak asymptotic completeness only means that the spaces of incoming and outgoing states are identical.

The following remarkable fact reduces completeness to an existence question.

Proposition 3.9. *Let A and B be self-adjoint operators and assume that the wave operators $\Omega_\pm(A, B)$ exist. Then $\Omega_\pm(A, B)$ are complete if and only if $\Omega_\pm(B, A)$ exist.*

Proof.

(1) We assume that both $\Omega_\pm(A, B)$ and $\Omega_\pm(B, A) = s - \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tB}\mathrm{e}^{-\mathrm{i}tA}P_{\text{ac}}(A)$ exist. By the chain rule (Proposition 3.6)

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

so that

$$\mathcal{H}_{\text{ac}}(A) = R(P_{\text{ac}}(A)) \subset R(\Omega_\pm(A, B)).$$

In view of Proposition 3.4,

$$\mathcal{H}_\pm = R(\Omega_\pm(A, B)) \subset \mathcal{H}_{\text{ac}}(A),$$

so that $\mathcal{H}_\pm = \mathcal{H}_{\text{ac}}(A)$.

(2) Conversely, suppose that $\Omega_\pm(A,B)$ exist and are complete. Let $\varphi \in \mathcal{H}_{\mathrm{ac}}(A) = R(P_{\mathrm{ac}}(A)) = P_{\mathrm{ac}}(A)\mathcal{H}$. As $\Omega_\pm(A,B)$ are complete, there is $\psi_\pm \in \mathcal{H}$ such that $\varphi = \Omega_\pm(A,B)\psi_\pm$. This implies that

$$\left\|\varphi - \mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}tB}P_{\mathrm{ac}}(B)\psi_\pm\right\| \to 0, \quad t \to \pm\infty.$$

As $\mathrm{e}^{\mathrm{i}tA}$ and $\mathrm{e}^{-\mathrm{i}tB}$ are unitary,

$$\left\|\mathrm{e}^{\mathrm{i}tB}\mathrm{e}^{-\mathrm{i}tA}\varphi - P_{\mathrm{ac}}(B)\psi_\pm\right\| \to 0, \quad t \to \pm\infty.$$

This shows that $\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tB}\mathrm{e}^{-\mathrm{i}tA}\varphi$ exists and is equal to $P_{\mathrm{ac}}(B)\psi_\pm$. □

Remark 3.10. At first sight Proposition 3.9 seems to say that completeness is no harder than existence. In fact, usually completeness is much harder.

One essential tool to prove the existence of $\Omega_\pm$ is *Cook's method* which is based on the observation that if f is a C^1-function on $\mathbb{R}$ with $f' \in L_1(\mathbb{R})$, then $\lim_{t\to\pm\infty} f(t)$ exists since

$$|f(t) - f(s)| = \left|\int_t^s f'(u)\,\mathrm{d}u\right| \le \int_t^s |f'(u)|\,\mathrm{d}u \to 0, \quad s,t \to \infty.$$

Theorem 3.11 (Cook's method). *Let A and B be self-adjoint operators in the Hilbert space $\mathcal{H}$ with $D(A) = D(B)$. Suppose that there is a set*

$$\mathcal{D} \subset D(B) \cap \mathcal{H}_{\mathrm{ac}}(B)$$

which is dense in $\mathcal{H}_{\mathrm{ac}}(B)$ so that for any $\varphi \in \mathcal{D}$ there is a $T_0 \in \mathbb{R}$ satisfying

$$\int_{T_0}^\infty \left\|(B - A)e^{\pm\mathrm{i}tB}\varphi\right\|\,\mathrm{d}t < \infty. \tag{3.4}$$

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

Proof.

(1) Let $\varphi \in \mathcal{D}$ and $\eta(t) := \mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}tB}\varphi$. We first show that $\eta(t)$ is differentiable and that

$$\eta'(t) = -\mathrm{i}\mathrm{e}^{\mathrm{i}tA}(B - A)\mathrm{e}^{-\mathrm{i}tB}\varphi. \tag{3.5}$$

As $\varphi \in D(B)$ we conclude that $\mathrm{e}^{-\mathrm{i}tB}\varphi \in D(B) = D(A)$. For $u, v \in \mathbb{R}$, $u \ne v$, u fixed, we consider the limit $v \to u$ of

$$\begin{aligned}\frac{\eta(v) - \eta(u)}{v - u} &= \frac{1}{v-u}\left(\mathrm{e}^{\mathrm{i}vA}\mathrm{e}^{-\mathrm{i}vB}\varphi - \mathrm{e}^{\mathrm{i}uA}\mathrm{e}^{-\mathrm{i}uB}\varphi\right)\\ &= \frac{1}{v-u}\left(\left(\mathrm{e}^{\mathrm{i}vA} - \mathrm{e}^{\mathrm{i}uA}\right)\mathrm{e}^{-\mathrm{i}vB}\varphi + \mathrm{e}^{\mathrm{i}uA}\left(\mathrm{e}^{-\mathrm{i}vB} - \mathrm{e}^{-\mathrm{i}uB}\right)\varphi\right)\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{v-u}\left(\mathrm{e}^{\mathrm{i}vA}-\mathrm{e}^{\mathrm{i}uA}\right)\mathrm{e}^{-\mathrm{i}uB}\varphi + \frac{1}{v-u}\left(\mathrm{e}^{\mathrm{i}vA}-\mathrm{e}^{\mathrm{i}uA}\right)\left(\mathrm{e}^{-\mathrm{i}vB}-\mathrm{e}^{-\mathrm{i}uB}\right)\varphi \\
&\quad + \frac{1}{v-u}\mathrm{e}^{\mathrm{i}uA}\left(\mathrm{e}^{-\mathrm{i}vB}-\mathrm{e}^{-\mathrm{i}uB}\right)\varphi.
\end{aligned}
$$

Using Theorem 2.2 we get that

$$\frac{1}{v-u}\left(\mathrm{e}^{\mathrm{i}vA}-\mathrm{e}^{\mathrm{i}uA}\right)\mathrm{e}^{-\mathrm{i}uB}\varphi \to \mathrm{i}\mathrm{e}^{\mathrm{i}uA}A\mathrm{e}^{-\mathrm{i}uB}, \quad v \to u,$$

and

$$\frac{1}{v-u}\left(\mathrm{e}^{-\mathrm{i}vB}-\mathrm{e}^{-\mathrm{i}uB}\right)\varphi \to -\mathrm{i}B\mathrm{e}^{-\mathrm{i}uB}\varphi, \quad v \to u,$$

so that

$$\frac{1}{v-u}\mathrm{e}^{\mathrm{i}uA}\left(\mathrm{e}^{-\mathrm{i}vB}-\mathrm{e}^{-\mathrm{i}uB}\right)\varphi \to -\mathrm{i}\mathrm{e}^{\mathrm{i}uA}B\mathrm{e}^{-\mathrm{i}uB}\varphi, \quad v \to u.$$

The second term may be rewritten as

$$\frac{1}{v-u}\left(\mathrm{e}^{\mathrm{i}vA}-\mathrm{e}^{\mathrm{i}uA}\right)\left(\mathrm{e}^{-\mathrm{i}vB}-\mathrm{e}^{-\mathrm{i}uB}\right)\varphi = \left(\mathrm{e}^{\mathrm{i}vA}-\mathrm{e}^{\mathrm{i}uA}\right)\frac{1}{v-u}\left(\mathrm{e}^{-\mathrm{i}vB}-\mathrm{e}^{-\mathrm{i}uB}\right)\varphi.$$

Here, $\left(\mathrm{e}^{\mathrm{i}vA}-\mathrm{e}^{\mathrm{i}uA}\right)$ converges strongly to 0 and $\frac{1}{v-u}\left(\mathrm{e}^{-\mathrm{i}vB}-\mathrm{e}^{-\mathrm{i}uB}\right)\varphi \to -\mathrm{i}\mathrm{e}^{-\mathrm{i}uB}B\varphi$ so that the second term in fact converges to zero. This achieves a proof of (3.5).

(2) We claim that for all $t > s > T_0$

$$\|\eta(t)-\eta(s)\| \le \int_s^t \|\eta'(u)\| \, \mathrm{d}u = \int_s^t \left\|(B-A)\mathrm{e}^{-\mathrm{i}uB}\varphi\right\| \, \mathrm{d}u. \tag{3.6}$$

For $\psi \in \mathcal{H}$, the map

$$\mathbb{R} \to \mathbb{C}, \quad t \mapsto \langle \eta(t), \psi \rangle$$

is continuous and differentiable and, in view of (3.5), its derivative is given by

$$d_\psi(t) := \left\langle (B-A)\mathrm{e}^{-\mathrm{i}tB}\varphi, \mathrm{i}\mathrm{e}^{-\mathrm{i}tA}\psi \right\rangle.$$

Clearly, $d_\psi(\cdot)$ depends continuously on t for $\psi \in D(A)$ as

$$
\begin{aligned}
d_\psi(t) &= \left\langle B\mathrm{e}^{-\mathrm{i}tB}\varphi, \mathrm{i}\mathrm{e}^{-\mathrm{i}tA}\psi \right\rangle - \left\langle A\mathrm{e}^{-\mathrm{i}tB}\varphi, \mathrm{i}\mathrm{e}^{-\mathrm{i}tA}\psi \right\rangle \\
&= \left\langle \mathrm{e}^{-\mathrm{i}tB}B\varphi, \mathrm{i}\mathrm{e}^{-\mathrm{i}tA}\psi \right\rangle - \left\langle \mathrm{e}^{-\mathrm{i}tB}\varphi, \mathrm{i}\mathrm{e}^{-\mathrm{i}tA}A\psi \right\rangle
\end{aligned}
$$

is obviously continuously in t. In view of the Fundamental Theorem of Calculus,

$$\langle (\eta(t)-\eta(s))\varphi, \psi \rangle = \int_s^t \left\langle (B-A)\mathrm{e}^{-\mathrm{i}uB}\varphi, \mathrm{i}\mathrm{e}^{-\mathrm{i}uA}\psi \right\rangle \mathrm{d}u.$$

As $D(A) \subset \mathcal{H}$ is dense,

$$\|(\eta(t)-\eta(s))\varphi\| = \sup_{\|\psi\|\le 1,\, \psi \in D(A)} |\langle (\eta(t)-\eta(s))\varphi, \psi \rangle|$$

$$
\begin{aligned}
&\leq \sup_{\|\psi\|\leq 1,\, \psi\in D(A)} \int_s^t \left|\left\langle (B-A)\mathrm{e}^{-\mathrm{i}uB}\varphi, \mathrm{i}\mathrm{e}^{-\mathrm{i}uA}\psi\right\rangle\right| \,\mathrm{d}u \\
&\leq \int_s^t \left\|(B-A)\mathrm{e}^{-\mathrm{i}uB}\varphi\right\| \,\mathrm{d}u.
\end{aligned}
$$

This achieves a proof of (3.6). Using (3.4) we infer that

$$
\|(\eta(t)-\eta(s))\varphi\| \to 0, \quad s,t\to\infty,
$$

and see that

$$
\lim_{t\to\infty} \mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}tB}P_{\mathrm{ac}}(B)\varphi = \lim_{t\to\infty}\eta(t)
$$

exists for all $\varphi\in\mathcal{D}$.

(3) For $\psi\in\mathcal{H}_{\mathrm{ac}}(B)^\perp=\mathcal{D}^\perp$ (as $\mathcal{D}\subset\mathcal{H}_{\mathrm{ac}}(B)$ is dense),

$$
\mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}tB}P_{\mathrm{ac}}(B)\psi = 0
$$

so that $\lim_{t\to\infty}\mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}tB}P_{\mathrm{ac}}(B)\psi$ exists trivially. We thus know that

$$
\lim_{t\to\infty}\mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}tB}P_{\mathrm{ac}}(B)f
$$

exists for all $f\in\mathcal{D}\oplus\mathcal{D}^\perp$. Let $g\in\mathcal{H}$ and $\varepsilon>0$. There is $f\in\mathcal{D}\oplus\mathcal{D}^\perp$ with $\|f-g\|<\varepsilon$. We write

$$
W(t) \coloneqq \mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}tB}P_{\mathrm{ac}}(B), \quad t\in\mathbb{R}.
$$

Thus

$$
\begin{aligned}
\|W(t)g-W(s)g\| &\leq \|W(t)f-W(s)f\| + \|W(t)(f-g)\| + \|W(s)(f-g)\| \\
&\leq \|W(t)f-W(s)f\| + 2\varepsilon \\
&\leq 3\varepsilon,
\end{aligned}
$$

for $s,t\geq t_0$, as $\|W(t)f-W(s)f\|\to 0$, $s,t\to\infty$. □

We now apply Cook's method to

$$
A=-\Delta+V, \quad B=-\Delta
$$

in $\mathbb{R}^3$. It will be crucial to obtain control on the term $\left|\left(\mathrm{e}^{\mathrm{i}t\Delta}\varphi\right)(x)\right|$.

Proposition 3.12. *Let* $H_0 \coloneqq \overline{-\Delta\restriction_{C_c^\infty(\mathbb{R}^3)}}$, $V\in L_2(\mathbb{R}^3)$ *and* V *bounded, and let* $H\coloneqq H_0+V$ *(so that* H_0 *and* H *are self-adjoint with* $D(H)=D(H_0)$*). Then* H_0 *is purely absolutely continuous, i.e.* $\mathcal{H}_{\mathrm{ac}}(H_0)=L_2(\mathbb{R}^3)$*, and the wave operators*

$$
\Omega_\pm(H,H_0) = s-\lim_{t\to\pm\infty}\mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}
$$

exist.

Lemma 3.13. *Assume that $h \in C^\infty(\mathbb{R}^d)$ is real-valued with $\nabla h(x) \neq 0$ for almost all $x \in \mathbb{R}^d$. Then the multiplication operator M_h in $L_2(\mathbb{R}^d)$ has purely absolutely continuous spectrum. In particular: Any non-trivial self-adjoint differential operator in $\mathbb{R}^d$ with constant coefficients has purely absolutely continuous spectrum.*

Proof. Exercise 9. □

The proof of the first part of Lemma 3.13 uses the Inverse Function Theorem (and the derivation of the Implicit Function Theorem from the Inverse Function Theorem). The second part is obtained via the Fourier transform: any (non-trivial) differential operator is unitarily equivalent to multiplication with a polynomial (different from the zero polynomial). Any non-trivial polynomial however satisfies the assumption of the first part of Lemma 3.13.

Lemma 3.14. *The free propagator $\mathrm{e}^{-\mathrm{i}tH_0}$ in $\mathbb{R}^3$ possesses a weak integral kernel*

$$K_t(x,y) \coloneqq \frac{1}{(4\pi \mathrm{i}t)^{3/2}} \mathrm{e}^{-\frac{|x-y|^2}{4\pi \mathrm{i}t}}, \quad x, y \in \mathbb{R}^3, \quad t \in \mathbb{R}\backslash\{0\},$$

in the sense that, for $f \in L_2(\mathbb{R}^3)$,

$$\left(\mathrm{e}^{-\mathrm{i}tH_0} f\right)(x) = L_2 - \lim_{R\to\infty} \frac{1}{(4\pi \mathrm{i}t)^{3/2}} \int_{|y|<R} \mathrm{e}^{-\frac{|x-y|^2}{4\pi \mathrm{i}t}} f(y)\,\mathrm{d}y, \quad \text{a.e.}$$

Proof. Exercise 13. □

We will only apply this Lemma for $f \in C_c^\infty(\mathbb{R}^3)$ where we do not need the L_2-limit.

Corollary 3.15. *For $t \neq 0$, $\mathrm{e}^{-\mathrm{i}tH_0}$ maps the space $L_1(\mathbb{R}^3)$ continuously to $L_\infty(\mathbb{R}^3)$ and*

$$\left\|\mathrm{e}^{-\mathrm{i}tH_0} u\right\|_\infty \leq \frac{c}{t^{3/2}} \|u\|_{L_1(\mathbb{R}^3)}, \quad u \in C_c^\infty(\mathbb{R}^3).$$

Proof. For $u \in C_c^\infty(\mathbb{R}^3)$,

$$\left(\mathrm{e}^{-\mathrm{i}tH_0} u\right)(x) = \frac{1}{(4\pi \mathrm{i}t)^{3/2}} \int_{\mathbb{R}^3} \mathrm{e}^{-\frac{|x-y|^2}{4\pi \mathrm{i}t}} u(y)\,\mathrm{d}y.$$

Hence

$$\left\|\mathrm{e}^{-\mathrm{i}tH_0} u\right\|_\infty = \sup_{x\in\mathbb{R}^3} \left|\mathrm{e}^{-\mathrm{i}tH_0} u(x)\right| \leq \frac{1}{(4\pi t)^{3/2}} \int_{\mathbb{R}^3} |u(y)|\,\mathrm{d}y \leq \frac{c}{t^{3/2}} \|u\|_{L_1(\mathbb{R}^3)}.$$

□

Proof of Proposition 3.12: We apply Cook's theorem with $\mathcal{D} := C_c^\infty(\mathbb{R}^3)$. For $u \in C_c^\infty(\mathbb{R}^3)$ we have that

$$\left\| V \mathrm{e}^{-\mathrm{i}tH_0} u \right\| \leq \|V\|_{L_2(\mathbb{R}^3)} \left\| \mathrm{e}^{-\mathrm{i}tH_0} u \right\|_\infty \leq \frac{c}{t^{3/2}} \|V\|_{L_2(\mathbb{R}^3)} \|u\|_{L_1(\mathbb{R}^3)} .$$

The function $t \mapsto t^{-3/2}$ is integrable at $\pm\infty$ so that the condition (3.4) in Cook's theorem is satisfied. $\square$

Suppose that

$$|V(x)| \leq c(1+|x|)^{-\beta}, \quad x \in \mathbb{R}^3.$$

If $\beta > 3/2$, then $V \in L_2(\mathbb{R}^3)$ as $\int_0^\infty \frac{r^2}{(1+r)^{2\beta}} \,\mathrm{d}r < \infty$. By a suitable choice of the space $\mathcal{D}$, the result of Proposition 3.12 can be improved regarding the case $\beta > 1$.

Theorem 3.16 (Cook-Hack). *Let $V \in L_2(\mathbb{R}^3) + L_r(\mathbb{R}^3)$ for some $r \in (2,3]$ and let V be bounded. Let $H_0 = \overline{-\Delta \restriction_{C_c^\infty(\mathbb{R}^3)}}$ in the Hilbert space $\mathcal{H} = L_2(\mathbb{R}^3)$ and $H = H_0 + V$. Then the wave operators $\Omega_\pm(H, H_0)$ exist.*

Proof. For $\gamma > 0$, we consider the functions

$$\varphi_\gamma(x) := \gamma^{3/4} \mathrm{e}^{-\gamma |x|^2/2}, \quad x \in \mathbb{R}^3,$$

and define

$$\mathcal{D} = \operatorname{span}\left\{ \varphi_\gamma(\cdot - a);\, \gamma > 0,\, a \in \mathbb{R}^3 \right\}.$$

Then $\mathcal{D} \subset D(H_0) = D(H)$ and $\overline{\mathcal{D}} = \mathcal{H}$, cf. Exercise 12.

(1) We first show that

$$\left(\mathrm{e}^{-\mathrm{i}tH_0} \varphi_\gamma \right)(x) = \alpha(t)^{3/4} \mathrm{e}^{-\frac{1}{2}(\alpha(t) + \mathrm{i}\beta(t))|x|^2} \tag{3.7}$$

with

$$\alpha(t) := \frac{\gamma}{(1 + 4t^2\gamma^2)}, \quad t \geq 0,$$

and some $\beta \colon \mathbb{R} \to \mathbb{R}$ (which is not interesting). To prove (3.7) we make use of the fact that

$$(\mathcal{F}\varphi_\gamma)(k) = \widehat{\varphi_\gamma}(k) = c_\gamma \mathrm{e}^{-\frac{|k|^2}{2\gamma}}, \quad k \in \mathbb{R}^3,$$

with suitable numbers c_γ, see Exercise 11; here $\mathcal{F}$ denotes the Fourier transform in $L_2(\mathbb{R}^3)$ given by

$$(\mathcal{F}\varphi)(k) = \hat{\varphi}(k) = L_2 - \lim_{R \to \infty} (2\pi)^{-3/2} \int_{|x|<R} \mathrm{e}^{-\mathrm{i}k \cdot x} \varphi(x) \,\mathrm{d}x,$$

for $\varphi \in L_2(\mathbb{R}^3)$. By Plancherel's Theorem, $\mathcal{F}$ is unitary with

$$(\mathcal{F}^{-1}\psi)(x) = (\mathcal{F}^*\psi)(x) = L_2 - \lim_{R \to \infty} (2\pi)^{-3/2} \int_{|k|<R} \mathrm{e}^{\mathrm{i}k \cdot x} \psi(k) \,\mathrm{d}k.$$

The Fourier transform allows for a functional calculus for the Laplacian, precisely

$$H_0 = \mathcal{F}^{-1} M_{|k|^2} \mathcal{F}, \quad \mathrm{e}^{-\mathrm{i}tH_0} = \mathcal{F}^{-1} M_{\mathrm{e}^{-\mathrm{i}t|k|^2}} \mathcal{F}.$$

We infer that

$$\mathcal{F}\mathrm{e}^{-\mathrm{i}tH_0}\varphi_\gamma = \mathrm{e}^{-\mathrm{i}t|k|^2}\widehat{\varphi_\gamma}(k) = c_\gamma \mathrm{e}^{-|k|^2(\mathrm{i}t+\frac{1}{2\gamma})} = c_\gamma \mathrm{e}^{-\frac{|k|^2}{2\gamma(t)}}$$

with $\gamma(t) \coloneqq (\gamma^{-1} + 2\mathrm{i}t)^{-1}$. Hence

$$\mathrm{e}^{-\mathrm{i}tH_0}\varphi_\gamma = \mathcal{F}^{-1}\left(c_\gamma \mathrm{e}^{-\frac{|k|^2}{2\gamma(t)}}\right) = c_\gamma c_{1/\gamma(t)} \mathrm{e}^{-\frac{\gamma(t)}{2}|x|^2}.$$

We set $\tilde{c}_\gamma(t) \coloneqq c_\gamma c_{1/\gamma(t)}$ and compute the real and imaginary part of $\gamma(t)$:

$$\gamma(t) = \frac{1}{\frac{1}{\gamma} + 2\mathrm{i}t} = \frac{\gamma^{-1} - 2\mathrm{i}t}{\gamma^{-2} + 4t^2} = \underbrace{\frac{\gamma}{1 + 4t^2\gamma^2}}_{=\alpha(t)} + \mathrm{i}\underbrace{\frac{-2t}{\gamma^{-2} + 4t^2}}_{=\beta(t)}.$$

As $\mathrm{e}^{-\mathrm{i}tH_0} \colon \mathcal{H} \to \mathcal{H}$ is unitary, we obtain the constant $\tilde{c}_\gamma(t)$ from

$$\left\|\mathrm{e}^{-\mathrm{i}tH_0}\varphi_\gamma\right\| = \|\varphi_\gamma\|,$$

where

$$\|\varphi_\gamma\|^2 = \gamma^{3/2}\int_{\mathbb{R}} \mathrm{e}^{-\gamma|x|^2}\,\mathrm{d}x = \int_{\mathbb{R}} \mathrm{e}^{-|x|^2}\,\mathrm{d}x$$

and

$$\left\|\mathrm{e}^{-\mathrm{i}tH_0}\varphi_\gamma\right\|^2 = \tilde{c}_\gamma^2(t)\int_{\mathbb{R}} \mathrm{e}^{-\alpha(t)|x|^2}\,\mathrm{d}x = \tilde{c}_\gamma^2(t)\alpha(t)^{-3/2}\int_{\mathbb{R}} \mathrm{e}^{-|x|^2}\,\mathrm{d}x$$

so that

$$\tilde{c}_\gamma^2(t)\alpha(t)^{-3/2} = 1 \quad\Longleftrightarrow\quad \tilde{c}_\gamma(t) = \alpha(t)^{3/4}.$$

This achieves a proof of (3.7).

(2) Using (3.7) we obtain for $M > 0$ and $|t| \geq 1/\gamma$ the bound

$$\left\|(1+|x|)^M \mathrm{e}^{-\mathrm{i}tH_0}\varphi_\gamma\right\|_\infty \leq c(\gamma)(1+|t|)^{M-3/2}. \tag{3.8}$$

This follows from

$$\begin{aligned}\left\|(1+|x|)^M \mathrm{e}^{-\mathrm{i}tH_0}\varphi_\gamma\right\|_\infty &\leq_{(3.7)} \sup_{x\in\mathbb{R}^3}\left((1+|x|)^M \alpha(t)^{3/4}\mathrm{e}^{-\frac{1}{2}\alpha(t)|x|^2}\right)\\ &\leq \frac{c_1}{(1+|t|)^{3/2}}\sup_{x\in\mathbb{R}^3}\left((1+|x|)^M \mathrm{e}^{-\frac{1}{2}\alpha(t)|x|^2}\right)\end{aligned}$$

and, for $|t| \geq \gamma^{-1}$,

$$\begin{aligned}\sup_{x\in\mathbb{R}^3}\left|(1+|x|)^M \mathrm{e}^{-\frac{1}{2}\alpha(t)|x|^2}\right| &\leq \sup_{y\in\mathbb{R}^3}\left|(1+|t||y|)^M \mathrm{e}^{-\frac{1}{2}\alpha(t)t^2|y|^2}\right|\\ &\leq \sup_{y\in\mathbb{R}^3}\left|(1+|t||y|)^M \mathrm{e}^{-\frac{1}{10\gamma}|y|^2}\right|\\ &\leq c_2|t|^M.\end{aligned}$$

This proves (3.8).

(3) We write $V = V_2 + V_r$ and deduce that

$$\begin{aligned}\left\|V\mathrm{e}^{-\mathrm{i}tH_0}\varphi_\gamma\right\|_2 &\le \left\|(1+|x|)^{-M}V\right\|_2 \left\|(1+|x|)^{M}\mathrm{e}^{-\mathrm{i}tH_0}\varphi_\gamma\right\|_\infty \\ &\le \left(\left\|(1+|x|)^{-M}V_2\right\|_2 + \left\|(1+|x|)^{-M}V_r\right\|_2\right) c(\gamma)(1+|t|)^{M-3/2} \\ &\le c'(\gamma)(\|V_2\|_2 + \|V_r\|_r)(1+|t|)^{M-3/2},\end{aligned}$$

for all $M \in (0, \frac{1}{2})$. Here we have used the trivial estimate

$$\left\|(1+|x|)^{-M}V_2\right\|_2 \le \|V_2\|_2$$

and

$$\left\|(1+|x|)^{-M}V_r\right\|_2 \le \left\|(1+|\cdot|)^{-M}\right\|_s \|V_r\|_r$$

provided

$$\frac{1}{2} = \frac{1}{r} + \frac{1}{s};$$

as $r \in (2,3]$, this defines some $s > 6$. We now choose $M \in (0, \frac{1}{2})$ with $Ms > 3$ so that $(1+|x|)^{-M} \in L_s(\mathbb{R}^3)$. Furthermore $M - \frac{3}{2} < -1$ and we see that $\left\|V\mathrm{e}^{-\mathrm{i}tH_0}\varphi\right\|_2$ is integrable at $t = \pm\infty$ for all $\varphi \in \mathcal{D}$. The desired result now follows from Cook's theorem. □

Remark 3.17.

(1) The proof of Theorem 3.16 shows that it is crucial to obtain precise estimates on $\mathrm{e}^{-\mathrm{i}tH_0}\varphi$. A systematic method to produce such estimates is the idea of *stationary phase*, cf. [RS-III, pp. 37-46].

(2) The Cook-Hack theorem enables to discuss potentials in $\mathbb{R}^3$ that satisfy

$$|V(x)| \le c(1+|x|)^{-1-\varepsilon}, \quad x \in \mathbb{R}^3,$$

with some $\varepsilon > 0$. Simple scattering theory yet breaks down at the Coulomb potential, cf. Section 9 in [RS-III] for how to modify quantum scattering theory to handle the Coulomb case.

Chapter 4

Kato-Birman Theory

We now turn to the complex of results that we designate as the *Kato-Birman Theory*. This theory uses the notion of trace class operators and aims at proving completeness of the wave operators. Typical assumptions on the perturbation are that $B - A$ or $(B+\mathrm{i})^{-1} - (A+\mathrm{i})^{-1}$ are trace class operators. A consequence of the completeness of the wave operators is that the absolutely continuous parts A_{ac} and B_{ac} are unitarily equivalent so that in particular $\sigma_{\mathrm{ac}}(A) = \sigma_{\mathrm{ac}}(B)$. This situation is quite similar to Weyl's essential spectrum theorem; however, instead of assuming that $A - B$ is compact, we need the much stronger assumption that $A - B$ is trace class here. From the technical point of view, the following results of the Kato-Birman Theory are obtained from *Pearson's Theorem*.

We begin with a brief overview about the trace class.

Definition 4.1. For $1 \leq p < \infty$ let

$$\mathcal{B}_p(\mathcal{H}) := \left\{ A \in \mathcal{B}_\infty(\mathcal{H});\ \sum_{j=1}^{\infty} \mu_j^p < \infty \right\}$$

be the *p-th Schatten-von Neumann class.* Here, $\mathcal{B}_\infty(\mathcal{H})$ denotes the class of compact operators on $\mathcal{H}$ and $(\mu_j)_{j\in\mathbb{N}}$ is the sequence of singular values of $A \in \mathcal{B}_\infty(\mathcal{H})$, i.e. the μ_j^2 are the eigenvalues of A^*A repeated according to their multiplicities and $\mu_j \geq 0$ (w.l.o.g.). We call $\mathcal{B}_1(\mathcal{H})$ the *trace class* and $\mathcal{B}_2(\mathcal{H})$ the *Hilbert-Schmidt class.*

Remark 4.2. There is an analogy between the spaces $\mathcal{B}_p(\mathcal{H})$ and ℓ_p, $1 \leq p \leq \infty$. However, ℓ_∞ corresponds to $\mathcal{L}(\mathcal{H})$ and not to the space of compact operators $\mathcal{B}_\infty(\mathcal{H})$; in this regard, the notation $\mathcal{B}_0$ for the class of compact operators would be more appropriate.

Theorem 4.3. *For $1 \leq p < \infty$, $\mathcal{B}_p(\mathcal{H})$ is a two-sided $*$-ideal in $\mathcal{L}(\mathcal{H})$,*

$$\begin{aligned} A \in \mathcal{B}_p(\mathcal{H}), \lambda \in \mathbb{C} &\Longrightarrow A^* \in \mathcal{B}_p(\mathcal{H}), \lambda A \in \mathcal{B}_p(\mathcal{H}), \\ A, B \in \mathcal{B}_p(\mathcal{H}) &\Longrightarrow A + B \in \mathcal{B}_p(\mathcal{H}), \\ A \in \mathcal{B}_p(\mathcal{H}), B \in \mathcal{L}(\mathcal{H}) &\Longrightarrow AB, BA \in \mathcal{B}_p(\mathcal{H}). \end{aligned}$$

Proof. See [RS-I, Thm. VI.19] for a proof for $p = 1$. $\square$

The space of compact operators $\mathcal{B}_\infty$ is closed with respect to the usual operator norm $\|\cdot\|_{\mathcal{L}(\mathcal{H})}$. However, the ideals $\mathcal{B}_p(\mathcal{H})$ only are closed with respect to certain stronger norms.

Theorem 4.4. *Let $1 \le p < \infty$ and define, for $A \in \mathcal{B}_p(\mathcal{H})$,*

$$\|A\|_{\mathcal{B}_p} := \left(\sum_{j=1}^{\infty} \mu_j^p\right)^{1/p}.$$

Then $\|\cdot\|_{\mathcal{B}_p}$ is a norm on $\mathcal{B}_p$ and $\mathcal{B}_p$ is closed with respect to this norm.

Proof. See [W-I, Thm. 3.22b]. $\square$

The spaces $\mathcal{B}_1$ and $\mathcal{B}_2$ have the following remarkable properties.

Theorem 4.5.

(1) *Let $A \in \mathcal{L}(\mathcal{H})$ and let $(e_j)_{j\in\mathbb{N}}$ be an orthonormal basis for $\mathcal{H}$. Then the sum $\sum_{j\in\mathbb{N}} \|Ae_j\|^2 \in [0,\infty]$ is independent of the choice of the $(e_j)_{j\in\mathbb{N}}$.*

(2) *For $A \in \mathcal{B}_2(\mathcal{H})$, $\|A\|_{\mathcal{B}_2}^2 = \sum_{j\in\mathbb{N}} \|Ae_j\|^2$ for any orthonormal basis $(e_j)_{j\in\mathbb{N}}$ for $\mathcal{H}$.*

(3) *$A \in \mathcal{B}_2(\mathcal{H})$ if and only if $\sum_{j\in\mathbb{N}} \|Ae_j\|^2 < \infty$ for some orthonormal basis $(e_j)_{j\in\mathbb{N}}$ for $\mathcal{H}$.*

Proof. Exercise 14. $\square$

Theorem 4.6. *Let $\Omega \subset \mathbb{R}^d$ be open and let $A \in \mathcal{L}(\mathcal{H})$ with $\mathcal{H} = L_2(\Omega)$. Then A is a Hilbert-Schmidt operator if and only if there is an integral kernel $K \in L_2(\Omega \times \Omega)$ such that*

$$(Af)(x) = \int_\Omega K(x,y) f(y)\,\mathrm{d}y \text{ a.e.}$$

Proof. See [W-I, Thm. 6.11], [RS-I, Thm. VI.23]. $\square$

Theorem 4.7. *$A \in \mathcal{B}_1(\mathcal{H})$ if and only if there are $B, C \in \mathcal{B}_2(\mathcal{H})$ with $A = BC$.*

Proof. Exercise 15. $\square$

Given a compact operator A with the singular values μ_j and the expansion

$$A^*A = \sum_{j=1}^{\infty} \mu_j^2 \langle \cdot, x_j\rangle\, x_j,$$

for some orthonormal system $(x_j)_{j\in\mathbb{N}}$, we define the absolute value $|A|$ by

$$|A| := \sum_{j=1}^{\infty} \mu_j \langle \cdot, x_j\rangle\, x_j = \sqrt{A^*A}.$$

Theorem 4.8.

(1) *$A \in \mathcal{B}_1(\mathcal{H})$ if and only if for any orthonormal basis $(e_j)_{j\in\mathbb{N}}$ for $\mathcal{H}$,*

$$\sum_{j\in\mathbb{N}} \langle |A|e_j, e_j\rangle < \infty.$$

(2) *For $A \in \mathcal{B}_1(\mathcal{H})$ and an orthonormal basis $(e_j)_{j\in\mathbb{N}}$ of $\mathcal{H}$, the trace*

$$\operatorname{tr}(A) := \sum_{j\in\mathbb{N}} \langle Ae_j, e_j\rangle$$

is well-defined, i.e. the sum converges absolutely and is independent of the choice of the orthonormal basis $(e_j)_{j\in\mathbb{N}}$ of $\mathcal{H}$.

Proof. Exercise 16. □

Remark 4.9. We denote the eigenvalues of a compact operator A by $\Lambda_j \in \mathbb{C}$, $j \in M$, where $M = \emptyset$, $M = \mathbb{N}$ or $M = \{1, \ldots, K\} \subset \mathbb{N}$. Note that a non-symmetric compact operator A may obtain no or only a very small number of eigenvalues. We denote the *algebraic multiplicity* of Λ_j by m_j,

$$m_j := \sup_{k\in\mathbb{N}} \dim N\left[(A - \Lambda_j I)^k\right];$$

this supremum is finite for any j as far as $\Lambda_j \neq 0$. More precisely: For any $\Lambda_j \neq 0$ there is a $k_j \in \mathbb{N}$ with

$$N\left[(A - \Lambda_j I)^{k_j+1}\right] = N\left[(A - \Lambda_j I)^{k_j}\right],$$

meaning that for $k \geq k_j$, the null spaces of $(A - \Lambda_j I)^k$ are equal. By Lidskii's theorem, for $A \in \mathcal{B}_1(\mathcal{H})$,

$$\operatorname{tr}(A) = \sum_{j\in M} m_j \Lambda_j,$$

see [RS-IV, p. 328]. However, we will not apply Lidskii's theorem henceforth.

Definition 4.10. Let $A\colon D(H) \to \mathcal{H}$ be self-adjoint. A vector $\varphi \in D(A)$ is called a *cyclic vector of* A if $\varphi \in D(A^k)$ for all $k \in \mathbb{N}$ and $\operatorname{span}\{\varphi, A\varphi, A^2\varphi, \ldots\}$ is dense in $\mathcal{H}$.

Remark 4.11. The existence of a cyclic vector is a strong claim. Nevertheless, for A self-adjoint and $\mathcal{H}$ separable, one always has a direct sum decomposition $\mathcal{H} = \oplus_{n=1}^{N} \mathcal{H}_n$, $N \in \mathbb{N}$ or $N = \infty$, so that A leaves each $\mathcal{H}_n$ invariant and for any n, there is φ_n which is cyclic for $A\restriction_{\mathcal{H}_n}$.

Let us provide the following version of the spectral theorem (multiplication operator form). We establish the unitary equivalence to multiplication with the variable λ in a suitable L_2-space. We assume that $\mathcal{H}$ is separable.

Theorem 4.12 (Spectral theorem). *Let $A\colon D(A) \to \mathcal{H}$ be a self-adjoint operator with the spectral family $(E(\lambda))_{\lambda\in\mathbb{R}}$ and assume that A has a cyclic vector φ. Let μ_φ be the Borel measure associated with the function $\mathbb{R} \to \mathbb{C}$, $\lambda \mapsto \langle E(\lambda)\varphi, \varphi\rangle$, i.e. $\mu_\varphi((-\infty, t]) = \langle E(t)\varphi, \varphi\rangle$, $t \in \mathbb{R}$. Then there is a unitary operator*

$$U\colon \mathcal{H} \to L_2(\mathbb{R}, \mathrm{d}\mu_\varphi)$$

with

$$Ax = U^{-1}M_\lambda Ux, \quad \forall x \in D(A).$$

Proof. We define the operator U by

$$U[f(A)\varphi] \coloneqq f, \quad f \in C_c(\mathbb{R})$$

and apply the spectral theorem (functional calculus version) to arrive at

$$\begin{aligned}
\|f(A)\varphi\|^2 &= \langle f(A)^* f(A)\varphi, \varphi\rangle \\
&= \left\langle |f(A)|^2\varphi, \varphi\right\rangle \\
&= \int_{\mathbb{R}} |f(\lambda)|^2 \,\mathrm{d}\,\langle E(\lambda)\varphi, \varphi\rangle \\
&= \int_{\mathbb{R}} |f(\lambda)|^2 \,\mathrm{d}\mu_\varphi(\lambda) \\
&= \|f\|^2_{L_2(\mathbb{R},\, \mathrm{d}\mu_\varphi)} .
\end{aligned}$$

Let $f, g \in C_c(\mathbb{R})$ with $f(A) = g(A)$. By the arguments above, $f(x) = g(x)$ a.e.; precisely, there is a Borel null set $N \subset \mathbb{R}$ with $\mu_\varphi(N) = 0$ so that $f(x) = g(x)$ for all $x \notin N$. This defines an equivalence relation on $C_c(\mathbb{R})$ so that U as a map on $\{f(A)\varphi; f \in C_c(\mathbb{R})\}$ to the set of equivalence classes is well-defined and isometric.

As φ is cyclic, $\{f(A)\varphi; f \in C_c(\mathbb{R})\}$ is dense in $\mathcal{H}$, and by the B.L.T. theorem, we can extend U to an isometric map $\mathcal{H} \to L_2(\mathbb{R}, \mathrm{d}\mu_\varphi)$. As $C_c(\mathbb{R})$ is dense in $L_2(\mathbb{R}, \mathrm{d}\mu_\varphi)$, the range $R(U)$ is dense in $L_2(\mathbb{R}, \mathrm{d}\mu_\varphi)$. As U is isometric, its range is closed so that

$$R(U) = L_2(\mathbb{R}, \mathrm{d}\mu_\varphi)$$

and U is unitary.

For $f \in C_c(\mathbb{R})$, the fact that $U^{-1}f = f(A)\varphi$ implies that

$$(UAU^{-1}f)(\lambda) = [UAf(A)\varphi](\lambda).$$

We now define $\tilde{f} \in C_c(\mathbb{R})$ by $\tilde{f}(\lambda) = \lambda f(\lambda)$, $\lambda \in \mathbb{R}$, so that $\tilde{f}(A) = Af(A)$ and

$$(UAU^{-1}f)(\lambda) = [U\tilde{f}(A)\varphi](\lambda) = \tilde{f}(\lambda) = \lambda f(\lambda).$$

As $C_c(\mathbb{R}) \subset L_2(\mathbb{R}, \mathrm{d}\mu_\varphi)$ is dense, this extends to all $f \in L_2(\mathbb{R}, \mathrm{d}\mu_\varphi)$. □

Remark 4.13. If there is no cyclic vector for A, there are Borel measures μ_n and there is a unitary operator

$$U\colon \mathcal{H} \to \bigoplus_{n=1}^{N} L_2(\mathbb{R}, \mathrm{d}\mu_n),$$

with $N \in \mathbb{N}$ or $N = \infty$, that provides a spectral representation of A,

$$(UAU^{-1}\varphi)_n(\lambda) = \lambda\varphi_n(\lambda),$$

so that any $\varphi \in \bigoplus_{n=1}^{N} L_2(\mathbb{R}, \mathrm{d}\mu_n)$ may be written as an N-tuple $(\varphi_1(\lambda), \varphi_2(\lambda), \dots)$, cf. [RS-I, Thm. VII.3]. If A has purely discrete spectrum, each eigenvector of A is associated with one copy of the $L_2(\mathbb{R}, \mathrm{d}\mu_n)$ and μ_n is a point measure concentrating its mass on the corresponding eigenvalue.

Let us recall some elementary properties of the Fourier transform: Let

$$\mathscr{S}(\mathbb{R}^d) := \left\{\varphi \in C^\infty(\mathbb{R}^d); (1 + |x|)^n D^\alpha \varphi(x) \text{ is bounded}, \forall n \in \mathbb{N}, \alpha \in \mathbb{N}_0^d\right\}$$

be the Schwartz space and define the Fourier transform $\mathcal{F}\colon \mathscr{S}(\mathbb{R}^d) \to \mathscr{S}(\mathbb{R}^d)$ by

$$(\mathcal{F}\varphi)(k) := (2\pi)^{-d/2} \int_{\mathbb{R}^d} \mathrm{e}^{-\mathrm{i}k\cdot x}\varphi(x)\,\mathrm{d}x.$$

By Plancherel's Theorem,

$$\|\mathcal{F}\varphi\| = \|\varphi\|, \quad \varphi \in \mathscr{S}(\mathbb{R}^d).$$

Furthermore, for any $\psi \in \mathscr{S}$, there is $\varphi \in \mathscr{S}$ with $\mathcal{F}\varphi = \psi$; this defines the inverse $\mathcal{F}^{-1}$ by

$$\varphi = \mathcal{F}^{-1}\psi := (2\pi)^{-d/2} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}k\cdot x}\psi(k)\,\mathrm{d}k.$$

As $\mathscr{S}(\mathbb{R}^d) \subset L_2(\mathbb{R}^d)$ is dense, the B.L.T. theorem yields a unique extension to an operator $\mathcal{F}\colon L_2(\mathbb{R}^d) \to L_2(\mathbb{R}^d)$. Here,

$$(\mathcal{F}u)(k) = L_2 - \lim_{R\to\infty} (2\pi)^{-d/2} \int_{|x|<R} \mathrm{e}^{-\mathrm{i}k\cdot x}u(x)\,\mathrm{d}x, \quad \forall u \in L_2(\mathbb{R}^d).$$

The Fourier transformation allows for a diagonalization of $H_0 := \overline{-\Delta\restriction_{C_c^\infty(\mathbb{R}^d)}}$, precisely

$$\mathcal{F}H_0\mathcal{F}^{-1} = M_{|\cdot|^2},$$

where $M_{|\cdot|^2}$ denotes the maximal multiplication operator in $L_2(\mathbb{R}^d)$ corresponding to the function $q(k) := |k|^2$. For all continuous and bounded functions $f\colon \mathbb{R} \to \mathbb{C}$,

$$\mathcal{F}f(H_0)\mathcal{F}^{-1} = M_{f(|\cdot|^2)}.$$

Theorem 4.14 (Riemann-Lebesgue). *The Fourier transform $\mathcal{F}$ maps $L_1(\mathbb{R}^d)$ continuously to $(C_0(\mathbb{R}^d), \|\cdot\|_\infty)$ where*

$$C_0(\mathbb{R}^d) := \left\{u \in C(\mathbb{R}^d); u(x) \to 0, |x| \to \infty\right\}$$

and $\|u\|_\infty = \sup_{x\in\mathbb{R}^d} |u(x)|$.

Remark 4.15. Note that $\mathcal{F}\colon L_1(\mathbb{R}^d) \to C_0(\mathbb{R}^d)$ is not surjective.

We now aim at proving the following two results: Let A and B be self-adjoint operators with $D(A) = D(B)$. Then:

- $A - B \in \mathcal{B}_1(\mathcal{H}) \implies$ The wave operators $\Omega_\pm(A, B)$ exist and are complete. (Kato-Rosenblum)
- $(A+\mathrm{i})^{-1} - (B+\mathrm{i})^{-1} \in \mathcal{B}_1(\mathcal{H}) \implies$ The wave operators $\Omega_\pm(A, B)$ exist and are complete. (Kuroda-Birman)

Both theorems will be derived from *Pearson's theorem.* Regarding Proposition 3.9, we know that it suffices to show that $\Omega_\pm(A, B)$ and $\Omega_\pm(B, A)$ exist. Nevertheless, the methods presented so far are not appropriate as they require that B is "simple" (cf. the Cook-Hack theorem).

To give a motivation for our approach, we consider the case that $B - A$ is an operator of rank 1, i.e.

$$(B - A)\varphi = \langle\varphi, \psi\rangle\, \psi, \quad \varphi \in D(A) = D(B),$$

for some fixed $\psi \in \mathcal{H}$. In order to apply Cook's method, we seek for $\varphi \in \mathcal{H}_{\mathrm{ac}}(B)$ satisfying

$$\left\langle \mathrm{e}^{-\mathrm{i}tB}\varphi, \psi\right\rangle \in L_1(\mathbb{R}).$$

Since $\varphi \in \mathcal{H}_{\mathrm{ac}}(B)$, the measure $\mathrm{d}\langle E(\lambda)\varphi, \varphi\rangle$ is absolutely continuous. Hence there is a measurable function $f\colon \mathbb{R} \to \mathbb{R}$ with $|f|^2 \in L_1(\mathbb{R})$ so that

$$\mathrm{d}\langle E(\lambda)\varphi, \varphi\rangle = |f(\lambda)|^2\,\mathrm{d}\lambda,$$

where $\mathrm{d}\lambda$ denotes the Lebesgue measure. Using Theorem 4.12 (for B) and the fact that $U\varphi = 1$ (from the identity $Uf(B)\varphi = f$) we get that

$$\left\langle e^{-\mathrm{i}tB}\varphi, \psi\right\rangle = \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}t\lambda} g(\lambda)|f(\lambda)|^2\,\mathrm{d}\lambda$$

where $g := U\psi \in L_2(\mathbb{R}, |f(\lambda)|^2\,\mathrm{d}\lambda)$. Therefore, $\left\langle e^{-\mathrm{i}tB}\varphi, \psi\right\rangle$ is the Fourier transform of $(2\pi)^{1/2} g|f|^2$. In general, it is not easy to see when a Fourier transform is in L_1 but to get it in L_2 is easy. We therefore begin by finding a set of $\varphi \in \mathcal{H}_{\mathrm{ac}}(B)$ with $\left\langle e^{-\mathrm{i}tB}\varphi, \psi\right\rangle \in L_2(\mathbb{R})$.

Definition 4.16. Let B be a self-adjoint operator with the spectral family $(E(\lambda))_{\lambda\in\mathbb{R}}$. We denote by $\mathcal{M}(B)$ the set of all $\varphi \in \mathcal{H}_{\mathrm{ac}}(B)$ for which there is $R = R_\varphi > 0$ and $f \in L_\infty(\mathbb{R})$ with $\operatorname{supp} f \subset [-R, R]$ so that

$$E(-R)\varphi = 0, E(R)\varphi = \varphi \quad \text{and} \quad \mathrm{d}\,\langle E(\lambda)\varphi, \varphi\rangle = |f(\lambda)|^2\,\mathrm{d}\lambda,$$

where $\mathrm{d}\lambda$ denotes the Lebesgue measure. Furthermore, we define

$$|\!|\!|\varphi|\!|\!| \coloneqq \|f\|_\infty\,, \quad \varphi \in \mathcal{M}.$$

Remark 4.17. For any $\varphi \in \mathcal{H}_{\mathrm{ac}}(B)$ there is $f \in L_2(\mathbb{R})$ such that $\mathrm{d}\,\langle E(\lambda)\varphi, \varphi\rangle = |f(\lambda)|^2\,\mathrm{d}\lambda$, as $\lambda \mapsto \langle E(\lambda)\varphi, \varphi\rangle$ is absolutely continuous. Hence $\mathcal{M}$ is the subspace of $\mathcal{H}_{\mathrm{ac}}(B)$ where the densities f are bounded and compactly supported.

Theorem 4.18. *$\mathcal{M}(B)$ is a linear subspace of $\mathcal{H}_{\mathrm{ac}}(B)$ and $\mathcal{M}(B)$ is dense in $\mathcal{H}_{\mathrm{ac}}(B)$ (in the $\mathcal{H}$-norm). Furthermore, $|\!|\!|\cdot|\!|\!|$ is a norm on $\mathcal{M}(B)$.*

Proof. Exercise 18. □

Lemma 4.19. *For $\varphi \in \mathcal{M}(B)$ and $\psi \in \mathcal{H}$,*

$$\int_{\mathbb{R}} \left|\left\langle \mathrm{e}^{-\mathrm{i}tB}\varphi, \psi\right\rangle\right|^2\,\mathrm{d}t \le 2\pi\,\|\psi\|^2\,|\!|\!|\varphi|\!|\!|^2\,.$$

Proof. Given $\varphi \in \mathcal{M}(B)$, there is $R > 0$ with $\varphi = (E(R) - E(-R))\varphi$. Hence $B^k\varphi$ is defined for all $k \in \mathbb{N}$. Let

$$\Phi \coloneqq \overline{\operatorname{span}\{\varphi, B\varphi, B^2\varphi, \dots\}}$$

and let Q be the projection on Φ. Trivially, $Q\mathcal{H} = R(Q) = \Phi$ is an invariant subspace for B, i.e. $QB \subset BQ$ and $B\restriction_{\Phi\cap D(B)}$ is self-adjoint. In Φ, the vector φ is cyclic for $B\restriction_{\Phi\cap D(B)}$. As $\varphi \in \mathcal{M}(B)$, there is $f \in L_\infty(\mathbb{R})$ with $f(\lambda) = 0$ for $|\lambda| > R$ and

$$\mathrm{d}\,\langle E(\lambda)\varphi, \varphi\rangle = |f(\lambda)|^2\,\mathrm{d}\lambda.$$

According to Theorem 4.12 there is a unitary map

$$U\colon Q\mathcal{H} \to L_2(\mathbb{R}, |f|^2\,\mathrm{d}\lambda)$$

with

$$\begin{aligned} U\varphi &= 1, \\ U\mathrm{e}^{-\mathrm{i}tB}v &= \mathrm{e}^{-\mathrm{i}t\lambda}Uv, \quad v \in Q\mathcal{H}. \end{aligned}$$

Let $\eta \coloneqq UQ\psi \in L_2(\mathbb{R}, |f|^2\,\mathrm{d}\lambda)$ so that

$$\left\langle \mathrm{e}^{-\mathrm{i}tB}\varphi, \psi\right\rangle = \left\langle \mathrm{e}^{-\mathrm{i}tB}\varphi, Q\psi\right\rangle$$

$$
\begin{aligned}
&= \left\langle U\mathrm{e}^{-\mathrm{i}tB}\varphi, UQ\psi \right\rangle_{L_2(\mathbb{R},|f|^2\,\mathrm{d}\lambda)} \\
&= \left\langle \mathrm{e}^{-\mathrm{i}t\lambda} U\varphi, \eta \right\rangle_{L_2(\mathbb{R},|f|^2\,\mathrm{d}\lambda)} \\
&= \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}t\lambda}\overline{\eta}(\lambda)|f(\lambda)|^2\,\mathrm{d}\lambda \\
&= (2\pi)^{1/2}\,\widehat{\overline{\eta}|f|^2}(t).
\end{aligned}
$$

Plancherel's Theorem now implies that

$$
\begin{aligned}
\int_{\mathbb{R}} \left|\left\langle \mathrm{e}^{-\mathrm{i}tB}\varphi, \psi\right\rangle\right|^2\,\mathrm{d}t &= 2\pi \left\| \widehat{\overline{\eta}|f|^2} \right\|^2 \\
&= 2\pi \left\| \overline{\eta}|f|^2 \right\|^2 \\
&\le 2\pi \left\| f \right\|_\infty^2 \int_{\mathbb{R}} |\eta(\lambda)|^2|f(\lambda)|^2\,\mathrm{d}\lambda.
\end{aligned}
$$

Now $\|f\|_\infty = \|\varphi\|$ and the fact that

$$
\int_{\mathbb{R}} |\eta(\lambda)|^2|f(\lambda)|^2\,\mathrm{d}\lambda = \|\eta\|^2_{L_2(\mathbb{R},|f|^2\,\mathrm{d}\lambda)} = \|Q\psi\|^2 \le \|\psi\|^2
$$

yield the desired result. □

Lemma 4.20. *For any $\varphi \in \mathcal{M}(B)$, $\mathrm{e}^{-\mathrm{i}tB}\varphi \xrightarrow{\mathrm{w}} 0$ as $t \to \pm\infty$. If C is compact, then $\left\|C\mathrm{e}^{-\mathrm{i}tB}\varphi\right\| \to 0$ as $t \to \pm\infty$.*

Proof. Let Q, U and $f \in L_2(\mathbb{R})$ be as in the proof of Lemma 4.19. Given $\psi \in \mathcal{H}$, we write $\eta := UQ\psi \in L_2(\mathbb{R}, |f|^2\,\mathrm{d}\lambda)$ again and recall that

$$
\left\langle \mathrm{e}^{-\mathrm{i}tB}\varphi, \psi \right\rangle = (2\pi)^{1/2}\,\widehat{\overline{\eta}|f|^2}(t).
$$

As $\eta \in L_2(\mathbb{R}, |f|^2\,\mathrm{d}\lambda)$, we infer that $\eta|f| \in L_2(\mathbb{R}, \mathrm{d}\lambda)$ and, as $f \in L_2(\mathbb{R}, \mathrm{d}\lambda)$, the Cauchy-Schwarz inequality implies that $\eta|f|^2 \in L_1(\mathbb{R}, \mathrm{d}\lambda)$. Hence $\left\langle \mathrm{e}^{-\mathrm{i}tB}\varphi, \psi \right\rangle$ is the Fourier transform of an L_1-function. By the Riemann-Lebesgue Lemma,

$$
\left\langle \mathrm{e}^{-\mathrm{i}tB}\varphi, \psi \right\rangle \to 0, \quad t \to \pm\infty,
$$

and as $\psi \in \mathcal{H}$ is arbitrary,

$$
\mathrm{e}^{-\mathrm{i}tB}\varphi \xrightarrow{\mathrm{w}} 0, \quad t \to \pm\infty.
$$

Let C be compact and assume for a contradiction that $\limsup_{t\to\infty} \left\|C\mathrm{e}^{-\mathrm{i}tB}\varphi\right\| > 0$. Then there exist $\delta > 0$ and a sequence $t_k \to \infty$ with $\left\|C\mathrm{e}^{-\mathrm{i}t_kB}\varphi\right\| > \delta$ for all $k \in \mathbb{N}$. The compactness of C and $\left\langle \mathrm{e}^{-\mathrm{i}tB}\varphi, \psi \right\rangle \to 0$ however imply that $C\mathrm{e}^{-\mathrm{i}t_kB}\varphi \to 0$ as $k \to \infty$. □

Lemma 4.21. *Let A and B be self-adjoint operators and let $C \in \mathcal{B}_1(\mathcal{H})$. Then the operator K defined by*

$$K\varphi := \int_0^1 \left(\mathrm{e}^{\mathrm{i}uA} C \mathrm{e}^{-\mathrm{i}uB} \varphi\right) \mathrm{d}u, \quad \varphi \in \mathcal{H},$$

is compact.

Proof. Let $(\varphi_n)_{n\in\mathbb{N}}$ with $\varphi_n \xrightarrow{\mathrm{w}} 0$ and $\|\varphi_n\| \le 1$ be given. We show that

$$\sup_{\|w\|\le 1} |\langle K\varphi_n, w\rangle| \to 0, \quad n \to \infty.$$

Assume that $\|w\| \le 1$ henceforth. Given $C \in \mathcal{B}_1(\mathcal{H})$, we can find $(\lambda_k)_{k\in\mathbb{N}} \subset (0, \infty)$ so that $\sum_{k\in\mathbb{N}} \lambda_k < \infty$ and orthonormal systems $(x_k)_{k\in\mathbb{N}}$, $(y_k)_{k\in\mathbb{N}}$ so that

$$C = \sum_{k\in\mathbb{N}} \lambda_k \langle \cdot, x_k\rangle \, y_k.$$

We now conclude that

$$\begin{aligned}
\left\langle \int_0^1 \left(\mathrm{e}^{\mathrm{i}uA} C \mathrm{e}^{-\mathrm{i}uB} \varphi_n\right) \mathrm{d}u, w \right\rangle &= \int_0^1 \left\langle \mathrm{e}^{\mathrm{i}uA} C \mathrm{e}^{-\mathrm{i}uB} \varphi_n, w \right\rangle \mathrm{d}u \\
&= \int_0^1 \left\langle C \mathrm{e}^{-\mathrm{i}uB} \varphi_n, \mathrm{e}^{-\mathrm{i}uA} w \right\rangle \mathrm{d}u \\
&= \int_0^1 \sum_{k\in\mathbb{N}} \lambda_k \left\langle \mathrm{e}^{-\mathrm{i}uB} \varphi_n, x_k \right\rangle \left\langle y_k, \mathrm{e}^{-\mathrm{i}uA} w \right\rangle \mathrm{d}u
\end{aligned}$$

and, as $|\left\langle y_k, \mathrm{e}^{-\mathrm{i}uA} w \right\rangle| \le \|y_k\| \left\|\mathrm{e}^{-\mathrm{i}uA} w\right\| \le 1$,

$$\left|\left\langle \int_0^1 \left(\mathrm{e}^{\mathrm{i}uA} C \mathrm{e}^{-\mathrm{i}uB} \varphi_n\right) \mathrm{d}u, w \right\rangle\right| \le \int_0^1 \sum_{k\in\mathbb{N}} \lambda_k \left|\left\langle \mathrm{e}^{-\mathrm{i}uB} \varphi_n, x_k \right\rangle\right| \mathrm{d}u.$$

Given $\varepsilon > 0$, we find $N \in \mathbb{N}$ so that $\sum_{k>N} \lambda_k < \varepsilon$. Let $\Lambda := \max_{k\in\mathbb{N}} \lambda_k$ so that

$$|\langle K\varphi_n, w\rangle| \le \Lambda \sum_{k=1}^{N} \int_0^1 \left|\left\langle \mathrm{e}^{-\mathrm{i}uB} \varphi_n, x_k \right\rangle\right| \mathrm{d}u + \varepsilon.$$

For any $k \in \mathbb{N}$ and all $u \in [0, 1]$, $\left\langle \mathrm{e}^{-\mathrm{i}uB} \varphi_n, x_k \right\rangle = \left\langle \varphi_n, \mathrm{e}^{\mathrm{i}uB} x_k \right\rangle \to 0$ as $n \to \infty$. By Lebesgue's dominated convergence theorem,

$$\int_0^1 \left|\left\langle \mathrm{e}^{-\mathrm{i}uB} \varphi_n, x_k \right\rangle\right| \mathrm{d}u \to 0, \quad n \to \infty.$$

This completes the proof. □

Remark 4.22. In the proof of Lemma 4.21, we could also make use of the compactness of the sets

$$M_k := \{e^{iuB} x_k, 0 \le u \le 1\}$$

which follows from the compactness of $[0, 1]$ and the continuity of the map $u \mapsto e^{iuB} x_k$. We then conclude that $\langle \varphi_n, z \rangle \to 0$ uniformly for all $z \in M_k$.

We will derive the key results of the Kato-Birman theory from the following theorem.

Theorem 4.23 (Pearson). *Let A and B be self-adjoint operators with $D(A) = D(B)$. Let J be a bounded operator so that*

$$C := AJ - JB \in \mathcal{B}_1(\mathcal{H}). \tag{4.1}$$

Then the strong limits

$$\Omega_\pm(A, B; J) := s - \lim_{t\to\pm\infty} e^{itA} J e^{-itB} P_{ac}(B)$$

exist.

Remark 4.24.

(1) We will apply Pearson's theorem with $J = I$ and $J = (A + i)^{-1}(B + i)^{-1}$.

(2) The assumption (4.1) in Pearson's theorem should be understood in the following manner: For $\varphi \in D(B) = D(A)$, $J\varphi \in D(B)$ and the closure of the operator $(AJ - JB)\restriction_{D(B)}$ is trace class.

Proof. We write

$$W(t) := e^{itA} J e^{-itB}$$

and consider the strong limit of $W(t)$ for $t \to \infty$. By Theorem 4.18, $\mathcal{M}(B)$ is dense in $\mathcal{H}_{ac}(B)$ so that it suffices to show that $\lim_{t\to\infty} W(t)\varphi$ exists for all $\varphi \in \mathcal{M}(B)$. Thus we have to show that

$$\lim_{t\to\infty} \sup_{s>t} \|(W(t) - W(s))\varphi\|^2 = 0, \quad \forall \varphi \in \mathcal{M}(B).$$

(1) Let $X \in \mathcal{L}(\mathcal{H})$. Then the map

$$\mathbb{R} \to \mathcal{L}(\mathcal{H}), \quad t \mapsto e^{itB} X e^{-itB} u$$

is strongly continuous for any $u \in \mathcal{H}$. In particular, the Riemann integral

$$F_{ab}(X)u := \int_a^b e^{itB} X e^{-itB} u \, dt, \quad a < b,$$

exists and defines an operator $F_{ab}(X) \in \mathcal{L}(\mathcal{H})$. Let us now prove that

$$W(t)^* W(s) - e^{iaB} W(t)^* W(s) e^{-iaB} = F_{0a}(Y(t, s)) \tag{4.2}$$

with
$$Y(t,s) := -\mathrm{i}\left[\mathrm{e}^{\mathrm{i}tB}J^*\mathrm{e}^{-\mathrm{i}(t-s)A}C\mathrm{e}^{-\mathrm{i}sB} - \mathrm{e}^{\mathrm{i}tB}C^*\mathrm{e}^{-\mathrm{i}(t-s)A}J\mathrm{e}^{-\mathrm{i}sB}\right].$$
Let
$$Q(b) := \mathrm{e}^{\mathrm{i}bB}W(t)^*W(s)\mathrm{e}^{-\mathrm{i}bB}$$
and observe that
$$\frac{\mathrm{d}}{\mathrm{d}b}Q(b) = \mathrm{i}\mathrm{e}^{\mathrm{i}bB}\left[B\mathrm{e}^{\mathrm{i}tB}J^*\mathrm{e}^{-\mathrm{i}(t-s)A}J\mathrm{e}^{-\mathrm{i}sB} - \mathrm{e}^{\mathrm{i}tB}J^*\mathrm{e}^{-\mathrm{i}(t-s)A}J\mathrm{e}^{-\mathrm{i}sB}B\right]\mathrm{e}^{-\mathrm{i}bB}.$$
As $JB = AJ - C$ and $BJ^* = J^*A - C^*$,
$$B\mathrm{e}^{\mathrm{i}tB}J^* = \mathrm{e}^{\mathrm{i}tB}BJ^* = \mathrm{e}^{\mathrm{i}tB}J^*A - \mathrm{e}^{\mathrm{i}tB}C^*$$
and
$$J\mathrm{e}^{-\mathrm{i}sB}B = JB\mathrm{e}^{-\mathrm{i}sB} = AJ\mathrm{e}^{-\mathrm{i}sB} - C\mathrm{e}^{-\mathrm{i}sB}.$$
Hence
$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}b}Q(b) = \mathrm{i}\mathrm{e}^{\mathrm{i}bB}\big[&\mathrm{e}^{\mathrm{i}tB}J^*A\mathrm{e}^{-\mathrm{i}(t-s)A}J\mathrm{e}^{-\mathrm{i}sB} - \mathrm{e}^{\mathrm{i}tB}C^*\mathrm{e}^{-\mathrm{i}(t-s)A}J\mathrm{e}^{-\mathrm{i}sB}\\ &- \mathrm{e}^{\mathrm{i}tB}J^*\mathrm{e}^{-\mathrm{i}(t-s)A}AJ\mathrm{e}^{-\mathrm{i}sB} + \mathrm{e}^{\mathrm{i}tB}J^*\mathrm{e}^{-\mathrm{i}(t-s)A}C\mathrm{e}^{-\mathrm{i}sB}\big]\mathrm{e}^{-\mathrm{i}bB}.\end{aligned}$$
Using that $\mathrm{e}^{-\mathrm{i}(t-s)A}A = A\mathrm{e}^{-\mathrm{i}(t-s)A}$, the first and the third term cancel out so that
$$\frac{\mathrm{d}}{\mathrm{d}b}Q(b) = -\mathrm{e}^{\mathrm{i}bB}Y(t,s)\mathrm{e}^{-\mathrm{i}bB}.$$
Finally,
$$\begin{aligned}W(t)^*W(s) - \mathrm{e}^{\mathrm{i}aB}W(t)^*W(s)\mathrm{e}^{-\mathrm{i}aB} &= Q(0) - Q(a)\\ &= -\int_0^a \frac{\mathrm{d}Q}{\mathrm{d}b}(b)\,\mathrm{d}b\\ &= \int_0^a \mathrm{e}^{\mathrm{i}bB}Y(t,s)\mathrm{e}^{-\mathrm{i}bB}\,\mathrm{d}b\\ &= F_{0a}(Y(t,s)).\end{aligned}$$

(2) As in the proof of Cook's theorem, cf. (3.5),
$$W(t) - W(s) = \mathrm{i}\int_s^t \mathrm{e}^{\mathrm{i}uA}C\mathrm{e}^{-\mathrm{i}uB}\,\mathrm{d}u.$$
By Lemma 4.21, $W(t) - W(s)$ is compact. Applying Lemma 4.20, we get that
$$\lim_{a\to\infty}\left\|\mathrm{e}^{\mathrm{i}aB}W^*(t)(W(t)-W(s))\mathrm{e}^{-\mathrm{i}aB}\varphi\right\| = 0, \quad \forall\varphi\in\mathcal{M}(B).$$
Eq. (4.2) shows that
$$W(t)^*(W(t)-W(s)) = F_{0a}(Y(t,t)-Y(t,s)) + \mathrm{e}^{\mathrm{i}aB}W(t)^*(W(t)-W(s))\mathrm{e}^{-\mathrm{i}aB}$$
so that for $\varphi\in\mathcal{M}(B)$,
$$\langle\varphi, W(t)^*(W(t)-W(s))\varphi\rangle = \lim_{a\to\infty}\langle\varphi, F_{0a}(Y(t,t)-Y(t,s))\varphi\rangle. \tag{4.3}$$

(3) As $C \in \mathcal{B}_1(\mathcal{H})$, we have the representation

$$C = \sum_{n\in\mathbb{N}} \lambda_n \langle \cdot, \varphi_n \rangle \psi_n$$

with $\lambda_n > 0$, $\sum_{n\in\mathbb{N}} \lambda_n < \infty$ and orthonormal systems $(\varphi_n)_{n\in\mathbb{N}}$ and $(\psi_n)_{n\in\mathbb{N}}$. In this step, we claim that if X is a bounded operator and $a > 0$, then

$$\left|\left\langle F_{0a}\left(\mathrm{e}^{\mathrm{i}uB} X C \mathrm{e}^{-\mathrm{i}uB}\right)\varphi, \varphi\right\rangle\right| \le \left(2\pi \|C\|_{\mathcal{B}_1(\mathcal{H})}\right)^{1/2} \|X\| \|\varphi\| \times \left[\sum_{n\in\mathbb{N}} \lambda_n \int_u^\infty \left|\left\langle \varphi_n, \mathrm{e}^{-\mathrm{i}xB}\varphi\right\rangle\right|^2 \mathrm{d}x\right]^{1/2}. \tag{4.4}$$

To prove (4.4), we observe that the left-hand side reads

$$\begin{aligned}
&\left|\left\langle \int_0^a \mathrm{e}^{\mathrm{i}tB}\mathrm{e}^{\mathrm{i}uB} X C \mathrm{e}^{-\mathrm{i}uB}\mathrm{e}^{-\mathrm{i}tB}\varphi \,\mathrm{d}t, \varphi\right\rangle\right| = \left|\int_0^a \left\langle C\mathrm{e}^{-\mathrm{i}(t+u)B}\varphi, X^*\mathrm{e}^{-\mathrm{i}(t+u)B}\varphi\right\rangle \mathrm{d}t\right| \\
&\quad = \left|\sum_{n\in\mathbb{N}} \int_0^a \lambda_n \left\langle \mathrm{e}^{-\mathrm{i}(t+u)B}\varphi, \varphi_n\right\rangle \left\langle \mathrm{e}^{\mathrm{i}(t+u)B} X\psi_n, \varphi\right\rangle \mathrm{d}t\right| \\
&\quad = \left|\sum_{n\in\mathbb{N}} \lambda_n \int_u^{u+a} \left\langle \mathrm{e}^{-\mathrm{i}xB}\varphi, \varphi_n\right\rangle \left\langle X\psi_n, \mathrm{e}^{-\mathrm{i}xB}\varphi\right\rangle \mathrm{d}x\right| \\
&\quad \le \sum_{n\in\mathbb{N}} \lambda_n \left(\int_u^{u+a} \left|\left\langle \mathrm{e}^{-\mathrm{i}xB}\varphi, \varphi_n\right\rangle\right|^2 \mathrm{d}x\right)^{1/2} \left(\int_u^{u+a} \left|\left\langle X\psi_n, \mathrm{e}^{-\mathrm{i}xB}\varphi\right\rangle\right|^2 \mathrm{d}x\right)^{1/2} \\
&\quad \le \left(\sum_{n\in\mathbb{N}} \lambda_n \int_u^{\infty} \left|\left\langle \mathrm{e}^{-\mathrm{i}xB}\varphi, \varphi_n\right\rangle\right|^2 \mathrm{d}x\right)^{1/2} \left(\sum_{n\in\mathbb{N}} \lambda_n \int_u^{\infty} \left|\left\langle X\psi_n, \mathrm{e}^{-\mathrm{i}xB}\varphi\right\rangle\right|^2 \mathrm{d}x\right)^{1/2}
\end{aligned}$$

where we have first used the Cauchy-Schwarz inequality for integrals and then for sums. In view of Lemma 4.19,

$$\int_{\mathbb{R}} \left|\left\langle X\psi_n, \mathrm{e}^{-\mathrm{i}xB}\varphi\right\rangle\right|^2 \mathrm{d}x \le 2\pi \|X\psi_n\|^2 \|\varphi\|^2,$$

so that

$$\begin{aligned}
\sum_{n\in\mathbb{N}} \lambda_n \int_u^\infty \left|\left\langle X\psi_n, \mathrm{e}^{-\mathrm{i}xB}\varphi\right\rangle\right|^2 \mathrm{d}x &\le \left(\sum_{n\in\mathbb{N}} \lambda_n\right) 2\pi \|X\|^2 \|\varphi\|^2 \\
&\le 2\pi \|C\|_{\mathcal{B}_1(\mathcal{H})} \|X\|^2 \|\varphi\|^2.
\end{aligned}$$

This completes the proof of (4.4).

(4) In this final step, we combine the results obtained so far. Observe that

$$\|((W(t) - W(s))\varphi\|^2 = \langle (W(t) - W(s))\varphi, (W(t) - W(s))\varphi\rangle$$

$$
\begin{aligned}
&= \langle W(t)^*(W(t)-W(s))\varphi,\varphi\rangle - \langle W(s)^*(W(t)-W(s))\varphi,\varphi\rangle \\
&=_{(4.3)} \lim_{a\to\infty} \langle F_{0a}(Y(t,t)-Y(t,s))\varphi,\varphi\rangle \\
&\qquad + \lim_{a\to\infty} \langle F_{0a}(Y(s,s)-Y(s,t))\varphi,\varphi\rangle
\end{aligned}
$$

so that

$$
\begin{aligned}
\|(W(t)-W(s))\varphi\|^2 \le{}& \limsup_{a\to\infty} |\,\langle F_{0a}(Y(t,t))\varphi,\varphi\rangle\,| + \limsup_{a\to\infty} |\,\langle F_{0a}(Y(t,s))\varphi,\varphi\rangle\,| \\
&+ \limsup_{a\to\infty} |\,\langle F_{0a}(Y(s,s))\varphi,\varphi\rangle\,| + \limsup_{a\to\infty} |\,\langle F_{0a}(Y(s,t))\varphi,\varphi\rangle\,|.
\end{aligned} \tag{4.5}
$$

By the definition of $Y(q,r)$,

$$
\begin{aligned}
\langle F_{0a}(Y(q,r))\varphi,\varphi\rangle ={}& -\mathrm{i}\left\langle F_{0a}\left(\mathrm{e}^{\mathrm{i}qB}J^*\mathrm{e}^{-\mathrm{i}(q-r)A}C\mathrm{e}^{-\mathrm{i}rB}\right)\varphi,\varphi\right\rangle \\
&+\mathrm{i}\left\langle F_{0a}\left(\mathrm{e}^{\mathrm{i}qB}C^*\mathrm{e}^{-\mathrm{i}(q-r)A}J\mathrm{e}^{-\mathrm{i}rB}\right)\varphi,\varphi\right\rangle
\end{aligned}
$$

so that the right-hand side of (4.5) yields 8 terms of the form

$$
\limsup_{a\to\infty} \left|\left\langle F_{0a}\left(\mathrm{e}^{\mathrm{i}qB}J^{(*)}\mathrm{e}^{-\mathrm{i}(q-r)A}C^{(*)}\mathrm{e}^{-\mathrm{i}rB}\right)\varphi,\varphi\right\rangle\right|,
$$

with $q,r\in\{s,t\}$, $J^{(*)}\in\{J,J^*\}$ and $C^{(*)}\in\{C,C^*\}$; note that the order of $J^{(*)}$ and $C^{(*)}$ may be interchanged. By (4.4), any of the 8 terms can be estimated by

$$
\begin{aligned}
&\left|\left\langle F_{0a}\left(\mathrm{e}^{\mathrm{i}qB}J^{(*)}\mathrm{e}^{-\mathrm{i}(q-r)A}C^{(*)}\mathrm{e}^{-\mathrm{i}rB}\right)\varphi,\varphi\right\rangle\right| \\
&\qquad\le \left(2\pi\,\|C\|_{\mathcal{B}_1(\mathcal{H})}\right)^{1/2}\|J\|\,\|\varphi\|\left(\sum_{n\in\mathbb{N}}\lambda_n\int_{\min\{q,r\}}^{\infty}\left|\left\langle \mathrm{e}^{-\mathrm{i}xB}\varphi,\varphi_n\right\rangle\right|^2\,\mathrm{d}x\right)^{1/2}.
\end{aligned} \tag{4.6}
$$

By virtue of Lemma 4.19,

$$
\|W(t)\varphi - W(s)\varphi\|^2 \le 16\pi\,\|C\|_{\mathcal{B}_1(\mathcal{H})}\,\|J\|\,\|\varphi\|^2.
$$

Furthermore, by Lemma 4.19, there is a constant c_0 so that

$$
\int_{\mathbb{R}}\left|\left\langle \mathrm{e}^{-\mathrm{i}xB}\varphi,\varphi_n\right\rangle\right|^2\mathrm{d}x \le c_0, \quad \forall n\in\mathbb{N}.
$$

Together with $\lambda_n\ge 0$ and $\sum_{n\in\mathbb{N}}\lambda_n<\infty$, Beppo Levi's monotone convergence theorem yields that the function

$$
\mathbb{R}\ni x\mapsto \sum_{n\in\mathbb{N}}\lambda_n\left|\left\langle \mathrm{e}^{-\mathrm{i}xB}\varphi,\varphi_n\right\rangle\right|^2
$$

is in $L_1(\mathbb{R})$. By Lebesgue's dominated convergence theorem, the last factor on the right-hand side of (4.6) becomes arbitrarily small,

$$
\sum_{n\in\mathbb{N}}\lambda_n\int_{\min\{s,t\}}^{\infty}\left|\left\langle \mathrm{e}^{-\mathrm{i}xB}\varphi,\varphi_n\right\rangle\right|^2\,\mathrm{d}x<\varepsilon,
$$

for t sufficiently large and $s>t$. This completes our proof. □

Theorem 4.25 (Kato-Rosenblum). *Let A and B be self-adjoint operators with $D(A) = D(B)$ and assume that $A - B \in \mathcal{B}_1(\mathcal{H})$. Then the wave operators $\Omega_\pm(A, B)$ exist and are complete.*

Proof. The assumptions of Pearson's theorem are satisfied for $J = I$. Hence the wave operators $\Omega_\pm(A, B)$ exist. As the assumptions are symmetric in A and B, the wave operators $\Omega_\pm(B, A)$ also exist. The theorem now follows from Proposition 3.9. $\square$

For applications to Schrödinger operators in $\mathbb{R}^3$, the following theorem is very suitable.

Theorem 4.26 (Kuroda-Birman). *Let A and B be self-adjoint with $D(A) = D(B)$ and assume that*

$$(A + \mathrm{i})^{-1} - (B + \mathrm{i})^{-1} \in \mathcal{B}_1(\mathcal{H}).$$

Then the wave operators $\Omega_\pm(A, B)$ exist and are complete.

Proof. We want to apply Pearson's theorem with

$$J := (A + \mathrm{i})^{-1}(B + \mathrm{i})^{-1}.$$

As $J : \mathcal{H} \to D(A) = D(B)$, one easily sees that for $\varphi \in D(A)$,

$$\begin{aligned}(AJ - JB)\varphi &= (A(A + \mathrm{i})^{-1}(B + \mathrm{i})^{-1} - (A + \mathrm{i})^{-1}(B + \mathrm{i})^{-1}B)\varphi \\ &= [((A + \mathrm{i}) - \mathrm{i})(A + \mathrm{i})^{-1}(B + \mathrm{i})^{-1} - (A + \mathrm{i})^{-1}(B + \mathrm{i})^{-1}((B + \mathrm{i}) - \mathrm{i})]\varphi \\ &= (B + \mathrm{i})^{-1}\varphi - \mathrm{i}(A + \mathrm{i})^{-1}(B + \mathrm{i})^{-1}\varphi - (A + \mathrm{i})^{-1}\varphi + \mathrm{i}(A + \mathrm{i})^{-1}(B + \mathrm{i})^{-1}\varphi \\ &= (B + \mathrm{i})^{-1}\varphi - (A + \mathrm{i})^{-1}\varphi.\end{aligned}$$

Hence

$$\overline{AJ - JB} = (B + \mathrm{i})^{-1} - (A + \mathrm{i})^{-1} \in \mathcal{B}_1(\mathcal{H}).$$

According to Pearson's theorem, the strong limits

$$s - \lim_{t \to \pm\infty} \mathrm{e}^{\mathrm{i}tA}(A + \mathrm{i})^{-1}(B + \mathrm{i})^{-1}\mathrm{e}^{-\mathrm{i}tB}P_{\mathrm{ac}}(B)$$

exist. We now consider vectors of type $(B + \mathrm{i})\varphi$ with $\varphi \in \mathcal{H}_{\mathrm{ac}}(B)$ as the subspace $\{(B + \mathrm{i})\varphi; \varphi \in \mathcal{H}_{\mathrm{ac}}(B) \cap D(B)\}$ is dense in $\mathcal{H}_{\mathrm{ac}}(B)$. It follows from

$$(B + \mathrm{i})^{-1}\mathrm{e}^{-\mathrm{i}tB}P_{\mathrm{ac}}(B)(B + \mathrm{i})\varphi = (B + \mathrm{i})^{-1}(B + \mathrm{i})\mathrm{e}^{-\mathrm{i}tB}P_{\mathrm{ac}}(B)\varphi = \mathrm{e}^{-\mathrm{i}tB}\varphi$$

that the strong limits

$$\Lambda_\pm(A) := s - \lim_{t \to \pm\infty} \mathrm{e}^{\mathrm{i}tA}(A + \mathrm{i})^{-1}\mathrm{e}^{-\mathrm{i}tB}P_{\mathrm{ac}}(B)$$

exist. The compactness of $(A+\mathrm{i})^{-1}-(B+\mathrm{i})^{-1}$ together with Lemma 4.20 and a simple approximation argument yields that

$$s-\lim_{t\to\pm\infty}\left[(A+\mathrm{i})^{-1}-(B+\mathrm{i})^{-1}\right]\mathrm{e}^{-\mathrm{i}tB}P_{\mathrm{ac}}(B)=0.$$

Thus the existence of $\Lambda_\pm(A)$ implies that

$$\Lambda_\pm(B):=s-\lim_{t\to\infty}\mathrm{e}^{\mathrm{i}tA}(B+\mathrm{i})^{-1}\mathrm{e}^{-\mathrm{i}tB}P_{\mathrm{ac}}(B)$$

exist. Applying $\Lambda_\pm(B)$ to elements of the form $(B+\mathrm{i})\varphi$, $\varphi\in\mathcal{H}_{\mathrm{ac}}(B)$, we conclude that $\Omega_\pm(A,B)$ exist. It follows from the symmetry of our assumption in A and B that $\Omega_\pm(B,A)$ exist and thus completeness holds. □

Let us consider a typical application of Theorem 4.26.

Example 4.27. Let $H_0:=\overline{-\Delta\restriction_{C_c^\infty(\mathbb{R}^3)}}$ and $H=H_0+V$ with $V\in L_1(\mathbb{R}^3)$ and V bounded. We show that

$$(H_0+1)^{-1}-(H+1)^{-1}\in\mathcal{B}_1(L_2(\mathbb{R}^3))$$

so that in view of Theorem 4.26 the wave operators $\Omega_\pm(H,H_0)$ exist and are complete. By the second resolvent equation,

$$\begin{aligned}(H+\mathrm{i})^{-1}-(H_0+\mathrm{i})^{-1}&=(H_0+\mathrm{i})^{-1}V(H+\mathrm{i})^{-1}\\&=(H_0+\mathrm{i})^{-1}V[(H_0+\mathrm{i})^{-1}+(H+\mathrm{i})^{-1}-(H_0+\mathrm{i})^{-1}]\\&=(H_0+\mathrm{i})^{-1}V(H_0+\mathrm{i})^{-1}+(H_0+\mathrm{i})^{-1}V(H_0+\mathrm{i})^{-1}V(H+\mathrm{i})^{-1}.\qquad(4.7)\end{aligned}$$

Fourier analysis shows that $(H_0+\mathrm{i})^{-1}$ has an integral kernel $G=G(x,y)$ satisfying

$$|G(x,y)|\le\frac{1}{4\pi}\frac{\mathrm{e}^{-|x-y|}}{|x-y|},$$

cf. [RS-II, p. 58f.]. Hence $|V|^{1/2}(H_0+\mathrm{i})^{-1}$ has the integral kernel $G_V(x,y):=|V|^{1/2}(x)G(x,y)$ with

$$|G_V(x,y)|\le\frac{1}{4\pi}|V(x)|^{1/2}\frac{\mathrm{e}^{-|x-y|}}{|x-y|}.$$

Furthermore, $G_V\in L_2(\mathbb{R}^{3\times3})$ as

$$\begin{aligned}\int_{\mathbb{R}^6}|G_V(x,y)|^2\,\mathrm{d}x\,\mathrm{d}y&\le\frac{1}{16\pi^2}\int_{\mathbb{R}^3}|V(x)|\int_{\mathbb{R}^3}\frac{\mathrm{e}^{-2|x-y|}}{|x-y|^2}\,\mathrm{d}y\,\mathrm{d}x\\&=\frac{1}{16\pi^2}\int_{\mathbb{R}^3}|V(x)|\left(\int_{\mathbb{R}^3}\frac{\mathrm{e}^{-2|y|}}{|y|^2}\,\mathrm{d}y\right)\mathrm{d}x\\&=c_0\int_{\mathbb{R}^3}|V(x)|\,\mathrm{d}x\end{aligned}$$

with a suitable constant $c_0 > 0$; note that $\int_0^\infty \frac{\mathrm{e}^{-2r}}{r^2} r^2 \,\mathrm{d}r < \infty$. As $V \in L_1(\mathbb{R}^3)$, the operator $|V|^{1/2}(H_0 + \mathrm{i})^{-1}$ is Hilbert-Schmidt and so

$$(H_0 + \mathrm{i})^{-1}|V|^{1/2}|V|^{1/2}(H_0 + \mathrm{i})^{-1} \in \mathcal{B}_1(L_2(\mathbb{R}^3)).$$

As $V(H + 1)^{-1}$ is bounded and $\mathcal{B}_1(L_2(\mathbb{R}^3))$ is an ideal, the second summand on the right-hand side of (4.7) is also trace class.

Remark 4.28.

(1) For $d \geq 4$, it is not possible to obtain $(H + 1)^{-1} - (H_0 + 1)^{-1} \in \mathcal{B}_1(L_2(\mathbb{R}^d))$. However, with suitable assumptions on V one can achieve that

$$(H + \mathrm{i})^{-k} - (H_0 + \mathrm{i})^{-k} \in \mathcal{B}_1(L_2(\mathbb{R}^d)),$$

for some $k \in \mathbb{N}$, $k > d/2$. Indeed, this suffices to obtain the existence and completeness of the wave operators, cf. [RS-III, Thm. XI.12].

(2) We have the following invariance principle for the wave operators, cf. [RS-III, Thm. XI.11] for a more sophisticated version: Let $\varphi \in C^2(\mathbb{R};\mathbb{R})$ with $\varphi' > 0$. Then

$$\Omega_\pm(\varphi(A), \varphi(B)) = \Omega_\pm(A, B)$$

and if the wave operators exist either on the left-hand or the right-hand side and are complete, the same holds true for the wave operators on the other side of the equation.

Chapter 5

A one-dimensional scattering problem

Let us consider a simple and (under suitable conditions) explicitly solvable scattering problem in $L_2(\mathbb{R})$. Let $V \in L_2(\mathbb{R})$ with compact support, i.e. there is $a > 0$ such that $\operatorname{supp} V \subset [-a, a]$. We define operators A and B by

$$Au \coloneqq -\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} + Vu, \quad Bu \coloneqq -\frac{\mathrm{d}^2 u}{\mathrm{d}x^2}$$

with

$$D(A) = D(B) = W_2^2(\mathbb{R}) = \{u \in L_2(\mathbb{R}); u, u' \in \mathrm{AC}_{\mathrm{loc}}(\mathbb{R}), u', u'' \in L_2(\mathbb{R})\}.$$

Then A and B are self-adjoint operators in $\mathcal{H} = L_2(\mathbb{R})$ (Friedrichs extension, Kato-Rellich theorem). By the arguments in Example 4.27, the wave operators $\Omega_\pm(A, B)$ exist and are complete. Let

$$U_1 \colon L_2(\mathbb{R}) \to L_2(0, \infty) \oplus L_2(0, \infty)$$

be defined by

$$(U_1 f)(k) = \hat{f}(k) = \begin{pmatrix} \hat{f}_1(k) \\ \hat{f}_2(k) \end{pmatrix} = \begin{pmatrix} L_2 - \lim_{N\to\infty} \frac{1}{\sqrt{2\pi}} \int_{-N}^{N} \mathrm{e}^{-\mathrm{i}k\cdot x} f(x)\,\mathrm{d}x \\ L_2 - \lim_{N\to\infty} \frac{1}{\sqrt{2\pi}} \int_{-N}^{N} \mathrm{e}^{\mathrm{i}k\cdot x} f(x)\,\mathrm{d}x \end{pmatrix}.$$

Then U_1 is unitary with the inverse

$$\left[U_1^{-1} \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}\right](x) = L_2 - \lim_{N\to\infty} \frac{1}{\sqrt{2\pi}} \int_0^N \left[\mathrm{e}^{\mathrm{i}k\cdot x} g_1(k) + \mathrm{e}^{-\mathrm{i}k\cdot x} g_2(k)\right] \mathrm{d}k$$

which follows from the fact that this is just a representation of the Fourier transform (and its inverse). In particular,

$$U_1 B U_1^{-1} = \begin{pmatrix} k^2 & 0 \\ 0 & k^2 \end{pmatrix} \quad \text{in } L_2(0,\infty)^2. \tag{5.1}$$

This is basically the spectral representation for B.

It is important to note that the functions $\mathrm{e}^{\pm \mathrm{i}k\cdot x}$ are solutions to the ordinary differential equation $-u'' - \lambda u = 0$, $\lambda = k^2$, but they are not elements of $L_2(\mathbb{R})$. We say that $\mathrm{e}^{\pm \mathrm{i}k\cdot x}$ are *generalized eigenfunctions* of B with the *generalized eigenvalue* $\lambda = k^2 > 0$. Let us now prove the existence of solutions $e_1(\cdot, k)$ and $e_2(\cdot, k)$ to $-u'' + Vu - k^2 u = 0$ of the form

$$e_1(x,k) = \begin{cases} \mathrm{e}^{\mathrm{i}k\cdot x} + r_1(k)\,\mathrm{e}^{-\mathrm{i}k\cdot x}, & x < -a, \\ t(k)\,\mathrm{e}^{\mathrm{i}k\cdot x}, & x > a, \end{cases} \tag{5.2}$$

$$e_2(x,k) = \begin{cases} t(k)\,\mathrm{e}^{-\mathrm{i}k\cdot x}, & x < -a, \\ \mathrm{e}^{-\mathrm{i}k\cdot x} + r_2(k)\,\mathrm{e}^{\mathrm{i}k\cdot x}, & x > a. \end{cases} \tag{5.3}$$

We will show that

$$\hat{S}(k) = \begin{pmatrix} t(k) & r_2(k) \\ r_1(k) & t(k) \end{pmatrix}$$

is the scattering matrix for our problem and hence $\hat{S}(k)$ is unitary. We will also need the unitary operator

$$U_2\colon L_2(\mathbb{R}) \to L_2(0,\infty) \oplus L_2(0,\infty)$$

given by

$$(U_2 f)(k) := \begin{pmatrix} L_2 - \lim_{N\to\infty} \frac{1}{\sqrt{2\pi}} \int_{-N}^{N} \overline{e_1(x,k)} f(x)\,\mathrm{d}x \\ L_2 - \lim_{N\to\infty} \frac{1}{\sqrt{2\pi}} \int_{-N}^{N} \overline{e_2(x,k)} f(x)\,\mathrm{d}x \end{pmatrix}.$$

Note that

$$\left[U_2^{-1} \begin{pmatrix} g_1 \\ g_2 \end{pmatrix} \right](x) = L_2 - \lim_{N\to\infty} \frac{1}{\sqrt{2\pi}} \int_0^N \left[e_1(x,k) g_1(k) + e_2(x,k) g_2(k) \right] \mathrm{d}k$$

as $\left\langle h, U_2^{-1} g \right\rangle_{L_2(\mathbb{R})} = \langle h, U_2^* g \rangle_{L_2(\mathbb{R})} = \langle U_2 h, g \rangle_{L_2(0,\infty)^2}$. Furthermore,

$$U_2 A_+ U_2^{-1} = \begin{pmatrix} k^2 & 0 \\ 0 & k^2 \end{pmatrix}, \quad A_+ = A E_A(0,\infty), \tag{5.4}$$

where $E_A(\cdot)$ denotes the family of spectral projections for A. A proof of this spectral representation and the fact that U_2 is unitary can be found in [W-II, Ch. 23.2]. We omit further details in order to be able to focus on the physical relevance of the quantities $r_1(k)$, $r_2(k)$ and $t(k)$.

In view of the representations (5.1) and (5.4), the wave operators $\Omega_\pm(A,B)$ obey for any $t \in \mathbb{R}$

$$\begin{aligned} U_2 \Omega_\pm(A,B) U_1^{-1} \begin{pmatrix} \mathrm{e}^{-\mathrm{i}tk^2} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}tk^2} \end{pmatrix} &= U_2 \Omega_\pm(A,B) \mathrm{e}^{-\mathrm{i}tB} U_1^{-1} \\ &= U_2 \mathrm{e}^{-\mathrm{i}tA} \Omega_\pm(A,B) U_1^{-1} \end{aligned}$$

$$= \begin{pmatrix} e^{-itk^2} & 0 \\ 0 & e^{-itk^2} \end{pmatrix} U_2\Omega_\pm(A,B)U_1^{-1};$$

here, we have used that

$$\begin{aligned}
\Omega_+(A,B)e^{-itB} &= s - \lim_{\tau\to\infty} e^{i\tau A}e^{-i\tau B}\underbrace{P_{ac}(B)}_{=I}e^{-itB} \\
&= s - \lim_{\tau\to\infty} e^{i\tau A}e^{-i(\tau+t)B}P_{ac}(B) \\
&= s - \lim_{\sigma\to\infty} e^{i(\sigma-t)A}e^{-i\sigma B}P_{ac}(B) \\
&= e^{-itA}\Omega_+(A,B)
\end{aligned}$$

and similarly $\Omega_-(A,B)e^{-itB} = e^{-itA}\Omega_-(A,B)$. Consequently, the operators

$$U_2\Omega_\pm(A,B)U_1^{-1} \quad \text{and} \quad \begin{pmatrix} e^{-itk^2} & 0 \\ 0 & e^{-itk^2} \end{pmatrix}$$

commute. But then $U_2\Omega_\pm(A,B)U_1^{-1}$ also commutes with M_k and hence with $M_{\chi_{(-\infty,s]}}$ for any $s \in \mathbb{R}$, as $(M_{\chi_{(-\infty,s]}})_{s\in\mathbb{R}}$ is the spectral family for M_k. This allows to apply [W-II, Thm. 21.14] saying that $U_2\Omega_\pm(A,B)U_1^{-1}$ is multiplication with a 2×2-matrix

$$\omega^\pm(k) = \begin{pmatrix} \omega_{11}^\pm(k) & \omega_{12}^\pm(k) \\ \omega_{21}^\pm(k) & \omega_{22}^\pm(k) \end{pmatrix}.$$

As $\Omega_\pm(A,B)$ are isometric, $\omega^\pm(k)$ is a.e. unitary. The scattering matrix

$$\hat{S} = U_1SU_1^{-1} = U_1\Omega_+^*\Omega_-U_1^{-1} = (U_1\Omega_+^*U_2^{-1})(U_2\Omega_-U_1^{-1}) = (U_2\Omega_+U_1^{-1})^*(U_2\Omega_-U_1^{-1})$$

corresponds to multiplication with $\omega^+(k)^*\omega^-(k)$.

We now make use of

$$U_2\Omega_\pm f = (U_2\Omega_\pm U_1^{-1})U_1 f = \omega^\pm(\cdot)\begin{pmatrix} \hat{f}_1(\cdot) \\ \hat{f}_2(\cdot) \end{pmatrix}$$

to obtain that, by the definition of the wave operators,

$$\begin{aligned}
0 &= \lim_{t\to\pm\infty} \left\| \Omega_\pm f - e^{itA}e^{-itB}f \right\|^2 \\
&= \lim_{t\to\pm\infty} \left\| \Omega_\pm f - U_2^{-1}e^{it\,\mathrm{diag}(k^2,k^2)}U_2U_1^{-1}e^{-it\,\mathrm{diag}(k^2,k^2)}U_1 f \right\|^2 \\
&= \lim_{t\to\pm\infty} \left\| U_2^{-1}e^{-it\,\mathrm{diag}(k^2,k^2)}U_2\Omega_\pm f - U_1^{-1}e^{-it\,\mathrm{diag}(k^2,k^2)}U_1 f \right\|^2 \\
&= \lim_{t\to\pm\infty} \frac{1}{2\pi}\int_{\mathbb{R}} |I(x,t)|^2\,dx
\end{aligned}$$

where

$$I(x,t) = \int_0^\infty \Big\{ e_1(x,k)e^{-itk^2}[\omega_{11}^\pm(k)\hat{f}_1(k) + \omega_{12}^\pm(k)\hat{f}_2(k)]$$

$$+ e_2(x,k)\mathrm{e}^{-\mathrm{i}tk^2}[\omega^{\pm}_{21}(k)\hat{f}_1(k) + \omega^{\pm}_{22}(k)\hat{f}_2(k)] - \mathrm{e}^{-\mathrm{i}k(kt-x)}\hat{f}_1(k) - \mathrm{e}^{-\mathrm{i}k(kt+x)}\hat{f}_2(x)\Big\}\,\mathrm{d}k.$$

In particular, we conclude that

$$\int_{-\infty}^{-a} |I(x,t)|^2\,\mathrm{d}x \to 0 \text{ and} \tag{5.5}$$

$$\int_{a}^{\infty} |I(x,t)|^2\,\mathrm{d}x \to 0 \text{ as } t \to \pm\infty. \tag{5.6}$$

We plug (5.2) and (5.3) into (5.5) to obtain

$$\begin{aligned}\int_{-\infty}^{-a}\Big|\int_0^{\infty}\Big\{&\mathrm{e}^{-\mathrm{i}k(kt-x)}[\omega^{\pm}_{11}(k)\hat{f}_1(k) + \omega^{\pm}_{12}(k)\hat{f}_2(k)]\\ &+ \mathrm{e}^{-\mathrm{i}k(kt+x)}r_1(k)[\omega^{\pm}_{11}(k)\hat{f}_1(k) + \omega^{\pm}_{12}(k)\hat{f}_2(k)]\\ &+ \mathrm{e}^{-\mathrm{i}k(kt+x)}t(k)[\omega^{\pm}_{21}(k)\hat{f}_1(k) + \omega^{\pm}_{22}(k)\hat{f}_2(k)]\\ &- \mathrm{e}^{-\mathrm{i}k(kt-x)}\hat{f}_1(k) - \mathrm{e}^{-\mathrm{i}k(kt+x)}\hat{f}_2(k)\Big\}\,\mathrm{d}k\Big|^2\,\mathrm{d}x \to 0, \quad t \to \pm\infty.\end{aligned} \tag{5.7}$$

According to Exercise 21, the terms with $\mathrm{e}^{-\mathrm{i}k(kt-x)}$ in (5.7) correspond to waves traveling from the left to the right, so that, as $t \to \infty$,

$$\begin{aligned}0 = \lim_{t\to\infty}\int_{-\infty}^{-a}\Big|\int_0^{\infty}&\mathrm{e}^{-\mathrm{i}k(kt+x)}\big\{r_1(k)[\omega^{+}_{11}(k)\hat{f}_1(k) + \omega^{+}_{12}(k)\hat{f}_2(k)]\\ &+ t(k)[\omega^{+}_{21}(k)\hat{f}_1(k) + \omega^{+}_{22}(k)\hat{f}_2(k)] - \hat{f}_2(k)\big\}\,\mathrm{d}k\Big|^2\,\mathrm{d}x.\end{aligned}$$

Similarly, as the terms with $\mathrm{e}^{-\mathrm{i}k(kt+x)}$ in (5.7) correspond to waves traveling from the right to the left, we get for $t \to -\infty$

$$0 = \lim_{t\to-\infty}\int_{-\infty}^{-a}\Big|\int_0^{\infty}\mathrm{e}^{-\mathrm{i}k(kt-x)}\big[\omega^{-}_{11}(k)\hat{f}_1(k) + \omega^{-}_{12}(k)\hat{f}_2(k) - \hat{f}_1(k)\big]\,\mathrm{d}k\Big|^2\,\mathrm{d}x.$$

As the remaining waves travel to $\pm\infty$, we may replace $\int_{-\infty}^{-a}\ldots\,\mathrm{d}x$ by $\int_{-\infty}^{\infty}\ldots\,\mathrm{d}x$ so that

$$\begin{aligned}\lim_{t\to\infty}\Big\|\mathcal{F}\big\{&\mathrm{e}^{-\mathrm{i}t|\cdot|^2}\big[r_1(\cdot)(\omega^{+}_{11}(\cdot)\hat{f}_1(\cdot) + \omega^{+}_{12}(\cdot)\hat{f}_2(\cdot))\big]\\ &+t(\cdot)\big[\omega^{+}_{21}(\cdot)\hat{f}_1(\cdot) + \omega^{+}_{22}(\cdot)\hat{f}_2(\cdot)\big] - \hat{f}_2(\cdot)\big\}\Big\| = 0,\\ \lim_{t\to-\infty}\Big\|\mathcal{F}^{-1}\big\{&\mathrm{e}^{-\mathrm{i}t|\cdot|^2}\big[\omega^{-}_{11}(\cdot)\hat{f}_1(\cdot) + \omega^{-}_{12}(\cdot)\hat{f}_2(\cdot) - \hat{f}_1(\cdot)\big]\big\}\Big\| = 0\end{aligned}$$

In view of Plancherel's Theorem and the fact that $|\mathrm{e}^{-\mathrm{i}tk^2}| = 1$, we conclude that

$$\hat{f}_1(k) = \omega^{-}_{11}(\cdot)\hat{f}_1(k) + \omega^{-}_{12}(k)\hat{f}_2(k), \tag{5.8}$$

$$\hat{f}_2(k) = r_1(k)[\omega^+_{11}(k)\hat{f}_1(k) + \omega^+_{12}(k)\hat{f}_2(k)] + t(k)[\omega^+_{21}(k)\hat{f}_1(k) + \omega^+_{22}(k)\hat{f}_2(k)]. \quad (5.9)$$

An analogous computation for $\int_a^\infty \dots \,\mathrm{d}x$ shows that

$$\hat{f}_2(k) = \omega^-_{21}(k)\hat{f}_1(k) + \omega^-_{22}(k)\hat{f}_2(k), \quad (5.10)$$

$$\hat{f}_1(k) = t(k)[\omega^+_{11}(k)\hat{f}_1(k) + \omega^+_{12}(k)\hat{f}_2(k)] + r_2(k)[\omega^+_{21}(k)\hat{f}_1(k) + \omega^+_{22}(k)\hat{f}_2(k)]. \quad (5.11)$$

Now (5.8) and (5.10) imply that

$$\omega^-(k) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

and by (5.9) and (5.11),

$$\begin{pmatrix} t(k) & r_2(k) \\ r_1(k) & t(k) \end{pmatrix} \omega^+(k) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Hence $\omega^+(k)$ is unitary and

$$\omega^+(k)^* = \omega^+(k)^{-1} = \begin{pmatrix} t(k) & r_2(k) \\ r_1(k) & t(k) \end{pmatrix}$$

and

$$\hat{S}(k) = \omega^+(k)^*\omega^-(k) = \begin{pmatrix} t(k) & r_2(k) \\ r_1(k) & t(k) \end{pmatrix}.$$

This also explains the physical relevance of the quantities $t(\cdot)$, $r_1(\cdot)$ and $r_2(\cdot)$: $t(k)$ is the *transmission coefficient*, i.e. $|t(k)|^2$ is the rate of an incoming wave that is transmitted by the potential. Concomitantly, arg $t(k)$ is the corresponding phase shift. We call $r_1(k)$ and $r_2(k)$ the *reflection coefficients* as $|r_1(k)|^2$ is the amount of a right traveling wave that is reflected and $|r_2(k)|^2$ is the amount of a left traveling wave that is reflected. Again, arg $r_j(k)$, $j \in \{1, 2\}$, is the corresponding phase shift.

Example 5.1. Let $L > 0$ and $U \in \mathbb{R}\backslash\{0\}$. The potential

$$V(x) = \begin{cases} 0, & x < 0 \text{ and } x > L, \\ U, & 0 \le x \le L \end{cases}$$

corresponds to a potential step for $U > 0$ and a potential well for $U < 0$. In [W-II], it is shown that the Schrödinger equation $-u'' + Vu - \lambda u = 0$, $\lambda > 0$, has a solution $u(x, \lambda)$ of the form

$$u(x,\lambda) = \begin{cases} a(\lambda)\mathrm{e}^{\mathrm{i}\sqrt{\lambda}x} + b(\lambda)\mathrm{e}^{-\mathrm{i}\sqrt{\lambda}x}, & x < 0, \\ c(\lambda)\mathrm{e}^{\mathrm{i}\sqrt{\lambda-U}x} + d(\lambda)\mathrm{e}^{-\mathrm{i}\sqrt{\lambda-U}x}, & 0 \le x \le L, \\ \mathrm{e}^{\mathrm{i}\sqrt{\lambda}x}, & x > L, \end{cases}$$

and that the transmission coefficient is $\frac{1}{|a(\lambda)|^2}$. It is an easy exercise to show that

$$\frac{1}{|a(\lambda)|^2} = \begin{cases} \frac{4\lambda(\lambda-U)}{4\lambda(\lambda-U)+U^2\sin^2 L\sqrt{\lambda-U}}, & U < 0, \\ \frac{4\lambda(\lambda-U)}{4\lambda(\lambda-U)+U^2\sin^2 L\sqrt{\lambda-U}}, & U > 0 \text{ and } \lambda > U, \\ \frac{4\lambda(U-\lambda)}{4\lambda(U-\lambda)+U^2\sinh^2 L\sqrt{U-\lambda}}, & U > 0 \text{ and } \lambda \in (0, U). \end{cases}$$

For the potential well ($U < 0$), one concludes that

$$\lim_{\lambda \downarrow 0} \frac{1}{|a(\lambda)|^2} = \begin{cases} 0, & L\sqrt{U} \neq k\pi, k \in \mathbb{N}_0, \\ 1, & L\sqrt{U} = k\pi, k \in \mathbb{N}_0. \end{cases}$$

For the potential step ($U > 0$), the transmission coefficient increases from 0 to $4(4 + UL^2)^{-1}$ on $[0, U]$, cf. Exercise 22.

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