Schrödinger Operators and their Spectra

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Priv.-Doz. Dr. Martin Kohlmann

GEORG-AUGUST-UNIVERSITÄT
GÖTTINGEN

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Preface

This lecture begins with a brief overview about the spectral theorem and its consequences for the spectrum of self-adjoint operators in Hilbert spaces. The key results are stated mainly without proofs to allow for a quick entry into the relevant aspects of spectral theory. Then our main goal is to study the spectrum of several classes of Schrödinger operators and to look at some important examples occurring in mathematical physics (e.g. the harmonic oscillator or the hydrogen atom). Searching for solutions of the IVP for the Schrödinger equation, we will discuss and prove Stone's theorem on strongly continuous unitary one-parameter groups. Finally, we will look at spectral measures that allow for a characterization and a decomposition of the spectrum of self-adjoint operators and the Hilbert space itself. The lecture will end with an outlook concerning some aspects of quantum scattering theory.

Chapter 1

Overview: The spectral theorem and the spectrum of self-adjoint operators in Hilbert space

Let $\mathcal{H}$ be a Hilbert space and denote by $\mathcal{L}(\mathcal{H})$ the space of bounded operators on $\mathcal{H}$. An operator $P \in \mathcal{L}(\mathcal{H})$ is called *(orthogonal) projection* if $P^2 = P = P^*$. For symmetric operators $A, B \in \mathcal{L}(H)$, we write $A \leq B$ if

$$\langle Au, u \rangle \leq \langle Bu, u \rangle , \quad \forall u \in \mathcal{H}.$$

For two projections P and Q,

$$P \leq Q \quad \Longleftrightarrow \quad R(P) \subset R(Q) \quad \Longleftrightarrow \quad PQ = QP = P.$$

We als comment on different notions of convergence of bounded operators: Let $(A_n)_{n\in\mathbb{N}} \in \mathcal{L}(\mathcal{H})$ be a sequence of bounded operators and let $A \in \mathcal{L}(\mathcal{H})$.

(i) *Norm convergence*: $\|A_n - A\| \to 0$, $n \to \infty$, i.e.

$$\sup\{\|A_n f - Af\| \,;\, \|f\| \leq 1\} \to 0, \quad n \to \infty.$$

(ii) *Strong convergence*: $\forall f \in \mathcal{H}\colon A_n f \to Af$, $n \to \infty$.

(iii) *Weak convergence*: $\forall f, g \in \mathcal{H}\colon \langle A_n f, g\rangle \to \langle Af, g\rangle$, $n \to \infty$.

Note: Norm convergence $\Longrightarrow$ strong convergence $\Longrightarrow$ weak convergence.

Definition 1.1. Let $(E(\lambda))_{\lambda\in\mathbb{R}} \subset \mathcal{L}(\mathcal{H})$ be a family of projections with 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 $E(\lambda)f \to 0$, $\lambda \to -\infty$.

Then $(E(\lambda))_{\lambda\in\mathbb{R}} \subset \mathcal{L}(\mathcal{H})$ is called a *spectral family.*

Remark 1.2. Why do we need strong convergence in (ii) und (iii)?

(1) Weak convergence + monotonicity imply strong convergence.

(2) Norm convergence + monotonicity of projections imply constance.

Remark 1.3. For any spectral family $(E(\lambda))_{\lambda\in\mathbb{R}}$ there also exists the strong limit from the left at $\lambda \in \mathbb{R}$,

$$E(\lambda - 0)f \coloneqq \lim_{\varepsilon\downarrow 0} E(\lambda - \varepsilon)f, \quad \forall f \in \mathcal{H}.$$

It is easy to see that $E(\lambda - 0)$ is a projection. It is possible that $E(\lambda - 0) \neq E(\lambda)$.

Example 1.4. Let $\mathcal{H} = L_2(\mathbb{R})$ and let $E(\lambda) = \chi_{(-\infty,\lambda]}(x)$ be multiplication with the characteristic function for the interval $(-\infty, \lambda]$. Then $(E(\lambda))_{\lambda\in\mathbb{R}}$ is a spectral family.

Example 1.5. Let $A \in \mathcal{L}(\mathcal{H})$ be symmetric and compact with $\dim R(A) = \infty$, the eigenvalues $\lambda_n \in \mathbb{R}\backslash\{0\}$ and an orthonormal basis $(u_n)_{n\in\mathbb{N}}$ of $R(A)$ with $Au_n = \lambda_n u_n$ for $n \in \mathbb{N}$. Let

$$\begin{aligned} E(\lambda) &\coloneqq \sum_{\lambda_n\leq\lambda} \langle \cdot, u_n\rangle\, u_n, \quad \lambda < 0, \\ E(\lambda) &\coloneqq P_{N(A)} + \sum_{\lambda_n\leq\lambda} \langle \cdot, u_n\rangle\, u_n, \quad \lambda \geq 0. \end{aligned}$$

Then $(E(\lambda))_{\lambda\in\mathbb{R}}$ is a spectral family.

Let $m\colon \mathbb{R} \to \mathbb{R}$ be monotonically increasing and right continuous. For $\varphi \in C_c(\mathbb{R})$ (i.e. φ is continuous and $\operatorname{supp}\varphi$ is compact, $\operatorname{supp}\varphi \subset (-R, R)$ for some $R > 0$), we define the *Riemann-Stieltjes integral*

$$\int_{-\infty}^{\infty} \varphi(x)\, \mathrm{d}m(x) \coloneqq \lim_{n\to\infty} \sum_{i=1}^{n} \varphi(x_i)[m(x_{i+1}) - m(x_i)];$$

the points x_i, $i = 1, \dots, n+1$, are an equidistant partition of $(-R, R)$ with $x_i < x_{i+1}$ and $x_1 = -R$, $x_{n+1} = R$.

For any fixed $f \in \mathcal{H}$, the function

$$\mathbb{R} \to [0, \infty), \quad \lambda \mapsto \langle E(\lambda)f, f\rangle$$

is monotonically non-decreasing and right continuous. For $\varphi \in C_c(\mathbb{R})$ with $\operatorname{supp}\varphi \subset (-R, R)$, the limit

$$\int_{\mathbb{R}} \varphi(\lambda)\, \mathrm{d}\, \langle E(\lambda)f, f\rangle \coloneqq \lim_{n\to\infty} \sum_{j=1}^{n} \varphi(\lambda_j)(\langle E(\lambda_{j+1})f, f\rangle - \langle E(\lambda_j)f, f\rangle)$$

exists; again the points λ_j, $j = 1, \dots, n+1$, are an equidistant partition of $(-R, R)$ with $\lambda_j < \lambda_{j+1}$ and $\lambda_1 = -R$, $\lambda_{n+1} = R$. For this Riemann-Stieltjes integral, we use the notation

$$\int \varphi(\lambda)\, \mathrm{d}\mu_f(\lambda) := \int_{\mathbb{R}} \varphi(\lambda)\, \mathrm{d}\left\langle E(\lambda)f, f\right\rangle.$$

We also say that the function $\lambda \mapsto \langle E(\lambda)f, f\rangle$ generates the *Riemann-Stieltjes measure* (or *Lebesgue-Stieltjes measure*) μ_f.

Given a spectral family $(E(\lambda))_{\lambda\in\mathbb{R}}$, we now look for a self-adjoint operator H so that

$$H = \int \lambda\, \mathrm{d}E(\lambda)$$

in a suitable sense. For this purpose, we first define the domain

$$\begin{aligned}\mathcal{D} &:= \left\{ f \in \mathcal{H};\ \int \lambda^2\, \mathrm{d}\mu_f(\lambda) < \infty \right\} \\ &= \left\{ f \in \mathcal{H};\ \limsup_{R\to\infty} \int_{-R}^{R} \lambda^2\, \mathrm{d}\left\langle E(\lambda)f, f\right\rangle < \infty \right\}. \end{aligned} \tag{1.1}$$

For $f \in \mathcal{D}$ and $g \in \mathcal{H}$ one shows that

$$\left| \int_{-\infty}^{\infty} \lambda\, \mathrm{d}\left\langle E(\lambda)f, g\right\rangle \right|^2 \le C_f \left\|g\right\|^2$$

with a constant $C_f \ge 0$. For all $f \in \mathcal{D}$,

$$\mathcal{H} \to \mathbb{C}, \quad g \mapsto \int \lambda\, \mathrm{d}\left\langle E(\lambda)f, g\right\rangle$$

is a continuous anti-linear functional on $\mathcal{H}$. By the Riesz representation theorem, there is $w \in \mathcal{H}$, $w = w_f$, such that

$$\langle w, g\rangle = \int \lambda\, \mathrm{d}\left\langle E(\lambda)f, g\right\rangle, \quad \forall g \in \mathcal{H}.$$

We now define

$$Hf := w_f, \quad \forall f \in \mathcal{D},$$

i.e. $H\colon \mathcal{D} \to \mathcal{H}$ is linear and

$$\langle Hf, g\rangle = \int \lambda\, \mathrm{d}\left\langle E(\lambda)f, g\right\rangle, \quad \forall g \in \mathcal{H}. \tag{1.2}$$

One shows that:

(1) $\mathcal{D} \subset \mathcal{H}$ is dense.

(2) $H\colon \mathcal{D} \to \mathcal{H}$ is symmetric.

(3) $H \pm \mathrm{i}\colon \mathcal{D} \to H$ is surjective.

This provides a proof of the following theorem.

Theorem 1.6. *Given a spectral family $(E(\lambda))_{\lambda\in\mathbb{R}}$ there exists a unique self-adjoint operator H such that*

$$H = \int \lambda \, \mathrm{d}E(\lambda)$$

in the sense of (1.1) *and* (1.2).

Contrariwise but much more difficult to prove we note the following theorem.

Theorem 1.7. *Let $H\colon D(H) \to \mathcal{H}$ be a self-adjoint operator in the Hilbert space $\mathcal{H}$. Then there is a unique spectral family $(E(\lambda))_{\lambda\in\mathbb{R}}$ such that*

$$H = \int \lambda \, \mathrm{d}E(\lambda),$$

i.e. the operator obtained for $(E(\lambda))_{\lambda\in\mathbb{R}}$ in Theorem 1.6 equals H.

Remark 1.8. Theorem 1.6 and Theorem 1.7 are the *Spectral Theorem for self-adjoint operators in Hilbert space*. This yields a "diagonalization" of H, in analogy to the principal axis transformation for symmetric matrices.

Definition 1.9. Let $T\colon D(T) \to \mathcal{H}$ be densely defined and let $A \in \mathcal{L}(H)$. We say that A *commutes with* T if $Au \in D(T)$ for all $u \in D(T)$ and if

$$[A, T]u := ATu - TAu = 0, \quad \forall u \in D(T).$$

Theorem 1.10. *Let $H\colon D(H) \to \mathcal{H}$ be self-adjoint, let $(E(\lambda))_{\lambda\in\mathbb{R}}$ be the associated spectral family and let $A \in \mathcal{L}(H)$. Then:*

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

Theorem 1.11. *Let $H\colon D(H) \to \mathcal{H}$ be self-adjoint and let $M \subset \mathcal{H}$ be a closed subspace with projection P. We assume that $[P, H] = 0$ and that there is $\lambda_0 \in \mathbb{R}$ such that $\langle Hu, u\rangle \le \lambda_0 \|u\|^2$ for all $u \in M \cap D(H)$ and $\langle Hu, u\rangle > \lambda_0 \|u\|^2$ for all $0 \ne u \in M^\perp \cap D(H)$. Then $P = E(\lambda_0)$.*

An important application of the spectral theorem for self-adjoint operators in Hilbert space is the option to study functions of operators: For certain classes of functions f, one studies

$$f(H) := \int f(\lambda) \, \mathrm{d}E(\lambda)$$

with the domain

$$D(f(H)) := \left\{ u \in \mathcal{H}; \int |f(\lambda)|^2 \, \mathrm{d} \langle E(\lambda)u, u\rangle < \infty \right\}.$$

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

Theorem 1.12. *Let $H \geq 0$ be self-adjoint with the spectral family $(E(\lambda))_{\lambda \in \mathbb{R}}$. We define an operator T by setting*

$$D(T) := \left\{ u \in \mathcal{H};\ \int_0^\infty \lambda \,\mathrm{d} \langle E(\lambda) u, v \rangle < \infty \right\}$$

and

$$T := \int_0^\infty \sqrt{\lambda}\, \mathrm{d}E(\lambda),$$

i.e.

$$\langle Tu, v \rangle := \int_0^\infty \sqrt{\lambda}\, \mathrm{d} \langle E(\lambda) u, v \rangle, \quad \forall u \in D(T), \forall v \in \mathcal{H}.$$

Then T is a non-negative self-adjoint operator with $T^2 = H$ and T is a square root of H, denoted as $T = \sqrt{H}$. The (non-negative) square root of H is unique.

Given a self-adjoint operator H in the Hilbert space $\mathcal{H}$ with the associated spectral family $(E(\lambda))_{\lambda \in \mathbb{R}}$, we now focus on the characterization of the spectrum $\sigma(H)$ with the aid of the properties of the $E(\lambda)$. First of all we recall the denfinition of the spectrum of some closed operator.

(1) **Spectrum and resolvent set.** Let $T \colon D(T) \to \mathcal{H}$ be closed. We define the *resolvent set* $\rho(T)$ by

$$\begin{aligned} \rho(T) &:= \left\{ z \in \mathbb{C}; (T - z) \colon D(T) \to \mathcal{H} \text{ bijective }, (T - z)^{-1} \in \mathcal{L}(\mathcal{H}) \right\} \\ &= \{ z \in \mathbb{C}; (T - z) \colon D(T) \to \mathcal{H} \text{ bijective} \}. \end{aligned}$$

For a closed operator $T \colon D(T) \to \mathcal{H}$, we call

$$\sigma(T) := \mathbb{C} \backslash \rho(T)$$

the *spectrum of* T.

(2) **Point spectrum and continuous spectrum.** Let $\sigma_{\mathrm{p}}(T)$ be the point spectrum of T given by the set of eigenvalues of T, i.e.

$$\lambda \in \sigma_{\mathrm{p}}(T) \quad :\Longleftrightarrow \quad N(T - \lambda) \neq \{0\},$$

and let $\sigma_{\mathrm{cont}}(T) := \sigma(T) \backslash \sigma_{\mathrm{p}}(T)$ be the *continuous spectrum of* T. Trivially,

$$\sigma(T) = \sigma_{\mathrm{p}}(T) \cup \sigma_{\mathrm{cont}}(T) \quad \text{(disjoint union)}.$$

A decomposition of this type holds in particular for self-adjoint operators, as for self-adjoint operators the residual spectrum is empty.

(3) **Discrete spectrum and essential spectrum.** Let $H\colon D(H) \to \mathcal{H}$ be self-adjoint. We define $\sigma_{\mathrm{disc}}(H)$, the *discrete spectrum of* H, as the set of eigenvalues of H having finite multiplicity and being isolated points of the spectrum. In other words, $\lambda \in \sigma_{\mathrm{disc}}(H)$ if and only if $0 < \dim N(H - \lambda) < \infty$ and if there is $\varepsilon > 0$ with the property $\sigma(H) \cap (\lambda - \varepsilon, \lambda + \varepsilon) = \{\lambda\}$. We define $\sigma_{\mathrm{ess}}(H)$, the *essential spectrum of* H, by

$$\sigma_{\mathrm{ess}}(H) := \sigma(H) \backslash \sigma_{\mathrm{disc}}(H).$$

We thus have the disjoint decomposition

$$\sigma(H) = \sigma_{\mathrm{disc}}(H) \cup \sigma_{\mathrm{ess}}(H).$$

Obviously, $\sigma_{\mathrm{ess}}(H)$ consists of all accumulation points of $\sigma(H)$ and all eigenvalues of infinite multiplicity. In particular, $\sigma_{\mathrm{ess}}(H)$ is a closed subset of $\mathbb{R}$ whereas $\sigma_{\mathrm{cont}}(H)$ is not necessarily closed. We will show later that $\sigma_{\mathrm{ess}}(H)$ is invariant under perturbations by symmetric and compact operators.

Theorem 1.13. *Let* H *be a self-adjoint operator in the Hilbert space* $\mathcal{H}$ *with the spectral family* $(E(\lambda))_{\lambda \in \mathbb{R}}$.

(1) *For* $\zeta \in \mathbb{R}$,

$$\zeta \in \rho(H) \quad \Longleftrightarrow \quad \exists \varepsilon > 0 : E(\zeta - \varepsilon) = E(\zeta + \varepsilon).$$

(2) *For* $\zeta \in \rho(H)$,

$$\left\| (H - \zeta)^{-1} \right\| = \frac{1}{\operatorname{dist}(\zeta, \sigma(H))}.$$

(3) *We have that*

$$H \geq 0 \quad \Longleftrightarrow \quad E(\lambda) = 0, \quad \forall \lambda < 0.$$

Proof. To prove "$\Longleftarrow$" in (1), let $\varepsilon > 0$ with $E(\zeta - \varepsilon) = E(\zeta + \varepsilon)$. Then

$$R_\zeta := \int_{-\infty}^{\infty} (\lambda - \zeta)^{-1} \, \mathrm{d}E(\lambda) \in \mathcal{L}(\mathcal{H})$$

with $\|R_\zeta\| \leq \varepsilon^{-1}$. It is easy to see that $(H - \zeta) R_\zeta = I$ and $R_\zeta (H - \zeta) = I\restriction_{D(H)}$. "$\Longrightarrow$": We assume that $E(\zeta - \varepsilon) \neq E(\zeta + \varepsilon)$ for any $\varepsilon > 0$ and choose for any $\varepsilon > 0$

a function $u_\varepsilon \in R(E(\zeta+\varepsilon)-E(\zeta-\varepsilon)) = R(E(\zeta+\varepsilon)) \cap R(E(\zeta-\varepsilon))^\perp$ with $\|u_\varepsilon\| = 1$. Then $u_\varepsilon \in D(H)$ with

$$\|(H-\zeta)u_\varepsilon\|^2 = \int_{\zeta-\varepsilon}^{\zeta+\varepsilon} |\lambda-\zeta|^2 \,\mathrm{d}\,\langle E(\lambda)u_\varepsilon, u_\varepsilon\rangle \le \varepsilon^2 \|u_\varepsilon\|^2 .$$

Hence $H-\zeta$ cannot be inverted continuously so that $\zeta \notin \rho(H)$. To prove (2), we use that

$$\left\|(H-\zeta)^{-1} f\right\|^2 = \int_{-\infty}^{\infty} |\lambda-\zeta|^{-2} \,\mathrm{d}\,\langle E(\lambda)f, f\rangle, \quad \forall f \in \mathcal{H},$$

and conclude

$$\left\|(H-\zeta)^{-1}\right\| \le \frac{1}{\operatorname{dist}(\zeta, \sigma(H))}.$$

As $\sigma(H)$ is closed, given $\zeta \in \rho(H)$, we can find some $\lambda_0 \in \sigma(H)$ such that

$$|\lambda_0 - \zeta| = \operatorname{dist}(\zeta, \sigma(H)).$$

From (1) we know that given $\varepsilon > 0$ there is $0 \neq u_\varepsilon \in R(E(\lambda_0+\varepsilon) - E(\lambda_0-\varepsilon))$. Hence

$$\begin{aligned}
\left\|(H-\zeta)^{-1}u_\varepsilon\right\|^2 &= \int_{\lambda_0-\varepsilon}^{\lambda_0+\varepsilon} |\lambda-\zeta|^{-2} \,\mathrm{d}\,\langle E(\lambda)u_\varepsilon, u_\varepsilon\rangle \\
&\ge \int_{\lambda_0-\varepsilon}^{\lambda_0+\varepsilon} (|\lambda_0-\zeta|+\varepsilon)^{-2} \,\mathrm{d}\,\langle E(\lambda)u_\varepsilon, u_\varepsilon\rangle \\
&= (|\lambda_0-\zeta|+\varepsilon)^{-2} \|u_\varepsilon\|^2 ,
\end{aligned}$$

as $|\lambda-\zeta| \le |\lambda_0-\zeta| + |\lambda-\lambda_0| \le |\lambda_0-\zeta|+\varepsilon$. Part (3) is trivial. □

We now show that the discontinuities of a spectral family correspond to the point spectrum of the associated self-adjoint operator whereas the strong continuity of the $E(\lambda)$ at $\lambda_0 \in \sigma(H)$ implies $\lambda_0 \in \sigma_{\mathrm{cont}}(H)$ (and vice versa).

Theorem 1.14. *For $\lambda_0 \in \sigma(H)$ we have that*

$$\lambda_0 \in \sigma_{\mathrm{p}}(H) \quad \Longleftrightarrow \quad E(\cdot) \textit{ is not strongly continuous at } \lambda_0,$$

and

$$\lambda_0 \in \sigma_{\mathrm{cont}}(H) \quad \Longleftrightarrow \quad E(\cdot) \textit{ is strongly continuous at } \lambda_0.$$

Proof. Obviously, $E(\lambda)$ is strongly continuous at λ_0 if and only if $E(\lambda_0-0) = E(\lambda_0)$. For $\lambda_0 \in \sigma_{\mathrm{p}}(H)$ and $u_0 \in N(H-\lambda_0)$ with $\|u_0\| = 1$,

$$0 = \|(H-\lambda_0)u_0\|^2 = \int_{-\infty}^{\infty} (\lambda-\lambda_0)^2 \,\mathrm{d}\,\langle E(\lambda)u_0, u_0\rangle .$$

Hence $\langle E(\cdot)u_0, u_0\rangle$ is constant for $\lambda < \lambda_0$ and $\lambda > \lambda_0$, i.e. $\langle E(\lambda)u_0, u_0\rangle = 0$ for $\lambda < \lambda_0$ and $\langle E(\lambda)u_0, u_0\rangle = 1$ for $\lambda > \lambda_0$. Then $E(\cdot)$ is not strongly continuous at

λ_0. On the contrary, assume that $E(\cdot)$ is not strongly continuous at λ_0. Then there is $u \in \mathcal{H}$ with $\|u\| = 1$ so that

$$E(\lambda_0 - 0)u = 0, \quad E(\lambda_0)u = u,$$

i.e. $u \in R(E(\lambda_0 - 0))^\perp \cap R(E(\lambda_0)) = R(E(\lambda_0) - E(\lambda_0 - 0))$, and hence

$$\|(H - \lambda_0)u\|^2 = \int_{\lambda_0 - 0}^{\lambda_0} (\lambda - \lambda_0)^2 \,\mathrm{d}\, \langle E(\lambda)u, u\rangle = 0,$$

i.e. $\lambda_0 \in \sigma_{\mathrm{p}}(H)$. □

The following theorem characterizes the essential and the discrete spectrum of a self-adjoint operator with the aid of its spectral family.

Theorem 1.15. *A number $\lambda \in \mathbb{R}$ belongs to $\sigma_{\mathrm{disc}}(H)$ if and only if the following two properties are satisfied:*

(1) *There is $\varepsilon > 0$ such that $E(\cdot)$ is constant in $(\lambda - \varepsilon, \lambda)$ and $[\lambda, \lambda + \varepsilon)$.*

(2) $0 < \dim R(E(\lambda) - E(\lambda - 0)) < \infty$.

Moreover, $\lambda \in \sigma_{\mathrm{ess}}(H)$ if and only if $\dim R(E(\lambda + \varepsilon) - E(\lambda - \varepsilon)) = \infty$ for any $\varepsilon > 0$.

Proof. The statement concerning $\sigma_{\mathrm{disc}}(H)$ is clear. If $\lambda \in \sigma_{\mathrm{ess}}(H)$, then $\lambda \in \sigma(H)$ and this implies that $E(\lambda - \varepsilon) \neq E(\lambda + \varepsilon)$ for any $\varepsilon > 0$. If $\dim R(E(\lambda + \varepsilon_0) - E(\lambda - \varepsilon_0))$ would be finite for some $\varepsilon_0 > 0$, then $\lambda \in \sigma_{\mathrm{disc}}(H)$. To prove the other direction, we assume for a contradiction that $\dim R(E(\lambda + \varepsilon) - E(\lambda - \varepsilon)) = \infty$ for any $\varepsilon > 0$ and that $\lambda \in \sigma_{\mathrm{disc}}(H)$. By (1) we can find $\eta > 0$ so that $E(\cdot)$ is constant in the intervals $(\lambda - \eta, \lambda)$ and $[\lambda, \lambda + \eta)$. Our assumption implies that $\dim R(E(\lambda) - E(\lambda - 0)) = \infty$ which contradicts the assumption $\lambda \in \sigma_{\mathrm{disc}}(H)$. □

To characterize the essential spectrum of self-adjoint operators, *singular sequences* are useful tools.

Definition 1.16. Let $H\colon D(H) \to \mathcal{H}$ be self-adjoint and let $\lambda \in \mathbb{R}$. A sequence $(u_n)_{n \in \mathbb{N}} \subset D(H)$ is called a *singular sequence for H and λ* if the following three properties are satisfied:

(1) $\|u_n\| = 1$ or $\liminf_{n \to \infty} \|u_n\| > 0$,

(2) $(u_n)_{n \in \mathbb{N}}$ is a weak null sequence, i.e. $u_n \xrightarrow{\mathrm{w}} 0$,

(3) $\|(H - \lambda)u_n\| \to 0$.

Singular sequences are sequences of approximate eigenfunctions. We have the following important theorem.

Theorem 1.17. $\lambda \in \sigma_{\text{ess}}(H) \Longleftrightarrow$ *There is a singular sequence for H and λ.*

Proof. We write
$$H = \int_{-\infty}^{\infty} \lambda \, \mathrm{d}E(\lambda)$$
and assume that $\lambda_0 \in \sigma_{\text{ess}}(H)$. By Theorem 1.15,
$$\dim R(E(\lambda_0+\varepsilon) - E(\lambda_0-\varepsilon)) = \infty, \quad \forall \varepsilon > 0.$$
Let $u_1 \in R(E(\lambda_0+1) - E(\lambda_0-1))$ with $\|u_1\| = 1$ be given. Then $u_1 \in D(H)$ and
$$\|(H-\lambda_0)u_1\|^2 = \int_{\lambda_0-1}^{\lambda_0+1} (\lambda-\lambda_0)^2 \, \mathrm{d}\langle E(\lambda)u_1, u_1\rangle \leq 1.$$
We then choose successively $u_k \in R(E(\lambda_0+1/k) - E(\lambda_0-1/k))$ with $\|u_k\| = 1$ and $\langle u_k, u_j\rangle = 0$ for all $j = 1, \ldots, k-1$; this is possible as
$$\dim R(E(\lambda_0+1/k) - E(\lambda_0-1/k)) = \infty, \quad \forall k \in \mathbb{N},$$
and $\dim \operatorname{span}\{u_1, \ldots, u_{k-1}\} < \infty$, i.e.
$$R(E(\lambda_0+1/k) - E(\lambda_0-1/k)) \cap \operatorname{span}\{u_1, \ldots, u_{k-1}\}^{\perp} \neq \{0\}.$$
Analogously, we get that $u_k \in D(H)$ with
$$\|(H-\lambda_0)u_k\| \leq k^{-1}.$$
Hence $(u_k)_{k\in\mathbb{N}} \subset D(H)$ is a singular sequence for H and λ_0. Contrariwise, we consider a singular sequence $(u_k)_{k\in\mathbb{N}}$ for H and λ_0, i.e.
$$\|u_k\| = 1, \quad u_k \xrightarrow{\mathrm{w}} 0, \quad \|(H-\lambda_0)u_k\| \to 0.$$
First, $\lambda_0 \in \sigma(H)$ since otherwise there would be $\eta > 0$ with $\|(H-\lambda_0)u\| \geq \eta \|u\|$ for all $u \in D(H)$. If $\lambda_0 \in \sigma_{\text{disc}}(H)$ then $E(\cdot)$ would be constant on the intervals $(\lambda_0-\varepsilon_0, \lambda_0)$ and $[\lambda_0, \lambda_0+\varepsilon_0)$ for some $\varepsilon_0 > 0$. Then the sequence $(u_k)_{k\in\mathbb{N}}$ satisfies
$$\begin{aligned}
\|(H-\lambda_0)u_k\|^2 &= \left(\int_{-\infty}^{\lambda_0-\varepsilon_0} + \int_{\lambda_0-\varepsilon_0}^{\lambda_0+\varepsilon_0} + \int_{\lambda_0+\varepsilon_0}^{\infty}\right) (\lambda-\lambda_0)^2 \, \mathrm{d}\langle E(\lambda)u_k, u_k\rangle \\
&\geq \varepsilon_0^2 \left(\int_{-\infty}^{\lambda_0-\varepsilon_0} + \int_{\lambda_0+\varepsilon_0}^{\infty}\right) \mathrm{d}\langle E(\lambda)u_k, u_k\rangle \\
&= \varepsilon_0^2 \int_{-\infty}^{\infty} \mathrm{d}\langle E(\lambda)u_k, u_k\rangle - \varepsilon_0^2 \int_{\lambda_0-\varepsilon_0}^{\lambda_0+\varepsilon_0} \mathrm{d}\langle E(\lambda)u_k, u_k\rangle \\
&= \varepsilon_0^2 \|u_k\|^2 - \varepsilon_0^2 \left(\langle E(\lambda_0+\varepsilon_0)u_k, u_k\rangle - \langle E(\lambda_0-\varepsilon_0)u_k, u_k\rangle\right).
\end{aligned}$$
By our assumption, $\dim R(E(\lambda_0) - E(\lambda_0-0)) < \infty$ and hence
$$\dim \left(R(E(\lambda_0+\varepsilon_0) - E(\lambda_0-\varepsilon_0)\right) < \infty.$$

Consequently $E(\lambda_0+\varepsilon_0)-E(\lambda_0-\varepsilon_0)$ is compact. As $u_k \xrightarrow{\mathrm{w}} 0$ we get that

$$E(\lambda_0+\varepsilon_0)u_k - E(\lambda_0-\varepsilon_0)u_k \to 0 \text{ (strongly).}$$

Thus

$$\liminf_{k\to\infty} \|(H-\lambda_0)u_k\|^2 \geq \varepsilon_0^2 \|u_k\|^2,$$

a contradiction. $\square$

Weyl's perturbation theorem says that the essential spectrum of a self-adjoint operator is invariant under symmetric and compact perturbations.

Theorem 1.18 (Weyl). *Let H be self-adjoint and let $A \in \mathcal{L}(\mathcal{H})$ be symmetric and compact. Then*

$$\sigma_{\text{ess}}(H+A) = \sigma_{\text{ess}}(H).$$

Remark 1.19. As A is bounded, $H+A$ is defined on $D(H+A)=D(H)$. It is easy to see that $H+A$ is self-adjoint for symmetric $A \in \mathcal{L}(\mathcal{H})$ (e.g. using the perturbation theorem of Kato and Rellich).

Proof. We show that (u_n) is a singular sequence for H and λ if and only if (u_n) is a singular sequence for $H+A$ and λ. Let $(u_n) \subset D(H) = D(H+A)$ be a sequence with $\|u_n\|=1$, $u_n \xrightarrow{\mathrm{w}} 0$ and $(H-\lambda)u_n \to 0$ (strongly). As A is compact, $Au_n \to 0$ (strongly) and thus $(H+A-\lambda)u_n \to 0$ (strongly), i.e. (u_n) ist a singular sequence for $H+A$ and λ. The other direction is proved similarly. We have shown that $\lambda \in \sigma_{\text{ess}}(H) \iff$ There is a singular sequence for H and $\lambda \iff$ There is a singular sequence for $H+A$ and $\lambda \iff \lambda \in \sigma_{\text{ess}}(H+A)$. $\square$

Theorem 1.20. *Let H be a self-adjoint operator with the spectral family $(E(\lambda))_{\lambda\in\mathbb{R}}$. Let λ_0 be an isolated point of $\sigma(H)$ and let $\varepsilon_0 > 0$ so that*

$$(\lambda_0 - 2\varepsilon_0, \lambda_0 + 2\varepsilon_0) \cap \sigma(H) = \{\lambda_0\}.$$

Furthermore, let $\Gamma := \partial B(\lambda_0, \varepsilon_0) \subset \mathbb{C}$ be the circle in $\mathbb{C}$ with middle point λ_0 and radius ε_0. Then

$$\frac{1}{2\pi\mathrm{i}} \int_\Gamma (H-\gamma)^{-1}\,\mathrm{d}\gamma = E(\lambda_0) - E(\lambda_0 - 0) = P_{N(H-\lambda_0)}.$$

Proof. As

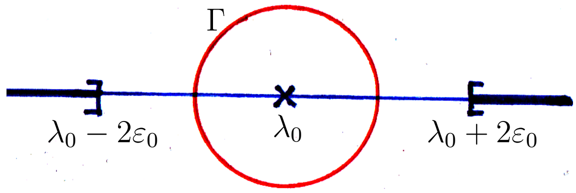
$$(H-\gamma)^{-1} = \int_{-\infty}^{\infty} (\lambda-\gamma)^{-1}\,\mathrm{d}E(\lambda), \quad \gamma \in \Gamma,$$

we obtain that

$$\begin{aligned}\frac{1}{2\pi\mathrm{i}} \int_\Gamma (H-\gamma)^{-1}\,\mathrm{d}\gamma &= \frac{1}{2\pi\mathrm{i}} \int_\Gamma \int_{-\infty}^{\infty} (\lambda-\gamma)^{-1}\,\mathrm{d}E(\lambda)\,\mathrm{d}\gamma \\ &= \int_{-\infty}^{\infty} \left\{ \frac{1}{2\pi\mathrm{i}} \int_\Gamma (\lambda-\gamma)^{-1}\,\mathrm{d}\gamma \right\} \mathrm{d}E(\lambda) =: J.\end{aligned}$$

The integrand can be estimated by $\frac{1}{|\lambda-\gamma|} \leq \frac{1}{\varepsilon_0}$ so that the order of the integrations can be interchanged according to Fubini's Theorem. We know from complex analysis that

$$\hat{\chi}_{\lambda_0,\varepsilon_0}(\lambda) := \frac{1}{2\pi \mathrm{i}} \int_\Gamma (\lambda-\gamma)^{-1} \,\mathrm{d}\gamma = \begin{cases} 1, & |\lambda-\lambda_0| < \varepsilon_0, \\ 1/2, & |\lambda-\lambda_0| = \varepsilon_0, \\ 0, & |\lambda-\lambda_0| > \varepsilon_0. \end{cases}$$



As $E(\lambda_0 - \varepsilon_0 - 0) = E(\lambda_0 - 0)$ and $E(\lambda_0) = E(\lambda_0 + \varepsilon_0)$,

$$J = \int_{-\infty}^{\infty} \hat{\chi}_{\lambda_0,\varepsilon_0}(\lambda) \,\mathrm{d}E(\lambda) = E(\lambda_0) - E(\lambda_0 - 0)$$

which completes our proof. $\square$

In some applications, an important characterization of the discrete eigenvalues below $\inf \sigma_{\mathrm{ess}}(H)$ is given by the *min-max-principle* (see [RS-IV, GS] for more details). For a self-adjoint and semi-bounded operator H, we define for arbitrary vectors $\varphi_1, \ldots, \varphi_m \in \mathcal{H}$ (not necessarily linearly independent) the auxiliary function

$$U_H(\varphi_1, \ldots, \varphi_m) := \inf \{\langle H\psi, \psi\rangle \,;\, \psi \in D(H),\ \|\psi\| = 1,\ \psi \perp \varphi_j,\ 1 \leq j \leq m\}$$

as well as

$$\mu_n(H) := \sup_{\varphi_1,\ldots,\varphi_{n-1}} U_H(\varphi_1, \ldots, \varphi_{n-1}), \quad n \in \mathbb{N},\, n \geq 2,$$

and

$$\mu_1 := \inf \{\langle H\psi, \psi\rangle \,;\, \psi \in D(H),\ \|\psi\| = 1\}\,.$$

For any $n \in \mathbb{N}$ we have: *Either* there are n eigenvalues (counting degenerate eigenvalues a number of times equal to their multiplicities) below $\sigma_{\mathrm{ess}}(H)$ and $\mu_n(H)$ is the n-th eigenvalue *or* $\mu_n(H) = \inf \sigma_{\mathrm{ess}}(H)$; in this case $\mu_n = \mu_{n+1} = \mu_{n+2} = \ldots$ and there are at most $n-1$ eigenvalues (counting multiplicities) below $\inf \sigma_{\mathrm{ess}}(H)$.

Remark 1.21. If $\dim R(E(\lambda)) < \infty$ for some $\lambda \in \mathbb{R}$, then $\dim R(E(\lambda))$ is precisely the number of eigenvalues below λ (counting multiplicities).

Chapter 2

Spectral properties of Schrödinger operators

In this section, we study some important examples of Schrödinger operators and determine their discrete and essential spectra. These operators mostly have the form

$$H = -\Delta + V$$

where $V\colon \mathbb{R}^d \to \mathbb{R}$ is the multiplication operator associated with the potential $V = V(x)$ in the Hibert space $\mathcal{H} := L_2(\mathbb{R}^d)$. Let $H_0\colon D(H_0) \to \mathcal{H}$ be the unique self-adjoint extension of

$$-\Delta\colon C_c^\infty(\mathbb{R}^d) \to \mathcal{H}, \quad -\Delta\varphi = -\sum_{k=1}^{d} \frac{\partial^2}{\partial x_k^2}\varphi(x).$$

The self-adjoint operator H_0 is equal to the closure of $-\Delta \restriction_{C_c^\infty(\mathbb{R}^d)}$ and also equals the Friedrichs extension of $-\Delta \restriction_{C_c^\infty(\mathbb{R}^d)}$. In the following, we will only discuss functions V such that the sum $-\Delta+V$ is defined on $C_c^\infty(\mathbb{R}^d)$, e.g. for V continuous. If $-\Delta+V$ is bounded from below, the Friedrichs extension yields a self-adjoint extension H of $(-\Delta + V) \restriction_{C_c^\infty(\mathbb{R}^d)}$. In many applications, V is bounded relative to H_0 with bound < 1. In this case, we may apply the Kato-Rellich Theorem to deduce that

$$-\Delta + V\colon C_c^\infty(\mathbb{R}^d) \to \mathcal{H}$$

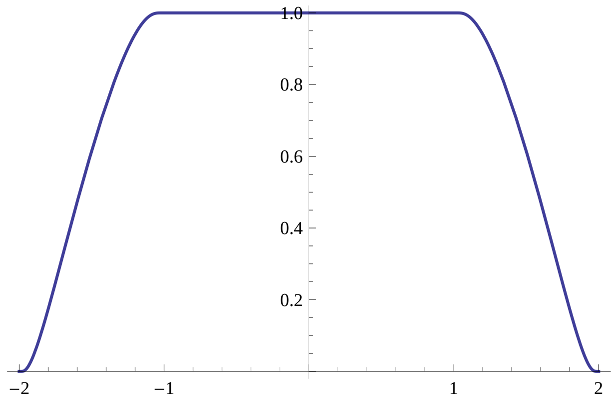
is essentially self-adjoint. The unique self-adjoint extension $H = H_0 + V$ satisfies $D(H) = D(H_0)$.

Let us first study the spectral properties of H_0.

2.1 The free Hamiltonian

We will frequently apply cut-off techniques so that it is useful to prepare some important features of appropriate cut-off functions.

Lemma 2.1. *Let $B_k := \{x \in \mathbb{R}^d; |x| < k\}$ be the open ball with radius $k > 0$ around zero in $\mathbb{R}^d$. There exists a function $\psi\colon \mathbb{R}^d \to \mathbb{R}$ satisfying the properties $\psi \in C_c^\infty(B_2)$, $0 \le \psi \le 1$ and $\psi \equiv 1$ on B_1.*



Proof. Let

$$f(x) := \begin{cases} \exp\left(\frac{1}{(x+4)(x+1)}\right), & -4 < x < -1, \\ 0, & \text{else.} \end{cases}$$

Let us first show that $f \in C^\infty(\mathbb{R})$. Therefor, we define an auxiliary function $g\colon \mathbb{R} \to [0,1)$ by

$$g(t) := \begin{cases} \exp\left(-\frac{1}{t}\right), & t > 0, \\ 0, & t \le 0, \end{cases}$$

and show that, for any $n \in \mathbb{N}$, g is n-times continuously differentiable with $g^{(n)}(0) = 0$. Moreover there exist polynomials p_n so that

$$g^{(n)}(t) := \begin{cases} p_n\left(\frac{1}{t}\right)\exp\left(-\frac{1}{t}\right), & t > 0, \\ 0, & t \le 0. \end{cases} \tag{2.1}$$

For $n = 0$ this is true with $p_0 \equiv 1$. Assuming that the representation (2.1) is true for some fixed $n \in \mathbb{N}$, we obtain, for $t > 0$, that

$$g^{(n+1)}(t) = \left(-p_n'\left(\frac{1}{t}\right) + p_n\left(\frac{1}{t}\right)\right)\frac{1}{t^2}\exp\left(-\frac{1}{t}\right) = p_{n+1}\left(\frac{1}{t}\right)\exp\left(-\frac{1}{t}\right)$$

where $p_{n+1}(\xi) := (p_n(\xi) - p_n'(\xi))\xi^2$. Furthermore,

$$\frac{g^{(n)}(t) - g^{(n)}(0)}{t} = p_n\left(\frac{1}{t}\right)\frac{1}{t}\exp\left(-\frac{1}{t}\right) \to 0, \quad t \to 0.$$

By induction, this shows that $g \in C^\infty(\mathbb{R})$. We can write f as the composition of the smooth functions

$$g_1(x) := g(3(x+4)), \quad g_2(x) := g(-3(x+1))$$

and hence $f \in C^\infty(\mathbb{R})$. We now let $F\colon \mathbb{R} \to \mathbb{R}$ be given by

$$F(t) := \frac{\int_{-4}^{t} f(s)\,\mathrm{d}s}{\int_{-4}^{-1} f(s)\,\mathrm{d}s}$$

and see that $F \in C^\infty(\mathbb{R})$, $F \equiv 0$ on $(-\infty, -4]$ and $F \equiv 1$ on $[-1, \infty)$. The function $\psi(x) := F(-|x|^2)$, $x \in \mathbb{R}^d$, satisfies the properties stated in our lemma. $\square$

Theorem 2.2. *We have that* $\sigma(H_0) = \sigma_{\mathrm{ess}}(H_0) = [0, \infty)$.

Proof. According to the Gauß-Green Theorem, we have for any $\varphi \in C_c^\infty(\mathbb{R}^d)$,

$$\langle H_0\varphi, \varphi\rangle = -\int_{\mathbb{R}^d} \Delta\varphi(x)\overline{\varphi(x)}\,\mathrm{d}x = \langle \nabla\varphi, \nabla\varphi\rangle = \int_{\mathbb{R}^d} |\nabla\varphi(x)|^2\,\mathrm{d}x \geq 0;$$

observe that φ has no contributions on the boundary as supp φ is compact. We write

$$\nabla\varphi = (\partial_1\varphi, \ldots, \partial_d\varphi)^T, \quad \partial_j\varphi = \frac{\partial}{\partial x_j}\varphi.$$

As $H_0 \restriction_{C_c^\infty(\mathbb{R}^d)}$ is essentially self-adjoint, given $f \in D(H_0)$ there exists a sequence $(\varphi_n) \subset C_c^\infty(\mathbb{R}^d)$ such that $\varphi_n \to f$ and $-\Delta\varphi_n \to H_0 f$. Then $\langle H_0 f, f\rangle \geq 0$ for all $f \in D(H_0)$. In particular, $H_0 \geq 0$ so that $E(\lambda) = 0$, $\lambda < 0$, for the associated spectral family, and the spectral theorem shows that $\sigma(H_0) \subset [0, \infty)$.

To complete the proof, we show that $\sigma_{\mathrm{ess}}(H_0) \supset [0, \infty)$. For this purpose, we construct, for any $\lambda \in [0, \infty)$ a suitable singular sequence. Pick $\xi \in \mathbb{R}^d$ so that $\xi \cdot \xi = \lambda$ and let w be the plane wave

$$w(x) := e^{\mathrm{i}\xi\cdot x}, \quad x \in \mathbb{R}^d.$$

Clearly $w \notin \mathcal{H}$, but we have pointwise

$$(-\Delta w)(x) = \lambda w(x), \quad x \in \mathbb{R}^d. \tag{2.2}$$

Let $\psi \in C_c^\infty(B_2)$ with $0 \leq \psi \leq 1$ and $\psi \restriction_{B_1} = 1$. We now define

$$\psi_k(x) := \psi(x/k), \quad x \in \mathbb{R}^d, \quad k \in \mathbb{N},$$

so that $\psi_k(x) = 1$ for $|x| \leq k$, $\psi_k(x) = 0$ for $|x| \geq 2k$ and

$$|\nabla\psi_k(x)| \leq C/k, \quad |\partial_{ij}\psi_k(x)| \leq C/k^2,$$

with a suitable constant $C > 0$ and $\partial_{ij} := \frac{\partial^2}{\partial x_i \partial x_j}$. We set

$$\eta_k := \psi_k w, \quad c_k := \frac{1}{\|\eta_k\|}, \quad k \in \mathbb{N},$$

and show that the functions

$$u_k := c_k\eta_k$$

are a singular sequence for H_0 and λ.

(1) Clearly, $\|u_k\| = 1$.

(2) To show that $u_k \xrightarrow{\mathrm{w}} 0$, we pick $f \in C_c^\infty(\mathbb{R}^d)$, write $\Omega_k \coloneqq B_{2k} \backslash B_k$ and observe that

$$\begin{aligned} |\langle f, u_k\rangle| &= \left| \int_{B_{2k}} f \frac{\eta_k}{\|\eta_k\|} \, \mathrm{d}x \right| \\ &\leq \left| \int_{B_k} f \frac{1}{\|\eta_k\|} \, \mathrm{d}x \right| + \left| \int_{\Omega_k} f \frac{\eta_k}{\|\eta_k\|} \, \mathrm{d}x \right| \\ &\leq \frac{\|f\|_{L_1}}{\|\eta_k\|} + \left| \int_{\Omega_k} f \frac{\eta_k}{\|\eta_k\|} \, \mathrm{d}x \right| \to 0 \end{aligned} \tag{2.3}$$

as $k \to \infty$. Here, we have used that

$$\|\eta_k\|^2 = \int_{\mathbb{R}^d} |\psi_k(x) w(x)|^2 \, \mathrm{d}x \geq \int_{B_k} |w(x)|^2 \, \mathrm{d}x = |B_k| \to \infty$$

and that the second term on the right-hand side of (2.3) vanishes for $k \geq K$ and $\operatorname{supp} f \subset B_K$. As $C_c^\infty(\mathbb{R}^d) \subset L_2(\mathbb{R}^d)$ is dense, we conclude that $\langle f, u_k\rangle \to 0$ for any $f \in \mathcal{H}$.

(3) It remains to show that $\|(H_0 - \lambda)u_k\| \to 0$, $k \to \infty$. For $f \in C^\infty(\mathbb{R}^d)$, we first prepare the identity

$$\begin{aligned} -\Delta(\psi_k f) &= -\sum_{j=1}^d \partial_j^2(\psi_k f) = -\sum_{j=1}^d \left[(\partial_j^2 \psi_k) f + 2\partial_j \psi_k \partial_j f + \psi_k \partial_j^2 f \right] \\ &= -(\Delta\psi_k) f - 2\langle \nabla\psi_k, \nabla f\rangle - \psi_k \Delta f. \end{aligned} \tag{2.4}$$

Again we decompose

$$\begin{aligned} \|(H_0 - \lambda)u_k\|^2 &= \int_{\mathbb{R}^d} \left| (-\Delta - \lambda) \frac{\eta_k}{\|\eta_k\|} \right|^2 \mathrm{d}x \\ &= \frac{1}{\|\eta_k\|^2} \left[\int_{B_k} \left| (-\Delta - \lambda) e^{\mathrm{i}\xi\cdot x} \right|^2 \mathrm{d}x + \int_{\Omega_k} \left| (-\Delta - \lambda)(\psi_k w) \right|^2 \mathrm{d}x \right]. \end{aligned} \tag{2.5}$$

The first term on the right-hand side of (2.5) vanishes according to (2.2). Using once again the identity (2.2) and equation (2.4), we get that

$$\begin{aligned} \|(H_0 - \lambda)u_k\|^2 &= \frac{1}{\|\eta_k\|^2} \int_{\Omega_k} \left| -\Delta(\psi_k w) + \psi_k \Delta w \right|^2 \mathrm{d}x \\ &= \frac{1}{\|\eta_k\|^2} \int_{\Omega_k} \left| 2\langle \nabla\psi_k, \nabla w\rangle + \Delta\psi_k w \right|^2 \mathrm{d}x \\ &\leq \frac{2}{\|\eta_k\|^2} \left[\int_{\Omega_k} \left| 2\langle \xi, \nabla\psi_k\rangle \right|^2 \mathrm{d}x + \int_{\Omega_k} |\Delta\psi_k|^2 \, \mathrm{d}x \right] \end{aligned}$$

$$\leq \frac{2}{\|\eta_k\|^2}\left[4\lambda \int_{\Omega_k} |\nabla\psi_k|^2 \,\mathrm{d}x + \int_{\Omega_k} |\Delta\psi_k|^2 \,\mathrm{d}x\right].$$

By our construction, there exist positive constants C_1, C_2 such that

$$\begin{aligned}\|(H_0-\lambda)u_k\|^2 &\leq \frac{|\Omega_k|}{|B_k|}\left(\frac{C_1}{k^2}+\frac{C_2}{k^4}\right) = \frac{(2k)^d - k^d}{k^d}\left(\frac{C_1}{k^2}+\frac{C_2}{k^4}\right) \\ &= (2^d-1)\left(\frac{C_1}{k^2}+\frac{C_2}{k^4}\right) \to 0,\end{aligned}$$

as $k \to \infty$. This completes the proof of our theorem. □

We will see later that H_0 does not have eigenvalues. Indeed, the spectrum of H_0 is purely absolutely continuous.

2.2 $V(x) \to \infty$ for $|x| \to \infty$

Next, we consider continuous potentials $V = V(x)$ with

$$V(x) \to \infty, \quad |x| \to \infty. \tag{2.6}$$

The most important example in this class is the harmonic oscillator for which

$$V(x) = |x|^2, \quad x \in \mathbb{R}^d.$$

Let $c_0 \in \mathbb{R}$ be a constant with the property $V(x) \geq c_0$ for all $x \in \mathbb{R}^d$. Then $(-\Delta + V)\colon C_c^\infty(\mathbb{R}^d) \to \mathcal{H}$ is semi-bounded and the Friedrichs extension yields a self-adjoint extension $H\colon D(H) \to \mathcal{H}$. Indeed, $(-\Delta+V)\restriction_{C_c^\infty(\mathbb{R}^d)}$ is also essentially self-adjoint (without giving a proof here) and hence it has a unique self-adjoint extension. We conclude that the Friedrichs extension equals $\overline{(-\Delta+V)\restriction_{C_c^\infty(\mathbb{R}^d)}}$.

For the class (2.6), compactness will play a decisive role. Our main theorem reads as follows.

Theorem 2.3. *Let $V : \mathbb{R}^d \to \mathbb{R}$ be continuous with $V(x) \to \infty$ for $|x| \to \infty$ and let $H = H_0 + V$ be the Friedrichs extension of $(-\Delta+V)\restriction_{C_c^\infty(\mathbb{R}^d)}$. Then:*

(1) *There is a constant c_0 such that $H + c_0 \geq 1$ and $(H+c_0)^{-1}$ is compact.*

(2) *The spectrum $\sigma(H)$ is an increasing sequence $(\lambda_k)_{k\in\mathbb{N}} \subset \mathbb{R}$ of eigenvalues of finite multiplicity and $\lambda_k \to \infty$ for $k \to \infty$. In particular, $\sigma(H) = \sigma_{\mathrm{disc}}(H)$ and $\sigma_{\mathrm{ess}}(H) = \emptyset$.*

(3) *The associated eigenfunctions form an orthonormal basis of the Hilbert space $L_2(\mathbb{R}^d)$.*

Concerning compactness, we will have to prepare some tools.

Definition 2.4. For $\varphi \in C_c^\infty(\mathbb{R}^d)$, let

$$\|\varphi\|_1^2 := \|\varphi\|^2 + \|\nabla\varphi\|^2 .$$

Then $\|\varphi\|_1 \geq \|\varphi\|$, for all $\varphi \in C_c^\infty(\mathbb{R}^d)$, $\|\cdot\|_1$ is a norm on $C_c^\infty(\mathbb{R}^d)$ and $\left(C_c^\infty(\mathbb{R}^d), \|\cdot\|_1\right)$ is a pre-Hilbert space. We denote its completion by $\mathring{\mathcal{H}}^1(\mathbb{R}^d)$. We have $\mathring{\mathcal{H}}^1(\mathbb{R}^d) \subset L_2(\mathbb{R}^d)$ with continuous embedding and $\mathring{\mathcal{H}}^1(\mathbb{R}^d)$ belongs to the class of *Sobolev spaces*. Similarly, we define, for $\Omega \subset \mathbb{R}^d$ open, the Sobolev spaces $\mathring{\mathcal{H}}^1(\Omega)$.

Remark 2.5. $\|\nabla u\|^2 = \sum_{k=1}^d \|\partial_k u\|^2 = \int_{\mathbb{R}^d} |\nabla u(x)|^2 \,\mathrm{d}x = \sum_{k=1}^d \int_{\mathbb{R}^d} |\partial_k u(x)|^2 \,\mathrm{d}x$.

Our aim is to give a proof of Rellich's compactness theorem which can be seen as the Hilbert space version of the Arzelà-Ascoli Theorem. Therefor, the following lemma will be crucial.

Lemma 2.6. *Let $Q := (0, 2\pi)^d \subset \mathbb{R}^d$ and let $(u_n)_{n\in\mathbb{N}} \subset C_c^\infty(Q)$ be a sequence with*

$$\|u_n\|_1 \leq c_0, \quad \forall n \in \mathbb{N}.$$

Then there exist a subsequence $(u_{n_k})_{k\in\mathbb{N}} \subset (u_n)_{n\in\mathbb{N}}$ and $u \in \mathring{\mathcal{H}}^1(Q)$ such that

$$\begin{aligned} &u_{n_k} \to u \text{ in } L_2(Q) \text{ and} \\ &u_{n_k} \xrightarrow{\mathrm{w}} u \text{ in } \mathring{\mathcal{H}}^1(Q), \end{aligned}$$

as $k \to \infty$.

Proof.

(1) As $L_2(Q)$ and $\mathring{\mathcal{H}}^1(Q)$ are Hilbert spaces, there are subsequences $\left(u_{n_j}^{(1)}\right)_{j\in\mathbb{N}} \subset (u_n)_{n\in\mathbb{N}}$ and $\left(u_{n_j}^{(2)}\right)_{j\in\mathbb{N}} \subset \left(u_{n_j}^{(1)}\right)_{j\in\mathbb{N}}$ and vectors $u \in L_2(Q)$ and $v \in \mathring{\mathcal{H}}^1(Q)$ such that

$$\begin{aligned} &u_{n_j}^{(1)} \xrightarrow{\mathrm{w}} u \text{ in } L_2(Q) \text{ and} \\ &u_{n_j}^{(2)} \xrightarrow{\mathrm{w}} v \text{ in } \mathring{\mathcal{H}}^1(Q), \end{aligned}$$

as $j \to \infty$. Let us show that $u = v$. For this purpose, we may assume without loss of generality that $v = 0$ since otherwise we would consider $\tilde{u}_n := u_n - v$. For $f \in L_2(Q)$, we define a linear functional $\ell_f \colon \mathring{\mathcal{H}}^1(Q) \to \mathbb{C}$ by setting

$$\ell_f(\varphi) := \langle \varphi, f \rangle, \quad \forall \varphi \in \mathring{\mathcal{H}}^1(Q).$$

As $|\ell_f(\varphi)| \leq \|\varphi\| \|f\| \leq \|\varphi\|_1 \|f\|$, we conclude that $\ell_f \in (\mathring{\mathcal{H}}^1(Q))^*$ and by the Riesz representation theorem, there exists a unique $\tilde{f} \in \mathring{\mathcal{H}}^1(Q)$ so that

$$\langle \varphi, f \rangle = \left\langle \varphi, \tilde{f} \right\rangle_1, \quad \forall \varphi \in \mathring{\mathcal{H}}^1(Q).$$

For arbitrary $f \in L_2(Q)$, we thus have that

$$\left\langle u_{n_j}^{(2)}, f \right\rangle = \left\langle u_{n_j}^{(2)}, \tilde{f} \right\rangle_1 \to 0, \quad n \to \infty$$

so that $u_{n_j}^{(2)} \xrightarrow{\text{w}} 0$ in $L_2(Q)$ and hence $u = v$. To simplify notation, we write henceforth

$$\begin{aligned} u_n &\xrightarrow{\text{w}} u \text{ in } L_2(Q) \text{ and} \\ u_n &\xrightarrow{\text{w}} u \text{ in } \mathring{\mathcal{H}}^1(Q), \end{aligned}$$

as $n \to \infty$.

(2) For $k \in \mathbb{Z}^d$, let

$$\varphi_k(x) := (2\pi)^{-d/2} e^{\mathrm{i}k\cdot x} = (2\pi)^{-d/2} \prod_{s=1}^{d} e^{\mathrm{i}k_s x_s}.$$

The family $(\varphi_k)_{k\in\mathbb{Z}^d}$ is an orthonormal basis of $L_2(Q)$ (Fourier series). By Parseval's Theorem,

$$\sum_{k\in\mathbb{Z}^d} \left|\left\langle u_n, e^{\mathrm{i}k\cdot x}\right\rangle\right|^2 = (2\pi)^d \left\|u_n\right\|^2 \le c_1.$$

But as $\|\partial_s u_n\| \le c_0$, $s = 1, \dots, d$, we may also conclude that

$$\sum_{k\in\mathbb{Z}^d} \left|\left\langle \partial_s u_n, e^{\mathrm{i}k\cdot x}\right\rangle\right|^2 = (2\pi)^d \left\|\partial_s u_n\right\|^2 \le c_2, \quad s = 1, \dots, d.$$

Using that

$$\left\langle \partial_s u_n, e^{\mathrm{i}k\cdot x}\right\rangle = -\left\langle u_n, \partial_s e^{\mathrm{i}k\cdot x}\right\rangle = \mathrm{i}k_s \left\langle u_n, e^{\mathrm{i}k\cdot x}\right\rangle,$$

we obtain that there exists a constant $c_3 \ge 0$ such that

$$\sum_{k\in\mathbb{Z}^d} \left(1 + |k|^2\right) \left|\left\langle u_n, e^{\mathrm{i}k\cdot x}\right\rangle\right|^2 \le c_3, \quad n \in \mathbb{N};$$

here, $|k|^2 = \sum_{s=1}^d k_s^2$.

(3) As $u_n \xrightarrow{\text{w}} u$, we also have, for $n \to \infty$,

$$\left\langle u_n, e^{\mathrm{i}k\cdot x}\right\rangle \to \left\langle u, e^{\mathrm{i}k\cdot x}\right\rangle, \quad \forall k \in \mathbb{Z}^d,$$

so that $\left(\left\langle u_n, e^{\mathrm{i}k\cdot x}\right\rangle\right)_{n\in\mathbb{N}} \subset \mathbb{C}$ is a Cauchy sequence for all $k \in \mathbb{Z}^d$.

(4) We claim that $(u_n)_{n\in\mathbb{N}}$ is a Cauchy sequence in $L_2(Q)$. Let $\varepsilon > 0$ and $R := \sqrt{c_3/\varepsilon}$. We note that there are only finitely many $k \in \mathbb{Z}^d$ such that $|k|^2 \le R^2$. According to (3), there is $J_\varepsilon \in \mathbb{N}$ such that

$$(2\pi)^{-d} \sum_{|k|\le R} \left|\left\langle u_j - u_m, e^{\mathrm{i}k\cdot x}\right\rangle\right|^2 \le \varepsilon, \quad j, m \ge J_\varepsilon. \tag{2.7}$$

By Parseval's Theorem, for $j, m \geq J_\varepsilon$,

$$\begin{aligned}
\|u_j - u_m\|^2 &= (2\pi)^{-d} \sum_{k \in \mathbb{Z}^d} \left|\left\langle u_j - u_m, e^{\mathrm{i}k\cdot x}\right\rangle\right|^2 \\
&= (2\pi)^{-d} \left(\sum_{|k| \leq R} + \sum_{|k| > R} \right) \left|\left\langle u_j - u_m, e^{\mathrm{i}k\cdot x}\right\rangle\right|^2 \\
&\leq_{(2.7)} \varepsilon + (2\pi)^{-d} \sum_{|k|>R} \frac{|k|^2}{R^2} \left|\left\langle u_j - u_m, e^{\mathrm{i}k\cdot x}\right\rangle\right|^2 \\
&\leq \varepsilon + (2\pi)^{-d} R^{-2} \sum_{k \in \mathbb{Z}^d} |k|^2 \left|\left\langle u_j - u_m, e^{\mathrm{i}k\cdot x}\right\rangle\right|^2 \\
&\leq \varepsilon + 2(2\pi)^{-d} R^{-2} \sum_{k \in \mathbb{Z}^d} |k|^2 \left[\left|\left\langle u_j, e^{\mathrm{i}k\cdot x}\right\rangle\right|^2 + \left|\left\langle u_m, e^{\mathrm{i}k\cdot x}\right\rangle\right|^2 \right] \\
&\leq \varepsilon + 4c_3 (2\pi)^{-d} R^{-2} \\
&\leq 2\varepsilon.
\end{aligned}$$

Now $u_n \xrightarrow{\mathrm{w}} u$ and the Cauchy property show that $\|u_n - u\| \to 0$. □

Theorem 2.7 (Rellich). *Let $\Omega \subset \mathbb{R}^d$ be open and bounded. Then for any bounded sequence $(u_n)_{n\in\mathbb{N}}$ in $\mathring{\mathcal{H}}^1(\Omega)$ there exists a subsequence $(u_{n_k})_{k\in\mathbb{N}} \subset (u_n)_{n\in\mathbb{N}}$ such that $(u_{n_k})_{k\in\mathbb{N}}$ converges strongly in $L_2(\Omega)$.*

Proof. Let $(u_n)_{n\in\mathbb{N}} \subset \mathring{\mathcal{H}}^1(\Omega)$ with $\|u_n\|_1 \leq c_1$ be given. Let $W \subset \mathbb{R}^d$ be an (open) cube such that $\overline{\Omega} \subset W$. For any u_n there exists $\varphi_n \in C_c^\infty(\Omega) \subset C_c^\infty(W)$ such that $\|u_n - \varphi_n\|_1 \leq \frac{1}{n}$. As $\|\varphi_n\|_1 \leq c_2$ and by Lemma 2.6, there exist a subsequence $(\varphi_{n_k})_{k\in\mathbb{N}} \subset (\varphi_n)_{n\in\mathbb{N}}$ and $u \in \mathring{\mathcal{H}}^1(W)$ such that

$$\varphi_{n_k} \to u \text{ in } L_2(W), \quad \varphi_{n_k} \xrightarrow{\mathrm{w}} u \text{ in } \mathring{\mathcal{H}}^1(W), \tag{2.8}$$

as $k \to \infty$. We let $u' := u\restriction_\Omega$. Then $u' \in L_2(\Omega)$ and $\varphi_{n_k} \to u'$ in $L_2(\Omega)$. By (2.8) and as $\mathring{\mathcal{H}}^1(\Omega) \subset \mathring{\mathcal{H}}^1(W)$,

$$\langle \varphi_{n_k}, \psi \rangle_1 \to \langle u, \psi \rangle_1, \quad \forall \psi \in \mathring{\mathcal{H}}^1(\Omega), \tag{2.9}$$

and hence $(\varphi_{n_k})_{k\in\mathbb{N}}$ converges weakly in $\mathring{\mathcal{H}}^1(\Omega)$. As Hilbert spaces are weakly sequentially closed, there is $v \in \mathring{\mathcal{H}}^1(\Omega)$ with $\varphi_{n_k} \xrightarrow{\mathrm{w}} v$ in $\mathring{\mathcal{H}}^1(\Omega)$. Now (2.9) implies that $v = u'$, in particular $u' \in \mathring{\mathcal{H}}^1(\Omega)$ and $\varphi_{n_k} \xrightarrow{\mathrm{w}} u'$ in $\mathring{\mathcal{H}}^1(\Omega)$. But then $u_{n_k} \to u'$ in $L_2(\Omega)$ and $u_{n_k} \xrightarrow{\mathrm{w}} u'$ in $\mathring{\mathcal{H}}^1(\Omega)$. □

Remark 2.8.

(1) Theorem 2.7 may also be stated as follows: For $\Omega \subset \mathbb{R}^d$ open and bounded the canonical embedding $\mathring{\mathcal{H}}^1(\Omega) \hookrightarrow L_2(\Omega)$ is compact (Rellich's embedding theorem).

(2) The strong limit u is in fact an element of $\mathring{\mathcal{H}}^1(\Omega)$ and additionally $u_{n_k} \xrightarrow{\text{w}} u$ in $\mathring{\mathcal{H}}^1(\Omega)$.

(3) The continuous embedding $\mathring{\mathcal{H}}^1(\Omega) \hookrightarrow L_2(\Omega)$ generates a self-adjoint and positive operator H with $D(H) \subset \mathring{\mathcal{H}}^1(\Omega)$ and

$$\langle Hu, v\rangle = \langle u, v\rangle_1, \quad \forall u \in D(H), \quad v \in \mathring{\mathcal{H}}^1(\Omega).$$

Moreover, H is the Friedrichs extension of $-\Delta \restriction_{C_c^\infty(\Omega)}$. We call H the Laplace operator with *(homogeneous) Dirichlet boundary conditions on* Ω and write $H_D^{(\Omega)} := H$.

To simplify notation, we assume henceforth (without loss of generality) that

$$V(x) \geq 0, \quad x \in \mathbb{R}^d.$$

Let $\mathring{\mathcal{H}}^1_V(\mathbb{R}^d)$ denote the completion of the pre-Hilbert space $(C_c^\infty(\mathbb{R}^d), \langle\cdot,\cdot\rangle_{1,V})$ where

$$\langle\varphi, \psi\rangle_{1,V} := \langle\varphi, \psi\rangle_1 + \int_{\mathbb{R}^d} V(x)\varphi(x)\overline{\psi(x)}\,\mathrm{d}x.$$

It is easy to see that

$$\begin{aligned}\mathring{\mathcal{H}}^1_V(\mathbb{R}^d) &= \left\{u \in \mathring{\mathcal{H}}^1(\mathbb{R}^d); \int_{\mathbb{R}^d} V(x)|u(x)|^2\,\mathrm{d}x < \infty\right\}\\ &= \mathring{\mathcal{H}}^1(\mathbb{R}^d) \cap \left\{u \in L_2(\mathbb{R}^d); \int_{\mathbb{R}^d} V(x)|u(x)|^2\,\mathrm{d}x < \infty\right\}.\end{aligned}$$

The Friedrichs extension $H = H_0 + V$ of $(-\Delta + V)\restriction_{C_c^\infty(\mathbb{R}^d)}$ is thus characterized by the properties

$$C_c^\infty(\mathbb{R}^d) \subset D(H) \subset \mathring{\mathcal{H}}^1_V(\mathbb{R}^d)$$

and

$$\langle Hu, v\rangle = \langle u, v\rangle_{1,V}, \quad \forall u \in D(H), \quad v \in \mathring{\mathcal{H}}^1_V(\mathbb{R}^d).$$

Furthermore, $D(H)$ is dense in $\mathring{\mathcal{H}}^1_V(\mathbb{R}^d)$ with respect to $\|\cdot\|_{1,V}$.

Theorem 2.9. *Let $V\colon \mathbb{R}^d \to \mathbb{R}$ be continuous with $V(x) \to \infty$ for $|x| \to \infty$ and let $H = H_0 + V$ be the Friedrichs extension of $(-\Delta + V)\restriction_{C_c^\infty(\mathbb{R}^d)}$. Then:*

(1) *$H \geq 0$ and $(H+1)^{-1}$ is compact.*

(2) *$\sigma(H)$ is an increasing sequence $(\lambda_k)_{k\in\mathbb{N}} \subset \mathbb{R}$ of eigenvalues of finite multiplicity and $\lambda_k \to \infty$ for $k \to \infty$. In particular, $\sigma(H) = \sigma_{\mathrm{disc}}(H)$ and $\sigma_{\mathrm{ess}}(H) = \emptyset$.*

(3) *The associated eigenfunctions form an orthonormal basis of the Hilbert space $L_2(\mathbb{R}^d)$.*

Proof. Our assumption $V(x) \geq 0$ implies that $H \geq 0$.

(1) Let $f_n \xrightarrow{\mathrm{w}} 0$ in $\mathcal{H} = L_2(\mathbb{R}^d)$ and let

$$u_n := (H+1)^{-1} f_n.$$

We show that there is a subsequence $(u_{n_j}) \subset (u_n)$ such that $\|u_{n_j}\| \to 0$, $j \to \infty$. First, the fact that (f_n) converges weakly implies that (f_n) is bounded in $\mathcal{H}$. As $(H+1)^{-1}$ is bounded, the sequence (u_n) is also bounded in $\mathcal{H}$ and converges weakly to zero in $\mathcal{H}$. Furthermore, $u_n \in D(H)$ and

$$\|Hu_n\| \le \left\|(H+1)(H+1)^{-1} f_n\right\| + \|u_n\| \le \|f_n\| + \|u_n\| \le C_1.$$

By the definition of H,

$$\|u_n\|_{1,V}^2 = \langle u_n, u_n \rangle_{1,V} = \langle Hu_n, u_n \rangle \le \|Hu_n\| \, \|u_n\| \le C_2. \tag{2.10}$$

Given $\varepsilon > 0$, we choose $R \ge 0$ such that

$$V(x) \ge \varepsilon^{-1}, \quad |x| \ge R.$$

By (2.10), $\int_{\mathbb{R}^d} V(x)|u_n(x)|^2 \, \mathrm{d}x \le C_2$ and hence $\int_{|x|\ge R} |u_n(x)|^2 \, \mathrm{d}x \le C_2 \varepsilon$. Let $\psi_R \in C_c^\infty(B_{2R})$ with $\psi_R \restriction_{B_R} = 1$ and $0 \le \psi_R \le 1$. We observe that

$$\|\psi_R u_n\|_1^2 \le 2 \int_{\mathbb{R}^d} \psi_R^2 |\nabla u_n|^2 \, \mathrm{d}x + 2 \int_{\mathbb{R}^d} |\nabla \psi_R|^2 |u_n|^2 \, \mathrm{d}x + \|u_n\|^2 \le_{(2.10)} C_3.$$

Consequently, $(\psi_R u_n)_{n \in \mathbb{N}}$ is a bounded sequence in $\mathring{\mathcal{H}}^1(B_{2R})$. Applying Rellich's compactness theorem, we obtain a subsequence $(u_{n_j}) \subset (u_n)$ such that $\|\psi_R u_{n_j}\| \to 0$, $j \to \infty$, as $u_n \xrightarrow{\mathrm{w}} 0$. Choose $j_0 \in \mathbb{N}$ so that

$$\left\|\psi_R u_{n_j}\right\|^2 < \varepsilon, \quad j \ge j_0.$$

We now obtain that $\left\|u_{n_j}\right\|^2 < C_2 \varepsilon + \varepsilon$ for $j \ge j_0$.

(2) Note that $(H+1)\colon D(H) \to L_2(\mathbb{R}^d)$ is bijective with compact inverse $(H+1)^{-1}$. This implies that $N((H+1)^{-1}) = \{0\}$ and thus the eigenfunctions of $(H+1)^{-1}$ form an orthonormal basis of $L_2(\mathbb{R}^d)$. Clearly, $\sigma_{\mathrm{ess}}(H) = \emptyset$. □

Remark 2.10.

(1) For any $z_1, z_2 \in \rho(H)$ one has

$$(H - z_1)^{-1} \text{ compact} \iff (H - z_2)^{-1} \text{ compact}.$$

This is an immediate consequence of the second resolvent equation as

$$(H - z_1)^{-1} - (H - z_2)^{-1} = (H - z_1)^{-1}(z_1 - z_2)(H - z_2)^{-1}.$$

(2) Criteria that H_0+V has compact resolvent: see, e.g., [A. Molchanov: On the discreteness of the spectrum conditions for self-adjoint differential equations of the second order; Trudy Mosk. Matem. Obshchestva **2** 169–199 (1953)], [V. Maz'ya & M. Shubin: Discreteness of spectrum and positivity criteria for Schrödinger operators; Ann. Math. **162** 919–942 (2005)] and [RS-IV, XIII.14]

(3) Asymptotic behavior of the eigenvalues λ_k for $k \to \infty$ (H. Weyl, see [RS-IV, XIII.15])

Let $V(x) \coloneqq x^2$, $x \in \mathbb{R}$. Then

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V \colon C_c^\infty(\mathbb{R}) \to L_2(\mathbb{R})$$

is essentially self-adjoint with the (unique) self-adjoint extension

$$H = H_0 + V = \overline{\left(-\tfrac{\mathrm{d}^2}{\mathrm{d}x^2} + V\right)\restriction_{C_c^\infty(\mathbb{R})}}.$$

Theorem 2.3 implies that $\sigma(H) = \sigma_{\mathrm{disc}}(H)$. Moreover, $\sigma(H)$ consists of a sequence of eigenvalues of finite multiplicity $0 < \lambda_1 < \lambda_2 < \dots$ with $\lambda_k \to \infty$ as $k \to \infty$. It is possible to calculate the eigenvalues of H explicitly; they are given by

$$\lambda_k \coloneqq 2k+1, \quad k \in \mathbb{N}_0.$$

The associated eigenfunctions are of the form

$$\Phi_k(x) = c_k P_k(x) e^{-\frac{1}{2}x^2}, \quad x \in \mathbb{R}, \quad k \in \mathbb{N}_0;$$

here, P_k is a polynomial of degree k and c_k is a constant such that

$$\langle \Phi_n, \Phi_k \rangle = \delta_{nk}, \quad k, n \in \mathbb{N}_0.$$

The family $(P_k)_{k\in\mathbb{N}}$ is the family of *Hermite polynomials* that is obtained from the Gram-Schmidt process applied to the scalar product

$$\langle p, q \rangle_{\mathrm{H}} \coloneqq \int_{\mathbb{R}} p(x)\overline{q(x)} e^{-x^2}\,\mathrm{d}x$$

and the polynomials $1, x, x^2, x^3, \dots$. Furthermore, the family $(\Phi_k)_{k\in\mathbb{N}}$ is an orthonormal basis of the Hilbert space $L_2(\mathbb{R})$. The eigenfunctions Φ_k are not elements of $C_c^\infty(\mathbb{R})$ but they are elements of the Schwartz space $\mathscr{S}(\mathbb{R})$.

Definition 2.11. We define the Schwartz space $\mathscr{S}(\mathbb{R})$ by

$$\mathscr{S}(\mathbb{R}) = \left\{ f \in C^\infty(\mathbb{R}); \forall k, m \in \mathbb{N}_0 \exists C \geq 0\colon \left(1 + |x|^k\right) \left|f^{(m)}(x)\right| \leq C. \right\}.$$

Remark 2.12. Obviously, $C_c^\infty(\mathbb{R}) \subset \mathscr{S}(\mathbb{R})$. It is easy to see that $\mathscr{S}(\mathbb{R}) \subset D(H)$. In particular, H is also essentially self-adjoint on $\mathscr{S}(\mathbb{R})$.

The eigenfunctions can be constructed applying the so-called *ladder operators*. In the following theorems we omit the norming constants for the sake of simplicity.

Theorem 2.13. *Let $\varphi_0 \in \mathscr{S}(\mathbb{R})$ be defined by*

$$\varphi_0(x) \coloneqq \frac{1}{\sqrt[4]{\pi}} e^{-\frac{1}{2}x^2}, \quad x \in \mathbb{R}.$$

Let $A, A^\dagger \colon \mathscr{S}(\mathbb{R}) \to \mathscr{S}(\mathbb{R})$ be defined by

$$A \coloneqq \frac{1}{\sqrt{2}}\left(x + \frac{\mathrm{d}}{\mathrm{d}x}\right), \quad A^\dagger \coloneqq \frac{1}{\sqrt{2}}\left(x - \frac{\mathrm{d}}{\mathrm{d}x}\right).$$

(1) *Let $N \coloneqq A^\dagger A$. Then $N = \frac{1}{2}(H-1)$, $[N, A] = -A$ and $[N, A^\dagger] = A^\dagger$.*

(2) *Let $\varphi_n \coloneqq (A^\dagger)^n \varphi_0$, for $n \in \mathbb{N}$. We have that $N\varphi_n = n\varphi_n$, $n \in \mathbb{N}_0$. Moreover, for $n, k \in \mathbb{N}_0$ and $n \neq k$, $\langle \varphi_n, \varphi_k \rangle = 0$.*

Proof. Let $M_x, \partial \colon \mathscr{S}(\mathbb{R}) \to \mathscr{S}(\mathbb{R})$ be defined by $(M_x f)(x) \coloneqq x f(x)$ and $(\partial f)(x) \coloneqq f'(x)$. We have

$$N = A^\dagger A = \frac{1}{2}(M_x - \partial)(M_x + \partial) = \frac{1}{2}\left(M_{x^2} - [\partial, M_x] - \partial^2\right) = \frac{1}{2}(H-1)$$

with $H \coloneqq (M_{x^2} - \partial^2)\restriction_{\mathscr{S}(\mathbb{R})}$ and $[\partial, M_x] = I_{\mathscr{S}(\mathbb{R})}$. Similarly, one sees that $AA^\dagger = \frac{1}{2}(H+1)$ so that $[A^\dagger, A] = -I_{\mathscr{S}(\mathbb{R})}$. Hence

$$\begin{aligned}
[N, A^\dagger] &= A^\dagger A A^\dagger - A^\dagger A^\dagger A = A^\dagger [A, A^\dagger] = A^\dagger, \\
[N, A] &= A^\dagger A A - A A^\dagger A = [A^\dagger, A] A = -A.
\end{aligned}$$

Note that $N\varphi_0 = 0$. Assuming that $N\varphi_n = n\varphi_n$, for some $n \in \mathbb{N}$, we compute

$$N\varphi_{n+1} = NA^\dagger \varphi_n = A^\dagger \varphi_n + A^\dagger N \varphi_n = (n+1)A^\dagger \varphi_n = (n+1)\varphi_{n+1}.$$

For $n \neq k$ we have that

$$n \langle \varphi_n, \varphi_k \rangle = \langle N\varphi_n, \varphi_k \rangle = \langle \varphi_n, N\varphi_k \rangle = k \langle \varphi_n, \varphi_k \rangle$$

so that $\langle \varphi_n, \varphi_k \rangle = 0$. □

Theorem 2.14. *Let $H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$ be the Schrödinger operator of the harmonic oscillator and let $\lambda_k = 2k+1$, $k \in \mathbb{N}_0$, and $(\varphi_k)_{k \in \mathbb{N}_0}$ be the sequence of eigenvalues and associated eigenfunctions as in Theorem 2.13.*

(1) *Let λ be some eigenvalue of H and let $u \in D(H)$ be an associated eigenfunction. We have $Au \in D(H)$ and $H(Au) = (\lambda - 2)Au$.*

(2) *There is $m \in \mathbb{N}_0$ so that $\lambda - 2m = 1$. In particular, $\sigma(H) = \{\lambda_k ; k \in \mathbb{N}_0\}$.*

(3) *The eigenvalues* $(\lambda_k)_{k\in\mathbb{N}_0}$ *are simple.*

Proof.

(1) First note that the fact that $\langle Hu, u\rangle = \langle \partial u, \partial u\rangle + \langle M_x u, M_x u\rangle < \infty$ implies that $Au \in L_2(\mathbb{R})$. Recall that $D(H) = D(N)$ and that $Nu = \frac{1}{2}(H-1)u = \frac{1}{2}(\lambda - 1)u$. We let $\mu := \frac{1}{2}(\lambda - 1)$ and pick $\varphi \in C_c^\infty(\mathbb{R})$. Now

$$\begin{aligned}\langle Au, (N-\mu)\varphi\rangle &= \left\langle u, A^\dagger(N-\mu)\varphi\right\rangle = \left\langle u, (N-\mu)A^\dagger\varphi\right\rangle - \left\langle u, A^\dagger\varphi\right\rangle\\ &= \left\langle (N-\mu)u, A^\dagger\varphi\right\rangle - \langle Au, \varphi\rangle = -\langle Au, \varphi\rangle\end{aligned}$$

so that

$$\langle Au, (N-(\mu-1))\,\varphi\rangle = 0, \quad \forall \varphi \in C_c^\infty(\mathbb{R}).$$

The fact that $N - (\mu - 1)$ is essentially self-adjoint implies that

$$Au \in (\operatorname{Ran}(N-(\mu-1)))^\perp = \ker(N-(\mu-1)) \subset D(N) = D(H)$$

so that finally $Au \in D(H)$ with $NAu = (\mu - 1)Au$. Moreover,

$$HAu = (2N+1)Au = (\lambda - 2)Au. \tag{2.11}$$

(2) As $\sigma(H) \subset [0,\infty)$, there is $m \in \mathbb{N}$ such that $A^m u \neq 0$ and $A^{m+1}u = 0$; otherwise, by (2.11), we could obtain a sequence of eigenvalues which is not bounded from below. Hence

$$HA^m u = (2N+1)A^m u = 2A^\dagger A^{m+1}u + A^m u = A^m u.$$

We get that $\lambda - 2m = 1$.

(3) It suffices to show that 1 is a simple eigenvalue. We use, without giving a proof, that any eigenfunction to H and $\lambda_0 = 1$ is in $C^2(\mathbb{R})$ and satisfies the homogeneous second-order equation $-y'' + x^2 y - y = 0$. By Picard-Lindelöf, the solution space has dimension 2 and we already know that $u_1(x) = e^{-\frac{1}{2}x^2} \in L_2(\mathbb{R})$ is a solution. We set $u_2(x) := \varphi(x)u_1(x)$ and observe that

$$0 = \left(-\partial^2 + x^2 - 1\right)u_2 = \varphi\left(-\partial^2 + x^2 - 1\right)u_1 - 2\varphi' u_1' - \varphi'' u_1 = -2\varphi' u_1' - \varphi'' u_1.$$

This implies $\varphi'' = 2x\varphi'$ and hence $\psi := \varphi'$ satisfies the first-order equation $\psi' = 2x\psi$. Integration yields $\ln|\psi| = x^2$ so that we may choose $\psi = e^{x^2}$. We therefore obtain

$$u_2(x) = e^{-\frac{1}{2}x^2}\int_1^x e^{t^2}\mathrm{d}t.$$

The function $f(x) := \int_1^x e^{t^2}\mathrm{d}t - e^{\frac{1}{2}x^2}$ is strictly increasing for $x \geq 2$ as $f'(x) = e^{x^2} - xe^{\frac{1}{2}x^2} > 0$ and $f(2) > 0$. Hence $\int_1^x e^{-t^2}\mathrm{d}t \geq e^{\frac{1}{2}x^2}$ for $x \geq 2$ so that $u_2 \notin L_2(\mathbb{R})$. $\square$

Our results can be generalized to $-\Delta+|x|^2$ in $L_2(\mathbb{R}^d)$. For this purpose, we need the tensor product of two operators. Let A and B be self-adjoint operators in $L_2(\mathbb{R})$. Then $A\otimes B$ operates on products $\varphi(x_1)\psi(x_2)$ with $\varphi\in D(A)$ and $\psi\in D(B)$ by

$$(A\otimes B)(\varphi(x_1)\psi(x_2)) = (A\varphi)(x_1)(B\psi)(x_2).$$

In addition, $A\otimes B$ can be extended to a self-adjoint operator in $L_2(\mathbb{R}^2)$ and

$$\sigma(A\otimes B) = \overline{\{\lambda\mu; \lambda\in\sigma(A), \mu\in\sigma(B)\}}.$$

One shows, for $d=2$ with $x=(x_1,x_2)$ and

$$-\Delta+|x|^2 = \left(-\frac{\mathrm{d}^2}{\mathrm{d}x_1^2}+x_1^2\right)\otimes I_{x_2} + I_{x_1}\otimes\left(-\frac{\mathrm{d}^2}{\mathrm{d}x_2^2}+x_2^2\right),$$

that $-\Delta+|x|^2$ is essentially self-adjoint on $C_c^\infty(\mathbb{R}^2)$ and that

$$\sigma(H) = \{\lambda_k+\mu_m; \lambda_k = 2k+1, \mu_m = 2m+1, k,m\in\mathbb{N}_0\}.$$

Here; H denotes the (unique) self-adjoint extension of $(-\Delta+|x|^2)\restriction_{C_c^\infty(\mathbb{R}^2)}$. The associated eigenfunctions are $\Phi_k(x_1)\Phi_m(x_2)$.

2.3 $V(x)\to 0$ for $|x|\to\infty$

Next we discuss the class of potentials V with $V(x)\to 0$ for $|x|\to\infty$. We will focus on relatively bounded potentials (with respect to H_0) with relative bound <1. Then $(-\Delta+V)\restriction_{C_c^\infty(\mathbb{R}^d)}$ is essentially self-adjoint and its unique self-adjoint extension is

$$H = H_0+V = \overline{(-\Delta+V)\restriction_{C_c^\infty(\mathbb{R}^d)}}.$$

Equivalently, it is possible to define H by means of the Friedrichs extension. Note that if V is relatively bounded with $(-\Delta)$-bound <1, then $(-\Delta+V)\restriction_{C_c^\infty(\mathbb{R}^d)}$ is already semi-bounded, cf. e.g. [T. Kato: Perturbation Theory for Linear Operators, Ch. V, Thm. 4.11].

The most prominent example in this class is the Schrödinger operator of the hydrogen atom,

$$H = -\Delta - \frac{1}{|x|} \quad \text{in } L_2(\mathbb{R}^3).$$

Hardy's inequality implies that the Coulomb potential $-1/|x|$ in $\mathbb{R}^3$ is relatively bounded with respect to $-\Delta$ with relative bound 0 and the perturbation theorem of Kato and Rellich shows that $-\Delta-1/|x|$ on $C_c^\infty(\mathbb{R}^3)$ is essentially self-adjoint. The unique self-adjoint extension H satisfies $D(H)=D(H_0)$. Hardy's inequality also implies that H is semi-bounded (although the potential $-1/|x|$ is not bounded from below).

Piecewise continuous and bounded potentials with compact support in $\mathbb{R}^d$ also belong to the class discussed here, e.g. so-called square well potentials.

Theorem 2.15. *Let $V\colon \mathbb{R}^d\backslash\{0\} \to \mathbb{R}$ be (piecewise) continuous with $V(x) \to 0$, $|x| \to \infty$. Let M_V be the multiplication operator associated with V and assume that M_V is relatively bounded with respect to H_0 with relative bound < 1. Then $H = H_0 + V\colon D(H_0) \to \mathcal{H}$ is self-adjoint and*

$$\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ess}}(H_0) = [0,\infty).$$

Proof. We will assume in addition that V is bounded so that there is $M \geq 0$ such that $|V(x)| \leq M$, for all $x \in \mathbb{R}^d$.

(1) By the second resolvent equation, for some $c \in \mathbb{R}$,

$$(H+c)^{-1} - (H_0+c)^{-1} = -(H+c)^{-1}V(H_0+c)^{-1}. \tag{2.12}$$

The right-hand side of (2.12) is compact as $(H+c)^{-1}$ is bounded and $V(H_0+c)^{-1}$ is compact, as we will show now: Let $(f_n) \subset \mathcal{H}$ with $f_n \xrightarrow{\mathrm{w}} 0$ be given and let $v_n \coloneqq (H_0+c)^{-1}f_n$. As in the proof of Theorem 2.3, one shows that

$$v_n \xrightarrow{\mathrm{w}} 0 \text{ in } L_2(\mathbb{R}^d)$$

and $\|v_n\| + \|H_0 v_n\| \leq c_1$ and hence

$$\|v_n\|_1^2 = \langle H_0 v_n, v_n\rangle + \|v_n\|^2 \leq c_2.$$

Hence for any $\varphi \in C_c^\infty(\mathbb{R}^d)$ there is a constant c_φ such that

$$\|\varphi v_n\|_1 \leq c_\varphi;$$

here we have used that

$$\int_{\mathbb{R}^d} |\nabla(\varphi v_n)|^2 \,\mathrm{d}x \leq 2\int_{\mathbb{R}^d} |v_n|^2|\nabla\varphi|^2 \,\mathrm{d}x + 2\int_{\mathbb{R}^d} |\varphi|^2|\nabla v_n|^2 \,\mathrm{d}x.$$

By Rellich's embedding theorem, we get from $\varphi v_n \xrightarrow{\mathrm{w}} 0$ and $\|\varphi v_n\|_1 \leq c_\varphi$ that $\varphi v_n \to 0$, for all $\varphi \in C_c^\infty(\mathbb{R}^d)$. Given $\varepsilon > 0$, we choose $R \geq 0$ so that

$$|V(x)| \leq \varepsilon, \quad |x| \geq R,$$

and let $\psi_R \in C_c^\infty(\mathbb{R}^d)$ with the properties $0 \leq \psi_R \leq 1$, $\psi_R\restriction_{B_R} = 1$ and $\operatorname{supp}\psi_R \subset B_{2R}$ be given. Then

$$\|Vv_n\| \leq \|V\psi_R v_n\| + \|V(1-\psi_R)v_n\| \leq M\|\psi_R v_n\| + \varepsilon\|(1-\psi_R)v_n\|. \tag{2.13}$$

There is $n_0 \in \mathbb{N}$ such that $\|\psi_R v_n\| \leq \varepsilon/M$ for $n \geq n_0$. For large n, the right-hand side of (2.13) thus is smaller than ε times a positive constant. This implies that $Vv_n \to 0$ for $n \to \infty$ and hence $V(H_0+c)^{-1}$ is compact.

(2) By virtue of Weyl's Theorem, we obtain that

$$\sigma_{\text{ess}}\left((H+c)^{-1}\right) = \sigma_{\text{ess}}\left((H_0+c)^{-1}\right).$$

By the spectral theorem, the essential spectra of H and $(H+c)^{-1}$ satisfy the relation

$$(\mu+c)^{-1} \in \sigma_{\text{ess}}\left((H+c)^{-1}\right) \quad \Longleftrightarrow \quad \mu \in \sigma_{\text{ess}}(H).$$

A similar relation holds true for H_0. This completes our proof. □

Remark 2.16. If V satisfies $V(x) \to 0$ for $|x| \to \infty$ and is relatively bounded with respect to H_0 with relative bound < 1, we still have $\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(H_0)$. On the one hand, it is easy to construct singular sequences for H_0 and $\lambda \geq 0$ that have support outside an arbitrarily large ball B_R. As $V(x) \to 0$ at ∞, it follows that $\sigma_{\text{ess}}(H) \supset \sigma_{\text{ess}}(H_0)$. If we assume that there is $\lambda < 0$ with $\lambda \in \sigma_{\text{ess}}(H)$, we can show for any singular sequence (u_k) for H and λ that $\psi_R u_k \to 0$ for $k \to \infty$ and arbitrary $R > 0$: Assuming for a contradiction that $\psi_R u_k$ does not converge to zero, we could find a sequence $(v_j)_{j\in\mathbb{N}} \subset (\psi_R u_k)_{k\in\mathbb{N}}$ and $d > 0$ such that

$$\|v_j\| \geq d, \quad \forall j \in \mathbb{N}. \tag{2.14}$$

Our assumption on V implies that there exist numbers $a < 1$ and $b \in \mathbb{R}$ such that

$$\langle H_0 u_k, u_k\rangle \leq \|H_0 u_k\| \leq \|(H-\lambda)u_k\| + |\lambda|\,\|u_k\| + a\,\|H_0 u_k\| + b\,\|u_k\|.$$

Hence $(\|u_k\|_1)$ is bounded and thus $(\|v_j\|_1)$ is also bounded. By Rellich's embedding theorem, we find another subsequence $(w_m)_{m\in\mathbb{N}} \subset (v_j)_{j\in\mathbb{N}}$ and $w \in \mathcal{H}$ such that $w_m \to w$. But as (u_k) is a singular sequence, $w = 0$ contradicting (2.14) so that indeed $\psi_R u_k \to 0$, $k \to \infty$, in $L_2(\mathbb{R}^d)$. Given $\varepsilon > 0$ we choose $R_\varepsilon > 0$ such that $|V(x)| < \varepsilon$ for $|x| \geq R_\varepsilon$. Then

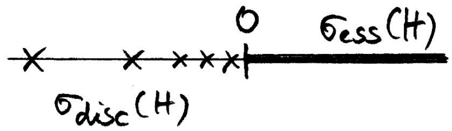
$$\|(H_0-\lambda)u_k\| \leq \|(H-\lambda)u_k\| + \|V\psi_R u_k\| + \|V(1-\psi_R)u_k\|.$$

As V is (piecewise) continuous, we conclude that

$$\limsup_{k\to\infty} \|(H_0-\lambda)u_k\| \leq \varepsilon.$$

Hence (u_k) is a singular sequence for H_0 and $\lambda < 0$ contradicting $\sigma_{\text{ess}}(H_0) = [0,\infty)$.

Under the assumptions of Theorem 2.15 we have that $\sigma_{\text{ess}}(H_0+V) = [0,\infty)$. Nevertheless, it is possible that H_0+V has discrete eigenvalues below 0 (and they are of importance in physics when thinking of spectroscopy etc.).



These eigenvalues are characterized by the min-max-principle, e.g.

$$\lambda_1 = \inf\{\langle Hu, u\rangle \,; u \in D(H), \|u\| = 1\}$$

for the lowest eigenvalue (Rayleigh-Ritz method) as described in Section 1. It is important to recall that the min-max-principle counts multiple eigenvalues with different indices. However, in this paragraph, eigenvalues are considered simply as points on the real line.

Proposition 2.17. *Let $H = H_0 + V$ as in Theorem 2.15. If there exists $u \in D(H)$ with $\langle Hu, u\rangle < 0$, then H has at least one negative eigenvalue.*

Proof. If the statement of the proposition was wrong, then $\sigma(H) \cap (-\infty, 0) = \emptyset$ meaning that $\sigma(H) \subset [0, \infty)$. By the spectral theorem, this would imply that $H \geq 0$, i.e. $\langle Hv, v\rangle \geq 0$ for all $v \in D(H)$ in contradiction to the assumption $\langle Hu, u\rangle < 0$. $\square$

Remark 2.18. A consequence of $\sigma_{\mathrm{ess}}(H) = [0, \infty)$ is that H can only have discrete eigenvalues in $(-\infty, 0)$.

Example 2.19. Assume that V is spherically symmetric, $V(x) = V(r)$, with $r = |x|$. We focus in particular on the Coulomb potential

$$V(x) = -\frac{1}{|x|}, \quad x \in \mathbb{R}^d \backslash \{0\}.$$

The main idea is to separate $H = H_0 + V(r)$ in spherical coordinates and to obtain the negative eigenvalues and the associated eigenfunctions in the following way:

(1) Find the eigenvalues and eigenfunctions of the negative Laplace-Beltrami operator $-\Delta_{\mathbb{S}^{d-1}}$ in $L_2(\mathbb{S}^{d-1})$ where $\mathbb{S}^{d-1} = \{\xi \in \mathbb{R}^d; |\xi| = 1\}$ is the $(d-1)$-dimensional unit sphere. The operator $-\Delta_{\mathbb{S}^{d-1}}$ has compact resolvent and purely discrete spectrum

$$0 = \kappa_0 < \kappa_1 < \ldots < \kappa_j \to \infty, \quad j \to \infty.$$

The eigenspaces belonging to the κ_j have a basis of C^∞-functions

$$\Psi_{j,k} \colon \mathbb{S}^{d-1} \to \mathbb{R}, \quad k = 1, \ldots, m_j,$$

where m_j denotes the dimension of the eigenspace belonging to the eigenvalue κ_j. In $\mathbb{R}^3$, one has $\kappa_j = j(j+1)$, $j \in \mathbb{N}_0$, with multiplicities $2j + 1$. For $d = 3$ the functions $\Psi_{j,k}$ are called the *spherical harmonics*. The information on $-\Delta_{\mathbb{S}^{d-1}}$ is independent of the potential V.

(2) Using separation of variables

$$u(x) = v(r)\Psi_{j,k}(\xi)$$

for the eigenfunctions u to eigenvalues λ of $-\Delta + V$ in the Hilbert space

$$L_2(\mathbb{R}^d) = L_2((0,\infty), r^{d-1}\,\mathrm{d}r) \otimes L_2(\mathbb{S}^{d-1}, \mathrm{d}\omega_{d-1})$$

leads to an ordinary differential equation for v,

$$-v''(r) - \frac{d-1}{r}v'(r) + V(r)v(r) + \frac{\kappa_j}{r^2}v(r) = \lambda v(r), \quad r \in (0,\infty).$$

If V is the Coulomb potential, this ODE becomes a *Bessel differential equation.* For any $j \in \mathbb{N}_0$ one gets a solution $v = v_j \in L_2((0,\infty), r^{d-1}\,\mathrm{d}r)$. The unitary transformation $v \mapsto r^{(d-1)/2}v$ produces an additional term including the factor $1/r^2$.

For the Coulomb potential in $\mathbb{R}^3$ one obtains an infinite sequence of negative eigenvalues. If the potential V decays faster than $-c_d(1+|x|)^{-2}$ for $|x| \to \infty$, the subspace spanned by the eigenfunctions of negative eigenvalues is finite-dimensional.

For many examples with $V(x) \to 0$ for $|x| \to \infty$, the number $N(V)$ of negative eigenvalues (counting multiplicities) can be estimated as follows.

Theorem 2.20 (Birman, Schwinger). *Let $V\colon \mathbb{R}^3 \to \mathbb{R}$ with $V(x) \to 0$ for $|x| \to \infty$. Then*

$$N(V) \leq \frac{1}{(4\pi)^2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|V(x)||V(y)|}{|x-y|^2}\,\mathrm{d}x\,\mathrm{d}y.$$

Proof. See [RS-IV, Thm. XIII.10, p. 98ff]. □

Of course, the Theorem of Birman and Schwinger is only helpful, if the integral is finite. The following theorem is of particular importance for the Thomas-Fermi-Theorie (atoms, molecules).

Theorem 2.21 (Cwikel-Lieb-Rozenblum bound). *Let $d \geq 3$ and let $N(V)$ be the number of negative eigenvalues of $H_0 + V$ in $L_2(\mathbb{R}^d)$. Let $V_- = \min\{V, 0\}$. Then there is a constant $c = c_d$ such that*

$$N(V) \leq c_d \int_{\mathbb{R}^d} |V_-(x)|^{d/2}\,\mathrm{d}x.$$

Proof. See [RS-IV, Thm. XIII.12, p. 101ff]. □

Theorem 2.22 (Weak coupling in $\mathbb{R}$ and $\mathbb{R}^2$). *Let $V \geq 0$ with compact support and $\int V(x)\,\mathrm{d}x > 0$. Then $H = H_0 - \mu V$ has a negative eigenvalue for any $\mu > 0$.*

Proof. For $d = 1$, we pick a cut-off function $\psi_k \in C_c^\infty(\mathbb{R})$ with $0 \leq \psi_k \leq 1$, $\psi_k \restriction_{(-k,k)} = 1$ and $\operatorname{supp} \psi_k \subset (-2k, 2k)$ and we choose $k \in \mathbb{N}$ so large so that $\operatorname{supp} V \subset (-k,k)$. Then

$$\langle H\psi_k, \psi_k\rangle = \int_{\mathbb{R}} |\psi_k'(x)|^2\,\mathrm{d}x - \mu \int_{\mathbb{R}} V(x)|\psi_k(x)|^2\,\mathrm{d}x$$

$$\leq \left(\int_{-2k}^{-k} + \int_{k}^{2k} \right) \frac{c}{k^2} \, \mathrm{d}x - \mu \int_{-k}^{k} V(x) \, \mathrm{d}x.$$

Sending $k \to \infty$, the above estimate shows that H cannot be nonnegative. But then the associated spectral family $E(\cdot)$ cannot be constant on the negative half-axis. This implies the existence of some $\lambda < 0$ with $\lambda \in \sigma(H)$. By Theorem 2.15, $\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ess}}(H_0) = [0, \infty)$ so that $\lambda \in \sigma_{\mathrm{disc}}(H)$. For a proof in $\mathbb{R}^2$ see [RS-IV, Thm. XIII.11, p. 100]. □

2.4 $V \colon \mathbb{R}^d \to \mathbb{R}$ bounded and continuous

If $V \colon \mathbb{R}^d \to \mathbb{R}$ is bounded and (piecewise) continuous, then $-\Delta + V$ on $C_c^\infty(\mathbb{R}^d)$ is essentially self-adjoint with the unique self-adjoint extension

$$H = H_0 + V := \overline{(-\Delta + V) \restriction_{C_c^\infty(\mathbb{R}^d)}}.$$

Let $\mu_- := \inf\{V(x); x \in \mathbb{R}^d\}$ and $\mu_+ := \sup\{V(x); x \in \mathbb{R}^d\}$. It is easy to see that

$$\inf \sigma(H) \in [\mu_-, \mu_+];$$

in particular $\sigma(H) \subset [\mu_-, \infty)$. We can also show that the gaps in the essential spectrum of H have at most the length $\gamma := \mu_+ - \mu_-$, i.e. for all $\lambda \geq \mu_-$, we have that

$$\sigma(H) \cap [\lambda - \tfrac{\gamma}{2}, \lambda + \tfrac{\gamma}{2}] \neq \emptyset.$$

Let us give a proof of the following version of this result.

Theorem 2.23. *Let $V \colon \mathbb{R}^d \to \mathbb{R}$ be bounded and continuous and let $\lambda \geq 0$. Then*

$$\sigma(H) \cap [\lambda - \mu_+, \lambda + \mu_+] \neq \emptyset.$$

Proof. As $\sigma_{\mathrm{ess}}(H_0) = [0, \infty)$, there exists a singular sequence $(u_n) \subset D(H_0)$ to H_0 and λ. The fact that $\|V u_n\| \leq \mu_+$, $n \in \mathbb{N}$, implies that $(u_n) \subset D(M_V)$. The spectral theorem yields

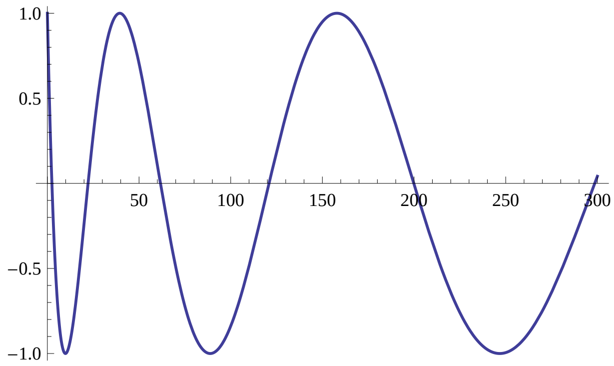
$$\begin{aligned} \inf_{\mu \in \sigma(H)} (\mu - \lambda)^2 \|u_n\|^2 &\leq \int_{-\infty}^{\infty} (\mu - \lambda)^2 \, \mathrm{d} \langle E(\mu) u_n, u_n \rangle \\ &= \|(H - \lambda) u_n\|^2 \leq \left(\|(H_0 - \lambda) u_n\| + \|V u_n\| \right)^2. \end{aligned}$$

As $\|u_n\| = 1$ for all $n \in \mathbb{N}$ and $\|(H_0 - \lambda) u_n\| \to 0$ for $n \to \infty$, we obtain that

$$\inf_{\mu \in \sigma(H)} (\mu - \lambda)^2 \leq \mu_+^2.$$

But then $\mathrm{dist}(\lambda, \sigma(H)) \leq \mu_+$ and $\sigma(H) \cap [\lambda - \mu_+, \lambda + \mu_+] \neq \emptyset$. □

An interesting example is the potential $V(x) = \cos\sqrt{|x|}$ which oscillates weakly at ∞.



Theorem 2.24. *Let $V : \mathbb{R} \to \mathbb{R}$ be defined by $V(x) := \cos\sqrt{|x|}$ and let $H = H_0 + V$. Then $\sigma(H) = [-1, \infty)$.*

Proof. Clearly, $\sigma(H) \subset [-1, \infty)$ as $V \geq -1$. In a first step, we show that $[-1, 1] \subset \sigma(H)$: For $x > 0$ we have that $V'(x) = -\frac{1}{2\sqrt{x}} \sin\sqrt{x} \to 0$, $x \to \infty$. Let $\lambda \in [-1, 1]$ and $\varepsilon_n := 1/n$. For any $n \in \mathbb{N}$, there exists $x_n > 0$ so that

$$|V(x) - \lambda| < \varepsilon_n, \quad \forall x \in B_{2n}(x_n).$$

The sequence (x_n) is monotonically increasing and $x_n \to \infty$. We can also assume that $B_{2n}(x_n) \cap B_{2(n+1)}(x_{n+1}) = \emptyset$. Let $\psi_n \in C_c^\infty(\mathbb{R})$ be a cut-off function with $0 \leq \psi_n \leq 1$, $\psi_n \restriction_{(-n,n)} = 1$ and $\operatorname{supp} \psi_n \subset (-2n, 2n)$. Let

$$\eta_n(x) := \frac{\psi_n(x - x_n)}{\|\psi_n(\cdot - x_n)\|}.$$

Clearly, $\|\eta_n\| = 1$ and $\eta_n \xrightarrow{\mathrm{w}} 0$. As

$$\|(H - \lambda)\eta_n\| \leq \|H_0\eta_n\| + \|(V - \lambda)\eta_n\| \leq \|H_0\eta_n\| + \varepsilon_n \to 0, \quad n \to \infty,$$

we see that $\lambda \in \sigma(H)$. Secondly, we show that $[1, \infty) \subset \sigma(H)$. Let $\lambda \in [1, \infty)$. Again we choose points x_n on the positive half-axis such that $|V(x)| < \varepsilon_n$ on $B_{2n}(x_n)$. Let u_n be the singular sequence to H_0 and λ obtained in the proof of Theorem 2.2. Then $v_n := u_n(\cdot - x_n)$ satisfies $\|v_n\| = 1$, $v_n \xrightarrow{\mathrm{w}} 0$ and

$$\|(H - \lambda)v_n\| \leq \|(H_0 - \lambda)v_n\| + \|Vv_n\| \leq \|(H_0 - \lambda)v_n\| + \varepsilon_n \to 0$$

so that $\lambda \in \sigma(H)$. Both results together show that $\sigma(H) = [-1, \infty)$. $\square$

2.5 V periodic

In solid state physics, periodic Schrödinger operators are suitable models to describe periodic crystals. The structure of a real crystal is periodic on a large (but not infinite) scale; a macroscopic crystal consists of 10^8 ions per edge length (Avogadro constant: $6.022 \cdot 10^{23}$ particles per mol). In a real crystal, periodicity is disturbed by several types of lattice defects (impurities, vacancies, dislocations, grain boundaries etc.). We will only discuss periodic crystals here for the sake of brevity. Defect models for periodic Schrödinger operators are an active area of research. From the historical point of view, Felix Bloch, a student of Erwin Schrödinger, was one of the first who studied periodic structures around 1929.

Here, we only skim some results for the periodic case and $d = 1$. For $d \geq 2$, we refer the reader to [RS-IV, Sec. XIII-16]. To be able to study models that apply more suitably to real crystals, quasi-periodic or random potentials are discussed in recent research papers. Let $d = 1$. A classical example is the *Mathieu operator*

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \cos x \quad \text{in } L_2(\mathbb{R}).$$

A function $V\colon \mathbb{R} \to \mathbb{R}$ is called *periodic* if there exists a number $a > 0$ such that $V(x + a) = V(x)$ for all $x \in \mathbb{R}$. The smallest positive number with this property is called the *period of* V. If V is periodic with period a, it thus suffices to study V on $[0, a]$. The *Floquet decomposition* considers this fact from the technical point of view: Let V be periodic with period 1 (without loss of generality). In $L_2[0, 1]$ one studies the family of operators

$$H_\vartheta \coloneqq -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V\colon D(H_\vartheta) \to L_2[0,1], \quad 0 \leq \vartheta \leq 2\pi,$$

with

$$D(H_\vartheta) \coloneqq \{u \in C^2[0,1]; u(1) = e^{\mathrm{i}\vartheta}u(0), u'(1) = e^{\mathrm{i}\vartheta}u'(0)\}.$$

In [RS-IV], it is shown that the $\overline{H_\vartheta}$ are well-defined and self-adjoint operators and that there is a unitary map U such that

$$U\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V\right)U^{-1} = \int_{[0,2\pi)}^{\oplus} H_\vartheta \frac{\mathrm{d}\vartheta}{2\pi}. \tag{2.15}$$

The representation (2.15) is called the *direct fiber integral decomposition* of the periodic Schrödinger operator $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$ on $L_2(\mathbb{R})$. The operators H_ϑ have compact resolvent and their spectra consist entirely of eigenvalues of finite multiplicity,

$$E_1(\vartheta) \leq E_2(\vartheta) \leq \cdots \leq E_k(\vartheta) \leq \cdots, \quad E_k(\vartheta) \to \infty, \quad k \to \infty.$$

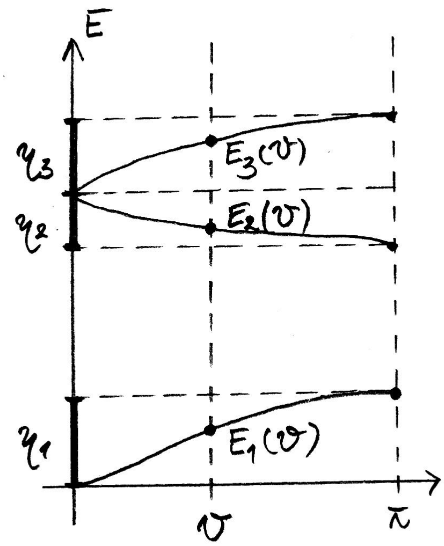
Moreover, H_ϑ and $H_{2\pi-\vartheta}$ are anti-unitarily equivalent under ordinary complex conjugation; in particular, their eigenvalues are identical and their eigenfunctions are complex conjugates. The $E_k(\vartheta)$ are sorted according to the min-max principle and depend continuously (in fact analytically) on ϑ. In solid state physics, the $E_k(\vartheta)$ are called *band functions* and they describe the possible electronic states in a crystal. The image of the $E_k(\vartheta)$,

$$\eta_k := \{E_k(\vartheta); 0 \le \vartheta \le 2\pi\},$$

are a compact intervals on the real axis, η_k is called a *spectral band* and

$$\sigma(H) = \cup_{k=1}^{\infty} \eta_k.$$

The sets $\eta_k \cap \eta_{k+1}$ contain a single point or they are empty. In the latter case, we have a *spectral gap* between the k-th and the $(k+1)$-th band.



2.6 Constant electric field

The potential for a constant electric field in $\mathbb{R}^d$ is given by $V(x) = c \cdot x$ with a fixed vector $c \in \mathbb{R}^d$. One shows that $-\Delta + c \cdot x$ is essentially self-adjoint on $C_c^\infty(\mathbb{R}^d)$. Let H_S be the self-adjoint extension which is obtained from taking the closure. The operator H_S is called the *Stark-Hamiltonian.*

Theorem 2.25. *Let $H_S = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \alpha x$, $\alpha \neq 0$, be the Stark-Hamiltonian in $L_2(\mathbb{R})$. We have that $\sigma_{\mathrm{ess}}(H_S) = \mathbb{R}$ and the operator H_S does not have eigenvalues.*

Proof. First of all, $\sigma(H_S) \neq \emptyset$. Otherwise the associated spectral family $E(\lambda)$ would be constant which would be in contradiction to $E(\lambda)f \to f$, $\lambda \to \infty$, and $E(\lambda)f \to 0$, $\lambda \to -\infty$, for any $f \in \mathcal{H}$. Let $\lambda \in \sigma(H_S)$ and pick some $\mu \in \mathbb{R}$. We aim at showing at $\mu \in \sigma(H_S)$. We define by $(U_t\varphi)(x) := \varphi(x-t)$, $\varphi \in L_2(\mathbb{R})$, the group of translations on $L_2(\mathbb{R})$. As $(U_t)_{t\in\mathbb{R}}$ is a unitary family, $\sigma(H_S) = \sigma(U_t H_S U_{-t})$, for all $t \in \mathbb{R}$, and $U_t(D(H_S)) = D(H_S)$. For $f \in D(H_S)$ we have that

$$\begin{aligned} U_t H_S U_{-t} f(x) &= U_t(-\Delta_x + M_{\alpha x}) f(x+t) \\ &= U_t((-\Delta_x f)(x+t) + \alpha x f(x+t)) \\ &= (-\Delta_x f)(x) + \alpha(x-t) f(x) \\ &= (H_S f)(x) - \alpha t f(x) \end{aligned}$$

so that $U_t H_S U_{-t} = H_S - \alpha t$, for all $t \in \mathbb{R}$. Choosing $t := \frac{\lambda-\mu}{\alpha}$, we find that $\mu = \lambda - \alpha t \in \sigma(H_S - \alpha t) = \sigma(H_S)$. To see that H_S does not have eigenvalues, we start with the assumption that $H_S u = \lambda u$ for some $u \neq 0$. Then also $H_S U_{-t} u = \lambda U_{-t} u$ and applying U_t, we find that $\lambda + \alpha t$ is also an eigenvalue of H_S for any $\alpha \neq 0$. This yields an over-countable orthonormal system of $L_2(\mathbb{R})$ which contradicts the fact that $L_2(\mathbb{R})$ is separable. □

Next, one considers the operator $H_S - \frac{1}{|x|}$ as a model for the hyrogen atom in a constant electric field for which one observes a splitting of the degenerate energy levels of $H_0 - \frac{1}{|x|}$. Note that $\sigma_{\mathrm{ess}}(H_S - \frac{1}{|x|}) = \mathbb{R}$. When the external electric field is switched on, the eigenvalues of $H_0 - \frac{1}{|x|}$ become *resonances* near the eigenvalues in the complex plane, cf. [HS, p. 263ff.].

2.7 Many-particle systems

We consider a model for an atom with a core of infinite weight placed at $0 \in \mathbb{R}^d$ with nuclear charge number Z and N electrons. For atoms, $Z = N$, otherwise we would have a model for an ion. Any electron feels the Coulomb potential of the core and the Coulomb repulsion of the other electrons. For any electron, we consider a space $L_2(\mathbb{R}^3)$ with coordinates $x_i := (\xi_i^1, \xi_i^2, \xi_i^3) \in \mathbb{R}^3$, $i = 1, \dots, N$. The energy states of the i-th electron are modeled by the Schrödinger operator

$$H_i := -\Delta_i - \frac{Z}{|x_i|} + \sum_{i\neq j=1,\dots,N} \frac{1}{|x_i - x_j|} \quad \text{in } L_2(\mathbb{R}^3).$$

The Schrödinger operator of the many-particle system reads

$$H := -\sum_{i=1}^N \Delta_i - \sum_{i=1}^N \frac{Z}{|x_i|} + \sum_{1\leq i<j\leq N} \frac{1}{|x_i - x_j|} \quad \text{in } L_2(\mathbb{R}^{3N}).$$

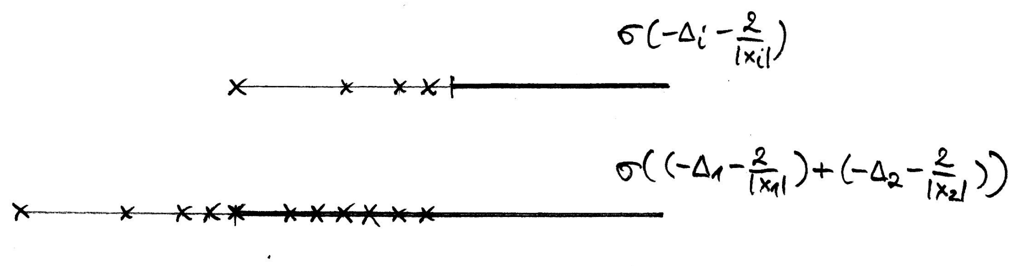
The operator H acts on functions $\Phi\colon \mathbb{R}^{3N} \to \mathbb{C}$ and is essentially self-adjoint on $C_c^\infty(\mathbb{R}^{3N})$. For $N = 2$, we obtain the Schrödinger operator of the helium atom,

$$H = -\Delta_1 - \Delta_2 - \frac{2}{|x_1|} - \frac{2}{|x_2|} + \frac{1}{|x_1 - x_2|} \quad \text{in } L_2(\mathbb{R}^6).$$

Neglecting the electron-electron interaction, one arrives at the operator

$$\left(-\Delta_1 - \frac{2}{|x_1|}\right) + \left(-\Delta_2 - \frac{2}{|x_2|}\right) = \left(-\Delta_1 - \frac{2}{|x_1|}\right) \otimes I_2 + I_1 \otimes \left(-\Delta_2 - \frac{2}{|x_2|}\right)$$

so that the associated spectrum is the sum of the spectra of two copies of $-\Delta - \frac{2}{|x|}$ in $L_2(\mathbb{R}^3)$; this operator has several *embedded eigenvalues.* Friedrichs showed that, when switching on the repulsion term, these embedded eigenvalues disappear.



For any $R > 0$ and $\alpha \in \rho(H)$, $\chi_{B_R(0)}(H - \alpha)^{-1}$ is compact. Concerning $\sigma_{\text{ess}}(H)$, we can thus assume without loss of generality that singular sequences on balls with increasing radii disappear. This allows the conclusion that $\inf \sigma_{\text{ess}}(H)$ is determined by the infimum of the spectrum of a $(N-1)$-particle system, precisely

$$\sigma_{\text{ess}}(H) = [\mu, \infty), \quad \mu := \inf \sigma\left(\tilde{H}_{N-1}\right)$$

with

$$\tilde{H}_{N-1} := -\sum_{i=1}^{N-1} \Delta_i - \sum_{i=1}^{N-1} \frac{Z}{|x_i|} + \sum_{1 \le i < j \le N-1} \frac{1}{|x_i - x_j|} \quad \text{in } L_2(\mathbb{R}^{3(N-1)}).$$

Indeed, the spectrum and the essential spectrum of H can be determined inductively. The results can be generalized to Coulomb-like potentials (Hunziker-van Winter-Zhislin-Theorem, cf. [RS-IV, W-II]).

Finally, it is important to note that the many-particle operators presented in this section describe bosons and not fermions. As electrons are fermions, they have to respect the Pauli exclusion principle and one is led to diminish the Hilbert space and to work with the anti-symmetric tensor product $A_N(L_2(\mathbb{R}^3) \otimes \cdots \otimes L_2(\mathbb{R}^3))$; here, A_N is the projection on the subspace of anti-symmetric tensors, cf. [RS-I].

2.8 Magnetic Schrödinger operators in $\mathbb{R}^2$

Let B be a constant magnetic field in $\mathbb{R}^2$ given by a vector potential $\vec{A}\colon \mathbb{R}^2 \to \mathbb{R}^2$ with $\vec{A} \in C^1(\mathbb{R}^2)$ and $\vec{A} = (A_1(x,y), A_2(x,y))$ such that

$$B = \operatorname{rot} \vec{A} = \partial_x A_2 - \partial_y A_1.$$

Then B is a continuous function. For instance, the constant magnetic field $B = 2$ is obtained from $\vec{A} = (-y, x)$. In Quantum Mechanics, magnetic Schrödinger operators are obtained from a *translation of momentum*,

$$\vec{p} = -\mathrm{i}\nabla \quad \longrightarrow \quad -\mathrm{i}\nabla - \vec{A}.$$

Then $H_0 = \vec{p}^{\,2}$ becomes

$$H_{\vec{A}} = (\vec{p} - \vec{A})^2 = (-\mathrm{i}\nabla - \vec{A})^2 = -\Delta + 2\mathrm{i}\,\vec{A} \cdot \nabla + \mathrm{i}(\nabla \cdot \vec{A}) + |\vec{A}|^2.$$

Given B there are many vector fields $\vec{A}$ such that $B = \operatorname{rot}\vec{A}$, but the spectrum of $H_{\vec{A}}$ only depends on B. If $\operatorname{rot}\vec{A} = \operatorname{rot}\vec{A}'$, the associated Schrödinger operators $H_{\vec{A}}$ and $H_{\vec{A}'}$ are unitarily equivalent (*gauge invariance*). For a constant magnetic field $B \neq 0$ in $\mathbb{R}^2$, the spectrum of $H_{\vec{A}}$ consists of a sequence of equidistant positive eigenvalues of infinite multiplicity (*Landau levels*). In $\mathbb{R}^3$ the spectrum is $[\mu, \infty)$ and μ is the first Landau level in $\mathbb{R}^2$ for the constant field B. The Schrödinger operator for the hydrogen atom in an external magnetic field yields a model for the *Zeeman effect*, i.e. the splitting of spectral lines into several components (analogous to the Stark effect in case of an electric field).

Theorem 2.26. *Let $\vec{A}\colon \mathbb{R}^2 \to \mathbb{R}^2$ be a C^1-vector field, $\vec{A} = (A_1, A_2)^T$ and let $B = \operatorname{rot}\vec{A}$ be the magnetic field induced by $\vec{A}$. If $B(x) > 0$ on $\mathbb{R}^2$, then $H_{\vec{A}} = (-\mathrm{i}\nabla - \vec{A})^2 \restriction_{C_c^\infty(\mathbb{R}^2)}$ satisfies the inequality*

$$\langle H_{\vec{A}}\varphi, \varphi\rangle \geq \int_{\mathbb{R}^2} B(x)|\varphi(x)|^2 \,\mathrm{d}x, \quad \forall \varphi \in C_c^\infty(\mathbb{R}^2).$$

Moreover, for $\chi \in C^2(\mathbb{R}^2)$ and $\vec{A}' = \vec{A} + \nabla\chi$, one has

$$e^{\mathrm{i}\chi}(-\mathrm{i}\nabla - \vec{A})e^{-\mathrm{i}\chi}\varphi = (-\mathrm{i}\nabla - \vec{A}')\varphi, \quad \forall \varphi \in C_c^\infty(\mathbb{R}^2).$$

Proof. Let $\Pi_j := -\mathrm{i}\partial_j - A_j$ for $j = 1, 2$. First, we claim that $[\Pi_1, \Pi_2] = \mathrm{i}\operatorname{rot}\vec{A}$ in $C_c^\infty(\mathbb{R}^2)$. For $f \in C_c^\infty(\mathbb{R}^2)$ the product rule and Schwarz's Theorem yield

$$\begin{aligned}
[\Pi_1, \Pi_2]f &= (-\mathrm{i}\partial_1 - A_1)(-\mathrm{i}\partial_2 - A_2)f - (-\mathrm{i}\partial_2 - A_2)(-\mathrm{i}\partial_1 - A_1)f \\
&= -\partial_1\partial_2 f + A_1A_2 f + \mathrm{i}A_1\partial_2 f + \mathrm{i}\partial_1(A_2 f) \\
&\quad - [-\partial_2\partial_1 f + A_1A_2 f + \mathrm{i}\partial_2(A_1 f) + \mathrm{i}A_2\partial_1 f] \\
&= \mathrm{i}(\partial_1 A_2 - \partial_2 A_1)f
\end{aligned}$$

so that indeed $[\Pi_1, \Pi_2] = \mathrm{i}\operatorname{rot}\vec{A} = \mathrm{i}B$. The operators Π_j are symmetric on $C_c^\infty(\mathbb{R}^2)$. Assuming $B > 0$, we find for any $\varphi \in C_c^\infty(\mathbb{R}^2)$ that

$$\begin{aligned}
\int_{\mathbb{R}^2} B|\varphi|^2 \,\mathrm{d}x &= \left|\int_{\mathbb{R}^2} B|\varphi|^2 \,\mathrm{d}x\right| = \left|\int_{\mathbb{R}^2} [\Pi_1, \Pi_2]\varphi\overline{\varphi} \,\mathrm{d}x\right| = |\langle [\Pi_1, \Pi_2]\varphi, \varphi\rangle| \\
&\leq 2|\,\langle \Pi_1\varphi, \Pi_2\varphi\rangle\,| \leq 2\,\|\Pi_1\varphi\|\,\|\Pi_2\varphi\| \leq \|\Pi_1\varphi\|^2 + \|\Pi_2\varphi\|^2
\end{aligned}$$

$$= \left\langle (\Pi_1^2 + \Pi_2^2)\varphi, \varphi \right\rangle = \langle H_{\vec{A}}\varphi, \varphi \rangle \, .$$

Finally, let $\vec{A}' = \vec{A} + \nabla\chi$ and let $\varphi \in C_c^\infty(\mathbb{R}^2)$. Then

$$\begin{aligned} e^{\mathrm{i}\chi}(-\mathrm{i}\nabla - \vec{A})e^{-\mathrm{i}\chi}\varphi &= e^{\mathrm{i}\chi}\left(-e^{-\mathrm{i}\chi}(\nabla\chi)\varphi - \mathrm{i}e^{-\mathrm{i}\chi}\nabla\varphi - e^{-\mathrm{i}\chi}\vec{A}\varphi\right) \\ &= -(\nabla\chi)\varphi - \mathrm{i}\nabla\varphi - \vec{A}\varphi \\ &= (-\mathrm{i}\nabla - \vec{A}')\varphi \end{aligned}$$

which completes our proof. $\square$

Chapter 3

The Schrödinger equation and Stone's Theorem

In this chapter, we consider the exponential function

$$e^{-\mathrm{i}tH}, \quad t \in \mathbb{R},$$

for a self-adjoint operator H in the Hilbert space $\mathcal{H}$. Stone's Theorem establishes a bijection between the class of self-adjoint operators and the class of strongly continuous unitary one-parameter groups: If $H\colon D(H) \to \mathcal{H}$ is self-adjoint, then $\{e^{-\mathrm{i}tH}; t \in \mathbb{R}\}$ is a strongly continuous group of unitary operators. The other way round, for any strongly continuous unitary group of operators $U(t)$ there exists a unique self-adjoint operator H such that $U(t) = e^{-\mathrm{i}tH}$, $t \in \mathbb{R}$. Recall that a bounded operator $U\colon \mathcal{H} \to \mathcal{H}$ is unitary if $\langle Ux, Uy\rangle = \langle x, y\rangle$, for all $x, y \in \mathcal{H}$, and if U is surjective. Equivalently: A bounded operator U is unitary if and only if U is bijective and $U^* = U^{-1}$.

If $H = -\Delta + V$ is a Schrödinger operator (with $H = H^*$) and $f_0 \in \mathcal{H} = L_2(\mathbb{R}^d)$ with $\|f_0\| = 1$ describes the state of a quantum-mechanical particle at time $t = 0$, then the solution of the initial value problem for the *Schrödinger equation*

$$\begin{aligned} \frac{\partial}{\partial t} f(x,t) &= \frac{1}{\mathrm{i}} \left(-\Delta_x f(x,t) + V(x) f(x,t)\right), \\ f(x,0) &= f_0(x) \end{aligned}$$

is given by

$$f(\cdot, t) = \left(e^{-\mathrm{i}tH} f_0\right)(\cdot).$$

The function $|f(\cdot,t)|^2$ can be interpreted as a probability density. As $e^{-\mathrm{i}tH}$ is unitary, indeed

$$\|f(\cdot,t)\|^2 = \|f_0\|^2 = 1, \quad \forall t \in \mathbb{R}.$$

If $\Omega \subset \mathbb{R}^d$ is measurable, $\int_\Omega |f(x,t)|^2 \, \mathrm{d}x$ is a measure for the probability to find the particle at time t in the set Ω.

Definition 3.1. Let $\mathcal{H}$ be a Hilbert space and let $\{U(t); t \in \mathbb{R}\}$ be unitary operators with the properties

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

(2) 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 $U(t_n)f \to U(t_0)f$,

is called a *strongly continuous unitary (one-parameter) group.*

Remark 3.2. Note that $I = U(0)^*U(0) = U(0)^*U(0+0) = [U^*(0)U(0)]U(0) = U(0)$ and that $U(-t) = U(t)^{-1} = U(t)^*$.

Theorem 3.3. *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*

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

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. As $|e^{\mathrm{i}t\lambda}| = 1$, the operators $U(t)$ are bounded with $\|U(t)\| \le 1$. Claim (1) follows from some straightforward calculations:

$$\begin{aligned}
\langle U(t)U(s)f, g\rangle &= \int_{-\infty}^{\infty} e^{\mathrm{i}\lambda t}\, \mathrm{d}\, \langle E(\lambda)U(s)f, g\rangle \\
&= \int_{-\infty}^{\infty} e^{\mathrm{i}\lambda t}\, \mathrm{d}_\lambda \int_{-\infty}^{\infty} e^{\mathrm{i}\mu s}\, \mathrm{d}_\mu\, \langle E(\mu)f, E(\lambda)g\rangle \\
&= \int_{-\infty}^{\infty} e^{\mathrm{i}\lambda t}\, \mathrm{d}_\lambda \int_{-\infty}^{\lambda} e^{\mathrm{i}\mu s}\, \mathrm{d}_\mu\, \langle E(\mu)f, g\rangle \\
&= \int_{-\infty}^{\infty} e^{\mathrm{i}\lambda t} e^{\mathrm{i}\lambda s}\, \mathrm{d}\, \langle E(\lambda)f, g\rangle \\
&= \langle U(t+s)f, g\rangle,
\end{aligned}$$

for all $f, g \in \mathcal{H}$, as $E(\cdot)$ is symmetric and monotonic ($E(\lambda)E(\mu) = E(\mu)E(\lambda) = E(\min\{\lambda, \mu\})$). Hence $U(t)U(s) = U(t+s)$. Furthermore

$$\begin{aligned}
\|U(t)f\|^2 &= \langle U(t)f, U(t)f\rangle \\
&= \int_{-\infty}^{\infty} e^{\mathrm{i}\lambda t}\, \mathrm{d}\, \langle E(\lambda)f, U(t)f\rangle
\end{aligned}$$

$$
\begin{aligned}
&= \int_{-\infty}^{\infty} e^{\mathrm{i}\lambda t}\,\mathrm{d}_\lambda \overline{\int_{-\infty}^{\infty} e^{\mathrm{i}\mu t}\,\mathrm{d}_\mu \langle E(\mu)f, E(\lambda)f\rangle} \\
&= \int_{-\infty}^{\infty} e^{\mathrm{i}\lambda t}\,\mathrm{d}_\lambda \overline{\int_{-\infty}^{\lambda} e^{\mathrm{i}\mu t}\,\mathrm{d}_\mu \langle E(\mu)f, f\rangle} \\
&= \int_{-\infty}^{\infty} e^{\mathrm{i}\lambda t} e^{-\mathrm{i}\lambda t}\,\mathrm{d}\langle E(\lambda)f, f\rangle \\
&= \|f\|^2 .
\end{aligned}
$$

Next, we prove that the $U(t)$ are surjective: Let $g \in \mathcal{H}$ be given. We claim that $f := U(-t)g$ satisfies $U(t)f = g$. Let $h \in \mathcal{H}$. We compute

$$
\begin{aligned}
\langle U(t)f, h\rangle &= \int_{-\infty}^{\infty} e^{\mathrm{i}\lambda t}\,\mathrm{d}\langle E(\lambda)f, h\rangle \\
&= \int_{-\infty}^{\infty} e^{\mathrm{i}\lambda t}\,\mathrm{d}\langle U(-t)g, E(\lambda)h\rangle \\
&= \int_{-\infty}^{\infty} e^{\mathrm{i}\lambda t}\,\mathrm{d}_\lambda \int_{-\infty}^{\lambda} e^{-\mathrm{i}\mu t}\,\mathrm{d}_\mu \langle E(\mu)g, h\rangle \\
&= \int_{-\infty}^{\infty} e^{\mathrm{i}\lambda t} e^{-\mathrm{i}\lambda t}\,\mathrm{d}\langle E(\lambda)g, h\rangle \\
&= \langle g, h\rangle .
\end{aligned}
$$

As h was arbitrary, we conclude that indeed $U(t)f = g$. To prove that the $U(t)$ are strongly continuous, we consider a sequence $(t_n)_{n\in\mathbb{N}} \subset \mathbb{R}$ with $t_n \to t_0$ and $f \in \mathcal{H}$. By the spectral theorem, for any continuous function $F\colon \mathbb{R} \to \mathbb{C}$ and all $f \in D(F(A))$,

$$
\|F(A)f\|^2 = \int_{\mathbb{R}} |F(\lambda)|^2\,\mathrm{d}\langle E(\lambda)f, f\rangle .
$$

We thus have that

$$
\|U(t_n)f - U(t_0)f\|^2 = \int_{\mathbb{R}} \left|e^{\mathrm{i}\lambda t_n} - e^{\mathrm{i}\lambda t_0}\right|^2\,\mathrm{d}\langle E(\lambda)f, f\rangle ,
$$

and applying Lebesgue's dominated convergence theorem, the desired result follows.

Proof of (2): Let $\psi \in D(A)$, i.e. $\int_{\mathbb{R}} \lambda^2\,\mathrm{d}\langle E(\lambda)\psi, \psi\rangle < \infty$. Then

$$
\begin{aligned}
\left\|\frac{1}{t}(U(t)\psi - \psi) - \mathrm{i}A\psi\right\|^2 &= \int_{-\infty}^{\infty} \left|\frac{1}{t}\left(e^{\mathrm{i}\lambda t} - 1\right) - \mathrm{i}\lambda\right|^2\,\mathrm{d}\langle E(\lambda)\psi, \psi\rangle \\
&= \int_{-\infty}^{\infty} \left|\mathrm{i}\lambda e^{\mathrm{i}\lambda\tau} - \mathrm{i}\lambda\right|^2\,\mathrm{d}\langle E(\lambda)\psi, \psi\rangle ,
\end{aligned}
$$

for some $\tau = \tau(\lambda, t) \in [-t, t]$. Again, applying the dominated convergence theorem, we see that the right hand side converges to zero as $t \to 0$.

Proof of (3): Let $\psi \in \mathcal{H}$ so that

$$\varphi := s - \lim_{t \to 0} \frac{1}{t}(U(t)\psi - \psi)$$

exists. We claim that $\psi \in D(A)$ and that $\mathrm{i}A\psi = \varphi$. Define an operator B by

$$\begin{aligned} D(B) &:= \left\{ u \in \mathcal{H};\ \lim_{t \to 0} \frac{1}{t}(U(t)u - u) \text{ exists} \right\}, \\ \mathrm{i}Bu &:= \lim_{t \to 0} \frac{1}{t}(U(t)u - u). \end{aligned}$$

As $U(-t) = U(t)^* = U(t)^{-1}$, one easily concludes that B is symmetric. By (2), $A \subset B$ and hence

$$A \subset B \subset B^* \subset A^*.$$

Since we have assumed that $A = A^*$, it follows that $B = A$, $\psi \in D(A)$ and $\mathrm{i}A\psi = \mathrm{i}B\psi = \lim_{t \to 0} \frac{1}{t}(U(t)\psi - \psi)$. $\square$

The other way round, any strongly continuous group is generated by a self-adjoint operator A.

Theorem 3.4 (Stone). *Let $\{U(t); t \in \mathbb{R}\}$ be a strongly continuous unitary group. Then there is a unique self-adjoint operator A satisfying*

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

Proof. For $f \in C_c^\infty(\mathbb{R})$ and $\varphi \in \mathcal{H}$ let

$$\varphi_f := \int_{-\infty}^{\infty} f(t) U(t) \varphi \, \mathrm{d}t;$$

this is a Riemann integral as the integrant depends continuously on t. We denote by $\mathcal{D}$ the set of all linear combinations of functions φ_f. Given $\varepsilon > 0$ we consider $j_\varepsilon \in C_c^\infty(\mathbb{R})$ with the properties

$$j_\varepsilon \geq 0, \quad \operatorname{supp} j_\varepsilon \subset [-\varepsilon, \varepsilon], \quad \int_{-\infty}^{\infty} j_\varepsilon(x) \, \mathrm{d}x = 1.$$

We then have

$$\begin{aligned} \|\varphi_{j_\varepsilon} - \varphi\| &= \left\| \int_{-\infty}^{\infty} j_\varepsilon(t)(U(t)\varphi - \varphi) \, \mathrm{d}t \right\| \\ &\leq \left(\int_{-\infty}^{\infty} j_\varepsilon(t) \, \mathrm{d}t \right) \cdot \sup_{-\varepsilon \leq t \leq \varepsilon} \|U(t)\varphi - \varphi\| \to 0, \quad \varepsilon \to 0, \end{aligned}$$

and hence $\mathcal{D}$ is dense in $\mathcal{H}$. Furthermore, for $\varphi_f \in \mathcal{D}$,

$$\frac{1}{s}(U(s) - I)\varphi_f = \int_{-\infty}^{\infty} f(t) \frac{1}{s}(U(s+t) - U(t))\varphi \, \mathrm{d}t$$

$$
\begin{aligned}
&= \int_{-\infty}^{\infty} \frac{1}{s}(f(\tau - s) - f(\tau))U(\tau)\varphi \, \mathrm{d}\tau \\
&\to - \int_{-\infty}^{\infty} f'(\tau)U(\tau)\varphi \, \mathrm{d}\tau \\
&= \varphi_{-f'}
\end{aligned}
$$

as $\frac{1}{s}(f(\tau - s) - f(\tau)) \to -f'(\tau)$ uniformly on supp f. For $\varphi_f \in \mathcal{D}$ we define

$$
A\varphi_f := -\mathrm{i}\varphi_{-f'} = \lim_{s\to 0} \frac{1}{\mathrm{i}s}(U(s) - I)\varphi_f.
$$

Note that $U(t)\colon \mathcal{D} \to \mathcal{D}$, $A\colon \mathcal{D} \to \mathcal{D}$ and that $U(t)A\varphi_f = AU(t)\varphi_f$, for all $\varphi_f \in \mathcal{D}$, as

$$
\begin{aligned}
U(t)\varphi_f = U(t) \int_{\mathbb{R}} f(s)U(s)\varphi \, \mathrm{d}s &=_{(*)} \int_{\mathbb{R}} f(s)U(t)U(s)\varphi \, \mathrm{d}s \\
&= \int_{\mathbb{R}} f(s)U(s)(U(t)\varphi) \, \mathrm{d}s = (U(t)\varphi)_f
\end{aligned}
$$

and

$$
AU(t)\varphi_f = A(U(t)\varphi)_f = \frac{1}{\mathrm{i}}(U(t)\varphi)_{-f'} = \frac{1}{\mathrm{i}}U(t)\varphi_{-f'} = U(t)\left(\frac{1}{\mathrm{i}}\varphi_{-f'}\right) = U(t)A\varphi_f.
$$

In $(*)$, we have approximated the Riemann integral by Riemann sums and have made use of the continuity of $U(t)$. The operator A with the domain $\mathcal{D}$ is symmetric since for $\varphi_f, \psi_g \in \mathcal{D}$ and with $U(s)^* = U(s)^{-1} = U(-s)$ we have that

$$
\begin{aligned}
\langle A\varphi_f, \psi_g \rangle &= \lim_{s\to 0} \left\langle \frac{1}{\mathrm{i}s}(U(s) - I)\varphi_f, \psi_g \right\rangle \\
&= \lim_{s\to 0} \left\langle \varphi_f, \frac{1}{\mathrm{i}s}(I - U(-s))\psi_g \right\rangle \\
&= \langle \varphi_f, A\psi_g \rangle .
\end{aligned}
$$

We now show that A is essentially self-adjoint as an operator on $\mathcal{D}$ by proving that $N(A^* \pm \mathrm{i}I) = \{0\}$. Let $u \in D(A^*)$ with $A^*u = -\mathrm{i}u$ be given. For all $\varphi \in \mathcal{D} = D(A)$,

$$
\frac{\mathrm{d}}{\mathrm{d}t} \langle U(t)\varphi, u \rangle = \langle \mathrm{i}AU(t)\varphi, u \rangle = \mathrm{i} \langle U(t)\varphi, A^*u \rangle = - \langle U(t)\varphi, u \rangle
$$

so that the function $F(t) := \langle U(t)\varphi, u \rangle$ satisfies the ODE $F' = -F$. Hence $F(t) = F(0)e^{-t}$. As $|F(t)| \le \|\varphi\| \, \|u\|$, we conclude that $F(0) = 0$. Using that $U(0) = I$ and that

$$
\langle U(0)\varphi, u \rangle = \langle \varphi, u \rangle = 0, \quad \forall \varphi \in \mathcal{D},
$$

the fact that $\mathcal{D}$ is dense implies that $u = 0$. Thus A is essentially self-adjoint on $\mathcal{D}$. Finally, let

$$
V(t) := e^{\mathrm{i}t\overline{A}}.
$$

By Theorem 3.3, $\{V(t); t \in \mathbb{R}\}$ is a strongly continuous unitary group. It remains to show that $U(t) = V(t)$ for all $t \in \mathbb{R}$. For all $\varphi \in \mathcal{D} \subset D(\overline{A})$ we have by means of Theorem 3.3, (2) that

$$\frac{\mathrm{d}}{\mathrm{d}t} V(t)\varphi = \mathrm{i}\overline{A}V(t)\varphi.$$

We also know that $U(t)\varphi \in \mathcal{D} \subset D(\overline{A})$ for all $t \in \mathbb{R}$. Let

$$w(t) := U(t)\varphi - V(t)\varphi, \quad t \in \mathbb{R}.$$

Then w is strongly differentiable with

$$w'(t) = \mathrm{i}AU(t)\varphi - \mathrm{i}\overline{A}V(t)\varphi = \mathrm{i}\overline{A}w(t)$$

and, as $\overline{A}$ is self-adjoint,

$$\frac{\mathrm{d}}{\mathrm{d}t} \|w(t)\|^2 = \mathrm{i}\left\langle \overline{A}w(t), w(t)\right\rangle - \mathrm{i}\left\langle w(t), \overline{A}w(t)\right\rangle = 0.$$

Using that $w(0) = 0$ implies that $w \equiv 0$ and hence

$$U(t)\varphi = V(t)\varphi, \quad \varphi \in \mathcal{D}, \quad t \in \mathbb{R}.$$

As $\mathcal{D}$ is dense, $U(t) = V(t)$ for all $t \in \mathbb{R}$. $\square$

Definition 3.5. We say that A is the *infinitesimal generator* of the strongly continuous group $\{U(t); t \in \mathbb{R}\}$ if $U(t) = e^{\mathrm{i}tA}$ for $t \in \mathbb{R}$.

Remark 3.6. If A is a bounded, symmetric operator in the Hilbert space $\mathcal{H}$, the generating unitary group $U(t)$ is norm-continuous: For $\varphi, \psi \in \mathcal{H}$, we have that

$$\begin{aligned}
\left\langle \mathrm{i}Ae^{\mathrm{i}As}\varphi, \psi\right\rangle &= \int_{-\infty}^{\infty} \mathrm{i}\lambda \,\mathrm{d}_\lambda \left\langle E(\lambda)e^{\mathrm{i}As}\varphi, \psi\right\rangle \\
&= \int_{-\infty}^{\infty} \mathrm{i}\lambda \,\mathrm{d}_\lambda \int_{-\infty}^{\infty} e^{\mathrm{i}\mu s} \,\mathrm{d}_\mu \left\langle E(\mu)\varphi, E(\lambda)\psi\right\rangle \\
&= \int_{-\infty}^{\infty} \mathrm{i}\lambda e^{\mathrm{i}\lambda s} \,\mathrm{d}_\lambda \left\langle E(\lambda)\varphi, \psi\right\rangle \\
&= \int_{-\infty}^{\infty} \frac{\mathrm{d}}{\mathrm{d}s} e^{\mathrm{i}\lambda s} \,\mathrm{d}_\lambda \left\langle E(\lambda)\varphi, \psi\right\rangle .
\end{aligned}$$

Integrating this equality with respect to s from 0 to t and Fubini's Theorem show that

$$\begin{aligned}
\left\langle \mathrm{i}\int_0^t AU(s)\varphi \,\mathrm{d}s, \psi\right\rangle &= \int_{-\infty}^{\infty} \left(\int_0^t \frac{\mathrm{d}}{\mathrm{d}s} e^{\mathrm{i}\lambda s} \,\mathrm{d}s\right) \mathrm{d}_\lambda \left\langle E(\lambda)\varphi, \psi\right\rangle \\
&= \int_{-\infty}^{\infty} (e^{\mathrm{i}\lambda t} - 1) \,\mathrm{d}_\lambda \left\langle E(\lambda)\varphi, \psi\right\rangle \\
&= \left\langle U(t)\varphi, \psi\right\rangle - \left\langle \varphi, \psi\right\rangle
\end{aligned}$$

for all $\psi \in \mathcal{H}$. Hence

$$\mathrm{i} \int_0^t AU(s)\varphi \, \mathrm{d}s = U(t)\varphi - \varphi, \quad \forall \varphi \in \mathcal{H}.$$

This implies

$$\|U(t)\varphi - \varphi\| \leq \int_0^t \|AU(s)\varphi\| \, \mathrm{d}s \leq \|A\| \, \|\varphi\| \, t$$

and

$$\sup\{\|U(t)\varphi - \varphi\| \, ; \|\varphi\| \leq 1\} = \|U(t) - I\| \leq \|A\| \, t \to 0, \quad t \to 0.$$

Thus $U(\cdot)$ is norm-continuous at $t = 0$ and hence at any $t \in \mathbb{R}$. In fact, a family $\{U(t); t \in \mathbb{R}\}$ of unitary operators is norm-continuous if and only if the infinitesimal generator A is bounded, see, e.g., [E.B. Davies, "One parameter semigroups", p. 19/20].

Remark 3.7. A family $\{U(t); t \in \mathbb{R}\}$ of unitary operators with

$$U(s)U(t) = U(s+t), \quad \forall s, t \in \mathbb{R},$$

and with the property that for all $f, g \in \mathcal{H}$ the map

$$\mathbb{R} \ni t \mapsto \langle U(t)f, g \rangle \in \mathbb{C}$$

is continuous (*weak continuity*) is in fact a strongly continuous group. This follows immediately from

$$\begin{aligned} \|U(t)\varphi - \varphi\|^2 &= \|U(t)\varphi\|^2 - \langle U(t)\varphi, \varphi \rangle - \langle \varphi, U(t)\varphi \rangle + \|\varphi\|^2 \\ &\to 2\|\varphi\|^2 - 2\|\varphi\|^2 = 0, \quad t \to 0. \end{aligned}$$

John von Neumann has show that in a *separable* Hilbert space, the strong continuity of a unitary group $\{U(t); t \in \mathbb{R}\}$ is already obtained from the *weak measurability*, i.e. it is enough to show that the map $t \mapsto \langle U(t)f, g \rangle$ is measurable. Measurability is relatively easy to prove as, for instance, it suffices to show that the map under consideration is the pointwise limit of a sequence of continuous functions.

Example 3.8. Let $\mathcal{H} = L_2(\mathbb{R})$ and let

$$(U(t)f)(x) := f(x+t), \quad f \in \mathcal{H}, \quad t \in \mathbb{R}.$$

Then $U(t)$ defines a strongly continuous unitary group: Clearly, $U(0) = I$ and U is invertible with $U(t)^{-1} = U(-t)$. As the Lebesgue integral is invariant under translations, $\langle U(t)f, U(t)g \rangle = \langle f, g \rangle$. To prove that $U(t)$ is strongly continuous, we fix $\varphi \in \mathcal{H}$ and choose a sequence $(t_n) \subset \mathbb{R}$ with $t_n \to t_0$, $n \to \infty$. We have to show that $U(t_n)\varphi \to U(t_0)\varphi$. For $f \in L_2(\mathbb{R})$, we write $f_n(x) := f(x+t_n)$. Let $\psi \in C_c^\infty(\mathbb{R})$

with $\|\psi - \varphi\| < \varepsilon$ be given. Then $|\psi_n(x) - \psi_0(x)| \to 0$, pointwise, $|\psi_n - \psi_0| \le 2\|\psi\|_\infty$ and

$$|\psi_n(x) - \psi_0(x)|^2 \le 4\|\psi\|_\infty^2 \chi_K(x) \in L_1(\mathbb{R}),$$

where $K \subset \mathbb{R}$ is compact and $\cup_{n\in\mathbb{N}} \operatorname{supp} \psi_n \cup \operatorname{supp} \psi_0 \subset K$. By the dominated convergence theorem, $\|\psi_n - \psi_0\| \to 0$ and consequently

$$\|\varphi_n - \varphi_0\| \le \|\varphi_n - \psi_n\| + \|\psi_n - \psi_0\| + \|\psi_0 - \varphi_0\| < 3\varepsilon, \quad n \to \infty.$$

This shows that $\varphi_n = U(t_n)\varphi \to U(t_0)\varphi = \varphi_0$, $n \to \infty$, strongly. We now claim that

$$U(t) = e^{\mathrm{i}tA}$$

where $A = \overline{A_0}$, $D(A_0) = C_c^\infty(\mathbb{R})$ and $A_0\varphi = -\mathrm{i}\varphi'$. Let φ_f and $\mathcal{D}$ be as in the proof of Theorem 3.4. We define $B\varphi_f := -\mathrm{i}\varphi_{-f'}$, $D(B) = \mathcal{D}$, and show that $A\restriction_{\mathcal{D}} = B$. This follows from

$$\varphi_f(x) = \int_{\mathbb{R}} f(t)\varphi(x+t)\,\mathrm{d}t = \int_{\mathbb{R}} f(t-x)\varphi(t)\,\mathrm{d}t$$

and

$$\begin{aligned} A\varphi_f &= -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}\int_{\mathbb{R}} f(t-x)\varphi(t)\,\mathrm{d}t = \mathrm{i}\int_{\mathbb{R}} f'(t-x)\varphi(t)\,\mathrm{d}t \\ &= \frac{1}{\mathrm{i}}\int_{\mathbb{R}} (-f')(t)\varphi(x+t)\,\mathrm{d}t = \frac{1}{\mathrm{i}}\varphi_{-f'} = Bf. \end{aligned}$$

We had shown in the proof of Stone's Theorem that B is essentially self-adjoint on the domain $\mathcal{D}$ and that $\overline{B}$ is the generator of the corresponding unitary group. As A is the unique self-adjoint extension of A_0 and $A\restriction_{\mathcal{D}} = A_0$, this yields that $A = \overline{B}$ and hence A is the infinitesimal generator of $\{U(t); t \in \mathbb{R}\}$. Note that

$$D(A) = \{u\colon \mathbb{R} \to \mathbb{C}; u \in \mathrm{AC}_{\mathrm{loc}}(\mathbb{R}), u, u' \in L_2(\mathbb{R})\}.$$

Here, $\mathrm{AC}_{\mathrm{loc}}(\mathbb{R})$ is the space of locally absolutely continuous functions on the real axis (see the next chapter).

Example 3.9. Let $\Omega \subset \mathbb{R}^d$ be open, $\mathcal{H} = L_2(\Omega)$ and $g\colon \Omega \to \mathbb{R}$ be measurable. Then

$$U(t)f(x) := e^{\mathrm{i}tg(x)}f(x), \quad f \in \mathcal{H}, \quad t \in \mathbb{R},$$

is a strongly continuous unitary group. Moreover,

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

and $A = M_g$ is the maximal multiplication operator induced by the function g in $L_2(\Omega)$. The proof is left as an exercise.

Chapter 4

Absolutely continuous and singularly continuous spectrum

We skim through some key facts concerning the fundamental results of H. Lebesgue about monotic functions on the real axis. For details, we refer to [A.N. Kolmogoroff & S.V. Fomin: Elements de la théorie des fonctions et de l'analyse fonctionelle] or [I.P. Natanson: Theory of functions of a real variable]. This yields a 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}:

$$f = f_{\mathrm{pp}} + f_{\mathrm{ac}} + f_{\mathrm{sc}}.$$

Concerning the absolutely continuous component, we may apply the Fundamental Theorem of Calculus

$$f_{\mathrm{ac}}(x) - f_{\mathrm{ac}}(x_0) = \int_{x_0}^{x} f'_{\mathrm{ac}}(t)\,\mathrm{d}t.$$

The study of monotonic functions is of particular interest for our goals as if $(E(\lambda))_{\lambda\in\mathbb{R}}$ is a spectral family, the function

$$\mathbb{R} \to [0,\infty), \quad \lambda \mapsto \langle E(\lambda)u, u\rangle$$

is monotonic. If H is a Schrödinger operator with the spectral family $(E(\lambda))_{\lambda\in\mathbb{R}}$, the elements $u \in \mathcal{H}$ for which $\langle E(\lambda)u, u\rangle$ is absolutely continuous correspond to the *scattering states*; the elements $u \in \mathcal{H}$ such that $\langle E(\lambda)u, u\rangle$ is a jump function correspond to the *bound states*. In fact, this yields a decomposition of the Hilbert space

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

A function $g\colon \mathbb{R} \to \mathbb{R}$ is called *integrable* if g is measurable and $\int_{\mathbb{R}} |g(x)|\,\mathrm{d}x < \infty$. Let $[a,b] \subset \mathbb{R}$ be a compact interval and let $f\colon [a,b] \to \mathbb{R}$ be monotonic and non-decreasing. Then:

(1) f is measurable and bounded and hence integrable.

(2) For $x \in (a,b)$, the limits $f(x+0) := \lim_{\varepsilon\to 0} f(x+\varepsilon)$, $f(x-0) := \lim_{\varepsilon\to 0} f(x-\varepsilon)$ exist. Either $f(x-0) = f(x+0)$ and f is continuous at x or $f(x-0) \neq f(x+0)$ and f is discontinuous at x and has a jump of height $f(x+0) - f(x-0) > 0$.

(3) The number of discontinuities of f is at most countable.

(4) Let f be monotonic and right-continuous. Then f has a unique decomposition into a continuous monotonic function g and a right-continuous jump function h in the sense that $f = g + h$. The function h is constant between the jump discontinuities.

(5) We can assume without loss of generality that a monotonic function is right-continuous.

Definition 4.1. A set $N \subset \mathbb{R}$ is called a *null set* if for any $\varepsilon > 0$ there exists a sequence of intervals $I_k \subset \mathbb{R}$, $k \in \mathbb{N}$, such that

$$N \subset \bigcup_{k\in\mathbb{N}} I_k \quad \text{and} \quad \sum_{k\in\mathbb{N}} |I_k| < \varepsilon.$$

Let $a < b$. We say that a property holds true *almost everywhere (a.e.) in* $[a,b]$ if it holds true for all $x \in [a,b]\backslash N$ with a null set N.

Remark 4.2. It is easy to see that the countable union of null sets is again a null set: If the null sets $\{N_i; i \in \mathbb{N}\}$ and $\varepsilon > 0$ are given, there exists $(I_{k,i})_{k\in\mathbb{N}}$ such that $N_i \subset \cup_{k\in\mathbb{N}} I_{k,i}$ and $\sum_{k\in\mathbb{N}} |I_{k,i}| < 2^{-i}\varepsilon$, for all $i \in \mathbb{N}$. Then $N := \cup_{i\in\mathbb{N}} N_i \subset \cup_{k,i\in\mathbb{N}} I_{k,i}$ and $\sum_{k,i\in\mathbb{N}} |I_{k,i}| < \varepsilon \sum_{i=1}^{\infty} 2^{-i} = \varepsilon$.

Theorem 4.3 (Lebesgue). *Let $f\colon [a,b] \to \mathbb{R}$ be monotonic. Then f is differentiable almost everywhere.*

The claim of Theorem 4.3 means that there exists a null set $N \subset [a,b]$ such that for $x \in (a,b)\backslash N$, the finite limit $\lim_{h\to 0} \frac{1}{h}(f(x+h) - f(x))$ exists.

Theorem 4.4 (Fubini). *Let $F_n\colon [a,b] \to \mathbb{R}$ be monotonic and non-decreasing and assume that $F := \sum_{n=1}^{\infty} F_n$ converges for all $x \in [a,b]$. Then*

$$F'(x) = \sum_{n=1}^{\infty} F_n'(x) \quad a.e.$$

Corollary 4.5. *Let $h\colon [a,b] \to \mathbb{R}$ be the jump function of a monotonic function f. Then $h' = 0$ a.e.*

Definition 4.6. A function $f\colon [a,b] \to \mathbb{R}$ is *of bounded variation* if there exists a constant C such that for all $n \in \mathbb{N}$

$$\sum_{k=1}^{n} |f(x_k) - f(x_{k-1})| \leq C \tag{4.1}$$

for any partition $a \le x_0 \le x_1 \le \cdots \le x_{n-1} \le x_n \le b$. The infimum of all constants $C \ge 0$ with the property (4.1) for all partitions $(x_i)_{i=1,\dots,n}$ of $[a,b]$ and all $n \in \mathbb{N}$ is called the *total variation* of f.

Theorem 4.7. *Any function of bounded variation can be written as the difference of two monotonically non-decreasing functions.*

Recall that the Fundamental Theorem of Calculus comprises the following two statements:

(a) If f is continuous, then $\frac{\mathrm{d}}{\mathrm{d}x}\int_a^x f(t)\,\mathrm{d}t = f(x)$.

(b) If F is continuously differentiable, then $F(x) = F(a) + \int_a^x F'(t)\,\mathrm{d}t$.

Is it possible to obtain analogous statements under weaker assumptions? This question has been answered by H. Lebesgue. First of all, let us consider the (easier) statement (a). If $\varphi\colon [a,b] \to \mathbb{R}$ is integrable, we write

$$\varphi = \varphi_+ - \varphi_-, \quad \varphi_\pm \ge 0, \quad \varphi_\pm \text{ integrable.}$$

Then the functions

$$x \mapsto \int_a^x \varphi_\pm(t)\,\mathrm{d}t$$

are monotonically increasing and according to Theorem 4.3 the derivatives

$$\frac{\mathrm{d}}{\mathrm{d}x}\int_a^x \varphi_\pm(t)\,\mathrm{d}t \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}x}\int_a^x \varphi(t)\,\mathrm{d}t$$

exist. Indeed, we have the following theorem.

Theorem 4.8. *Let $f\colon [a,b] \to \mathbb{R}$ be integrable. Then*

$$\frac{\mathrm{d}}{\mathrm{d}x}\int_a^x f(t)\,\mathrm{d}t = f(x) \ \ a.e.$$

Concerning part (b), we make use of the following inequality.

Theorem 4.9. *Let $f\colon [a,b] \to \mathbb{R}$ be monotonically increasing. Then f' is integrable and*

$$\int_a^b f'(t)\,\mathrm{d}t \le f(b) - f(a). \tag{4.2}$$

Proof. For $h > 0$ let $\varphi_h(x) := \frac{1}{h}(f(x+h) - f(x))$; to this end, f may be extended by the constant function $f(b)$ at b. Then

$$\begin{aligned}\int_a^b \varphi_h(x)\,\mathrm{d}x &= \frac{1}{h}\left(\int_a^b f(x+h)\,\mathrm{d}x - \int_a^b f(x)\,\mathrm{d}x\right)\\ &= \frac{1}{h}\left(\int_{a+h}^{b+h} f(x)\,\mathrm{d}x - \int_a^b f(x)\,\mathrm{d}x\right)\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{h}\left(\int_b^{b+h} f(x)\,\mathrm{d}x - \int_a^{a+h} f(x)\,\mathrm{d}x\right) \\
&\le f(b+h) - f(a) = f(b) - f(a),
\end{aligned}
$$

as f is monotonically increasing. Clearly, $\varphi_h \geq 0$ so that we may deduce that $\varphi_h \in L_1(a,b)$ and $\liminf_{h\to 0} \|\varphi_h\|_{L_1} \leq f(b) - f(a)$. Furthermore,

$$
f'(x) = \liminf_{h\to 0} \varphi_h(x) \text{ a.e.}
$$

By Fatou's lemma, $f' \in L_1(a,b)$ and, as $f'(x) \geq 0$,

$$
\int_a^b f'(t)\,\mathrm{d}t = \|f'\|_{L_1} \leq \liminf_{h\to 0} \|\varphi_h\|_{L_1} \leq f(b) - f(a)
$$

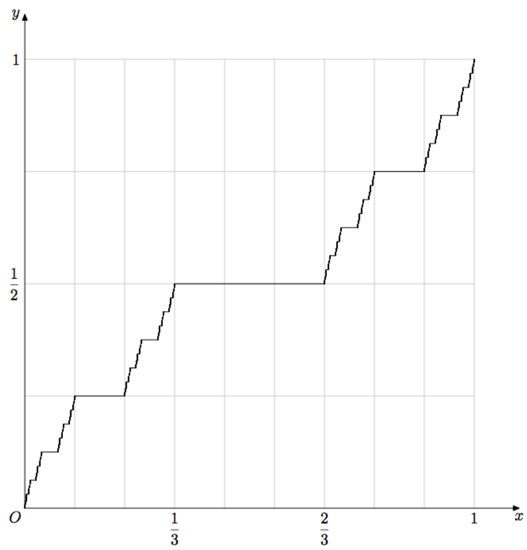
which completes our proof. □

In general, we do not have equality in (4.2); consider a jump function, for instance. More interestingly, there exist continuous functions for which we do not have equality in (4.2).

Example 4.10 (Cantor function). There exists a continuous and monotonic function $f\colon [0,1] \to [0,1]$ satisfying

$$
f(0) = 0, \quad f(1) = 1, \quad f'(t) = 0 \text{ a.e.}
$$

This function satisfies $\int_0^1 f'(t)\,\mathrm{d}t = 0 \neq f(1) - f(0) = 1$, see [RS-I, p. 21].



Definition 4.11. A function $f\colon [a,b] \to \mathbb{R}$ is called *absolutely continuous* if for any $\varepsilon > 0$ there exists $\delta > 0$ with the following property: If $\{I_k; k = 1,\dots,n\}$ is a finite family of pairwise disjunct open intervals $I_k = (a_k, b_k) \subset [a,b]$ then

$$
\sum_{k=1}^n (b_k - a_k) < \delta \quad \Longrightarrow \quad \sum_{k=1}^n |f(b_k) - f(a_k)| < \varepsilon.
$$

Remark 4.12.

(1) Any absolutely continuous function is uniformly continuous, but the reverse statement is not true; consider once more the Cantor function of Example 4.10.

(2) In Definition 4.11, we may replace "finite family" by "countable family".

(3) Any absolutely continuous function is of bounded variation.

(4) The set of absolutely continuous functions on $[a, b]$ is a vector space, denoted as $\mathrm{AC}[a, b]$.

(5) Any absolutely continuous function can be written as the difference of two monotonic and absolutely continuous functions.

Theorem 4.13. *If $f\colon [a, b] \to \mathbb{R}$ is integrable, then the integral function*

$$F(x) := \int_a^x f(t)\,\mathrm{d}t, \quad x \in [a, b],$$

is absolutely continuous.

Theorem 4.14 (Vitali, 1906). *Let $F\colon [a, b] \to \mathbb{R}$ be absolutely continuous. Then F is a.e. differentiable, the derivative $f := F'$ is integrable and for all $x \in [a, b]$ we have that*

$$\int_a^x f(t)\,\mathrm{d}t = F(x) - F(a).$$

Remark 4.15.

(1) Vitali's Theorem can be applied to prove that absolutely continuous functions are of bounded variation, see Remark 4.12(3): Let $a = x_0 < x_1 < \ldots < x_{n+1} = b$ be a partition of $[a, b]$. If f is absolutely continuous on $[a, b]$, there is a function $g \in L_1(a, b)$ such that $f' = g$ a.e. It follows from

$$\sum_{k=0}^{n} |f(x_{k+1}) - f(x_k)| = \sum_{k=0}^{n} \left| \int_{x_k}^{x_{k+1}} g(y)\,\mathrm{d}y \right| \le \sum_{k=0}^{n} \int_{x_k}^{x_{k+1}} |g(y)|\,\mathrm{d}y = \|g\|_{L_1(a,b)}$$

that the total variation of f on $[a, b]$ is finite.

(2) We also obtain that any Lipschitz continuous function is absolutely continuous: Assume that there exists $L > 0$ such that, for all $x, y \in [a, b]$, $|f(x) - f(y)| \le L|x - y|$. Let $\varepsilon > 0$ and define $\delta := \varepsilon/L$. Furthermore, let $I_k = (a_k, b_k) \subset [a, b]$, $k = 1, \ldots, n$, with $\sum_{k=1}^{n} |b_k - a_k| < \delta$ be given. As

$$\sum_{k=1}^{n} |f(b_k) - f(a_k)| \le L \sum_{k=1}^{n} |b_k - a_k| < L\delta = \varepsilon,$$

we obtain that f is absolutely continuous. And as

$$\frac{|f(x) - f(y)|}{|x - y|} \leq L, \quad \forall x \neq y,$$

it is also clear that $|f'(x)| \leq L$ a.e.

(3) A more stronger result is *Rademacher's Theorem*: A function $f\colon [a,b] \to \mathbb{R}$ is Lipschitz continuous if and only if f is almost everywhere differentiable with bounded derivative f'.

We already know that any function f of bounded variation can be decomposed in the sense that it can be written as a sum of a jump function h and a continuous function φ of bounded variation,

$$f = h + \varphi.$$

We now define the function

$$\psi(x) \coloneqq \int_a^x \varphi'(t)\,\mathrm{d}t.$$

According to Theorem 4.9, φ' is indeed integrable and hence, by Theorem 4.13, ψ is absolutely continuous. In consequence, the difference $\chi \coloneqq \varphi - \psi$ is of bounded variation and

$$\frac{\mathrm{d}}{\mathrm{d}x}\chi = \varphi'(x) - \frac{\mathrm{d}}{\mathrm{d}x}\int_a^x \varphi'(t)\,\mathrm{d}t = 0 \text{ a.e.}$$

Definition 4.16. A continuous, non-constant function $\chi\colon [a,b] \to \mathbb{R}$ of bounded variation is called *singularly continuous* if $\chi'(x) = 0$ a.e.

Remark 4.17. The Lebesgue-Stieltjes measure corresponding to χ is localized on a Borel null set and hence it is singular with respect to the Lebesgue measure.

Theorem 4.18 (Lebesgue, 1904). *Any function $f\colon [a,b] \to \mathbb{R}$ of bounded variation allows for a unique decomposition*

$$f = h + \psi + \chi,$$

where h is a jump function, ψ is absolutely continuous and χ is singularly continuous.

Let $T\colon D(T) \to \mathcal{H}$ be a self-adjoint operator in the Hilbert space $\mathcal{H}$ with the spectral family $(E(\lambda))_{\lambda\in\mathbb{R}}$. For all $f \in \mathcal{H}$, the function

$$\mathbb{R} \to \mathbb{R}, \quad \lambda \mapsto \langle E(\lambda)f, f\rangle = \|E(\lambda)f\|^2$$

is monotonically non-decreasing and right-continuous. Hence the above results apply and we will define the following subspaces of $\mathcal{H}$:

$$\mathcal{H}_{\mathrm{pp}} \coloneqq \overline{\operatorname{span}\{u \in D(T); u \text{ is an eigenvector of } T\}},$$

$$\mathcal{H}_{\text{ac}} := \{f \in \mathcal{H}; \|E(\cdot)f\|^2 \text{ is absolutely continuous}\},$$
$$\mathcal{H}_{\text{sc}} := \{f \in \mathcal{H}; \|E(\cdot)f\|^2 \text{ is singularly continuous}\};$$

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

$$\mathcal{H} = \mathcal{H}_{\text{pp}} \oplus \mathcal{H}_{\text{ac}} \oplus \mathcal{H}_{\text{sc}}. \tag{4.3}$$

Denote by I_{pp}, I_{ac} and I_{sc} the projections on $\mathcal{H}_{\text{pp}}$, $\mathcal{H}_{\text{ac}}$ and $\mathcal{H}_{\text{sc}}$. Then T commutes with I_{pp}, I_{ac} and I_{sc} and hence

$$T_{\text{pp}} := TI_{\text{pp}}, \quad T_{\text{ac}} := TI_{\text{ac}}, \quad T_{\text{sc}} := TI_{\text{sc}}$$

are self-adjoint operators in the subspaces $\mathcal{H}_{\text{pp}}$, $\mathcal{H}_{\text{ac}}$ and $\mathcal{H}_{\text{sc}}$. We define

$$\sigma_{\text{ac}}(T) := \sigma(T_{\text{ac}}), \quad \sigma_{\text{sc}}(T) := \sigma(T_{\text{sc}})$$

and our final goal is to show that $\sigma(T) = \overline{\sigma_{\text{p}}(T)} \cup \sigma_{\text{ac}}(T) \cup \sigma_{\text{sc}}(T)$, where $\sigma_{\text{p}}(T)$ is the point spectrum of T.

We now shed light on some aspects concerning the decomposition (4.3) omitting some of the proofs, cf. [W-II; Ch. 12] and [RS-I; Thm. VII.4] for more details.

Definition 4.19. Let T be a self-adjoint operator in the Hilbert space $\mathcal{H}$. We call

$$\mathcal{H}_{\text{pp}} := \overline{\operatorname{span}\{u \in D(T); u \text{ is an eigenvector of } T\}}$$

the *discontinuous subspace of $\mathcal{H}$ with respect to T* and $\mathcal{H}_{\text{c}}(T) := \mathcal{H}_{\text{pp}}(T)^{\perp}$ the *continuous subspace.*

Obviously, $\mathcal{H}_{\text{pp}}$ and $\mathcal{H}_{\text{c}}$ are closed subspaces of $\mathcal{H}$. Our definition is motivated by the following theorem.

Theorem 4.20. *We have that* $\mathcal{H}_{\text{pp}}(T) = \{f \in \mathcal{H}; \|E(\cdot)f\|^2 \text{ is a jump function}\}$ *and* $\mathcal{H}_{\text{c}}(T) = \{f \in \mathcal{H}; \|E(\cdot)f\|^2 \text{ is continuous}\}$. *Moreover,*

$$\mathcal{H}_{\text{sc}} := \{f \in \mathcal{H}; \|E(\cdot)f\|^2 \textit{ is singularly continuous}\}$$

is a closed subspace of $\mathcal{H}$.

Proof. We only give a sketch of the proof of the last statement. For any interval (a, b), $a < b$, one defines

$$E_{(a,b)} = E(b - 0) - E(a).$$

Next one shows that we can associate a spectral projection E_B with a Borel set $B \subset \mathbb{R}$. Afterwards, one proves that $f \in \mathcal{H}_{\text{sc}}$ if and only if there is a Borel null set $N \subset \mathbb{R}$ such that $E_N f = f$. It follows that $f, g \in \mathcal{H}_{\text{sc}}$ implies that $f + g \in \mathcal{H}_{\text{sc}}$: First $f, g \in \mathcal{H}_{\text{sc}}$ implies that there exist null sets N, N' with $E_N f = f$ and $E_{N'} g = g$. Then $\tilde{N} = N \cup N'$ is a null set and as $E_{\tilde{N}} \geq E_N$ and $E_{\tilde{N}} \geq E_{N'}$, we conclude that

$$E_{\tilde{N}}(f + g) = E_{\tilde{N}} f + E_{\tilde{N}} g = E_{\tilde{N}} E_N f + E_{\tilde{N}} E_{N'} g = E_N f + E_{N'} g = f + g;$$

here we have used that, for two projections P and Q, $P \geq Q \iff R(P) \supset R(Q) \iff PQ = QP = Q$. If $(f_n) \subset \mathcal{H}_{\mathrm{sc}}$ is a convergent sequence, $f_n \to f \in \mathcal{H}$, there exist Borel null sets $N_n \subset \mathbb{R}$ with $E_{N_n} f_n = f_n$. Then $N := \cup_{n\in\mathbb{N}} N_n$ is a Borel null set and

$$E_N f = E_N \left(\lim_{n\to\infty} f_n \right) = \lim_{n\to\infty} E_N f_n = \lim_{n\to\infty} E_N E_{N_n} f_n = \lim_{n\to\infty} E_{N_n} f_n = \lim_{n\to\infty} f_n = f,$$

meaning that $f \in \mathcal{H}_{\mathrm{sc}}$. □

Definition 4.21. Let T, $\mathcal{H}_{\mathrm{c}}$ and $\mathcal{H}_{\mathrm{sc}}$ as above. The orthogonal complement of $\mathcal{H}_{\mathrm{sc}}$ in $\mathcal{H}_{\mathrm{c}}$ is denoted by $\mathcal{H}_{\mathrm{ac}}$, the *absolutely continuous subspace of $\mathcal{H}$ with respect to T*,

$$\mathcal{H}_{\mathrm{ac}} := \mathcal{H}_{\mathrm{c}} \cap \mathcal{H}_{\mathrm{sc}}^{\perp} = \mathcal{H}_{\mathrm{c}} \ominus \mathcal{H}_{\mathrm{sc}}.$$

Finally let $\mathcal{H}_{\mathrm{s}} := \mathcal{H}_{\mathrm{pp}} \oplus \mathcal{H}_{\mathrm{sc}}$ be the *singular continuous subspace of $\mathcal{H}$* so that

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

Finally, one shows that indeed $\mathcal{H}_{\mathrm{ac}} = \{f \in \mathcal{H}; \|E(\cdot)f\|^2 \text{ is absolutely continuous}\}$. We now intend to decompose T into its components with respect to the subspaces $\mathcal{H}_{\mathrm{pp}}$, $\mathcal{H}_{\mathrm{sc}}$ and $\mathcal{H}_{\mathrm{ac}}$.

Definition 4.22. Let M be a closed subspace of $\mathcal{H}$ and let $P = P_M$ be the projection on M. We say that M *reduces* T if

$$PT \subset TP$$

i.e. if $u \in D(T)$ implies $Pu \in D(T)$ and $TPu = PTu$. If M reduces T, then

$$D(T_M) := D(T) \cap M, \quad T_M f := Tf, \quad \forall f \in D(T_M)$$

is an operator in M. As M reduces T if and only if $M^\perp$ reduces T, we obtain an operator $T_{M^\perp}$ similarly.

Theorem 4.23. *Let T be a self-adjoint operator in the Hilbert space $\mathcal{H}$ and assume that M reduces T. Then T_M and $T_{M^\perp}$ are self-adjoint operators in M and $M^\perp$ respectively. Furthermore $\sigma(T) = \sigma(T_M) \cup \sigma(T_{M^\perp})$.*

Proof.

(1) We first show that $D(T_M) \subset M$ is dense. Let $v \in M$ with $v \perp D(T_M)$ be given. As $D(T) = D(T_M) \oplus D(T_{M^\perp})$ and $v \in D(T_{M^\perp})^\perp$, $v \in D(T)^\perp$ and hence $v = 0$, since $D(T) \subset \mathcal{H}$ is dense. Similarly, one sees that $D(T_{M^\perp}) \subset M^\perp$ is dense.

(2) Clearly, $T_M = T\restriction_M$ and $T_{M^\perp} = T\restriction_{M^\perp}$ are symmetric.

(3) We show that $R(T_M \pm \mathrm{i}I_M) = M$. Let $f \in M$. As T is self-adjoint, there exists $u \in D(T)$ such that $(T + \mathrm{i})u = f$. We want to show that in fact $u \in M$ and make use of the decomposition $u = v + w \in M \oplus M^\perp$. Using that M and $M^\perp$ are invariant under the action of T, we obtain that $(T+\mathrm{i})v \in M$ and $(T+\mathrm{i})w \in M^\perp$. As $f = (T + \mathrm{i})v + (T + \mathrm{i})w$, we obtain that $(T + \mathrm{i})w = 0$ and as $(T + \mathrm{i})$ is injective, we see that $w = 0$. It is shown similarly that $R(T_M - \mathrm{i}I_M) = M$ and that $R(T_{M^\perp} \pm \mathrm{i}I_{M^\perp}) = M^\perp$. Hence T_M and $T_{M^\perp}$ are self-adjoint.

(4) To prove the decomposition of the spectrum, we start from $z \in \sigma(T_M) \cup \sigma(T_{M^\perp})$ and assume without loss of generality that $z \in \sigma(T_M)$. This implies the existence of a sequence $(u_n) \subset D(T_M)$, $\|u_n\| = 1$ such that $\|(T_M - z)u_n\| \to 0$. But then also $\|(T - z)u_n\| \to 0$ and $z \in \sigma(T)$. To prove the other direction, we start from the assumption $z \in \rho(T_M) \cap \rho(T_{M^\perp})$ to obtain that

$$T - z = (T_M - zI_M) \oplus (T_{M^\perp} - zI_{M^\perp})\colon D(T) \to \mathcal{H}$$

is bijective and hence $z \in \rho(T)$. □

Theorem 4.24. *Let T be a self-adjoint operator with the spectral family $(E(\lambda))_{\lambda\in\mathbb{R}}$ and let M be a closed subspace of $\mathcal{H}$ with the associated projection P. Then:*

$$M \text{ reduces } T \quad \iff \quad \forall\lambda \in \mathbb{R}\colon [P, E(\lambda)] = 0. \tag{4.4}$$

Proof. This follows from [M. Kohlmann: Spectral Theory; Exercise 9.7]. □

Theorem 4.25. *Let T be a self-adjoint operator in the Hilbert space $\mathcal{H}$. Then the subspaces $\mathcal{H}_{\mathrm{pp}}$, $\mathcal{H}_{\mathrm{sc}}$ and $\mathcal{H}_{\mathrm{ac}}$ reduce T.*

Proof. By Theorem 4.24, it suffices to show that, for $P \in \{P_{\mathrm{pp}}, P_{\mathrm{ac}}, P_{\mathrm{sc}}\}$ and $E_\lambda \coloneqq E_{(-\infty,\lambda]}$,

$$\forall\lambda \in \mathbb{R}\colon [P, E_\lambda] = 0.$$

(1) Let $x \in \mathcal{H}_{\mathrm{pp}}$. Then there exists $A \coloneqq (\lambda_n)_{n\in\mathbb{N}} \subset \mathbb{R}$ such that

$$E_A x \coloneqq \sum_{n=1}^{\infty} E_{\{\lambda_n\}} x = \sum_{n=1}^{\infty} (E_{\lambda_n} - E_{\lambda_n - 0})\, x = x = P_{\mathrm{pp}} x.$$

As E_λ is a bounded operator and $E_\lambda E_\mu = E_\mu E_\lambda$, for all $\lambda, \mu \in \mathbb{R}$, we conclude that $E_\lambda P_{\mathrm{pp}} x = P_{\mathrm{pp}} E_\lambda x$, for all $x \in \mathcal{H}_{\mathrm{pp}}$. Hence $E_\lambda P_{\mathrm{pp}} = P_{\mathrm{pp}} E_\lambda P_{\mathrm{pp}}$ and taking the adjoint yields $P_{\mathrm{pp}} E_\lambda = P_{\mathrm{pp}} E_\lambda P_{\mathrm{pp}} = E_\lambda P_{\mathrm{pp}}$ so that indeed $[P_{\mathrm{pp}}, E_\lambda] = 0$.

(2) As explained in the proof of Theorem 4.20, given $f \in \mathcal{H}_{\mathrm{sc}}$, there exists a Borel null set $N \subset \mathbb{R}$ such that $f = P_{\mathrm{sc}} f = E_N f$ and $E_N = \int_{-\infty}^{\infty} \chi_N(\lambda)\, \mathrm{d}E_\lambda$. We show that $[E_N, E_\lambda] = 0$. Let $g \in \mathcal{H}$ and observe that

$$\langle E_N E_\lambda f, g\rangle = \int_{-\infty}^{\infty} \chi_N(\mu)\, \mathrm{d}_\mu \langle E_\mu E_\lambda f, g\rangle$$

$$\begin{aligned}
&= \int_{-\infty}^{\infty} \chi_N(\mu)\,\mathrm{d}_\mu \int_{-\infty}^{\infty} \chi_{(-\infty,\lambda]}(\xi)\,\mathrm{d}_\xi \,\langle E_\xi f, E_\mu g\rangle \\
&= \int_{-\infty}^{\infty} \chi_N(\mu)\chi_{(-\infty,\lambda]}(\mu)\,\mathrm{d}_\mu \,\langle E_\mu f, g\rangle \,.
\end{aligned}$$

Similarly,

$$\begin{aligned}
\langle E_\lambda E_N f, g\rangle &= \int_{-\infty}^{\infty} \chi_{(-\infty,\lambda]}(\mu)\,\mathrm{d}_\mu \,\langle E_\mu E_N f, g\rangle \\
&= \int_{-\infty}^{\infty} \chi_{(-\infty,\lambda]}(\mu)\,\mathrm{d}_\mu \int_{-\infty}^{\infty} \chi_N(\xi)\,\mathrm{d}_\xi \,\langle E_\xi f, E_\mu g\rangle \\
&= \int_{-\infty}^{\infty} \chi_{(-\infty,\lambda]}(\mu)\chi_N(\mu)\,\mathrm{d}_\mu \,\langle E_\mu f, g\rangle
\end{aligned}$$

so that, as in step (1), $E_\lambda P_{\mathrm{sc}} = P_{\mathrm{sc}} E_\lambda P_{\mathrm{sc}}$. Writing down the adjoint of the left-hand and the right-hand side, we also get that $P_{\mathrm{sc}} E_\lambda = P_{\mathrm{sc}} E_\lambda P_{\mathrm{sc}}$ and hence $[P_{\mathrm{sc}}, E_\lambda] = 0$.

(3) Using the decomposition $\mathcal{H} = \mathcal{H}_{\mathrm{pp}} \oplus \mathcal{H}_{\mathrm{ac}} \oplus \mathcal{H}_{\mathrm{sc}}$, it follows from $P_{\mathrm{ac}} = 1 - P_{\mathrm{pp}} - P_{\mathrm{sc}}$ that also $[P_{\mathrm{ac}}, E_\lambda] = 0$. □

Definition 4.26. We denote by T_{pp}, T_{c}, T_{sc}, T_{ac} and T_{s} the restrictions of T to the subspaces $\mathcal{H}_{\mathrm{pp}}$, $\mathcal{H}_{\mathrm{c}}$, $\mathcal{H}_{\mathrm{sc}}$, $\mathcal{H}_{\mathrm{ac}}$ and $\mathcal{H}_{\mathrm{s}}$ and call them the *(spectrally) discontinuous, continuous, singularly continuous, absolutely continuous* and the *singular part of* T. Moreover, we define

$$\begin{aligned}
\sigma_{\mathrm{c}}(T) &\coloneqq \sigma(T_{\mathrm{c}}), \text{ the continuous spectrum of } T, \\
\sigma_{\mathrm{sc}}(T) &\coloneqq \sigma(T_{\mathrm{sc}}), \text{ the singularly continuous spectrum of } T, \\
\sigma_{\mathrm{ac}}(T) &\coloneqq \sigma(T_{\mathrm{ac}}), \text{ the absolutely continuous spectrum of } T, \\
\sigma_{\mathrm{s}}(T) &\coloneqq \sigma(T_{\mathrm{s}}), \text{ the singular spectrum of } T.
\end{aligned}$$

We define $\sigma_{\mathrm{pp}}(T)$ as the set of eigenvalues of T, i.e. $\sigma_{\mathrm{pp}}(T) \coloneqq \sigma_{\mathrm{p}}(T)$, and

$$\sigma(T_{\mathrm{pp}}) \coloneqq \overline{\sigma_{\mathrm{p}}(T)}.$$

In particular,

$$\begin{aligned}
\mathcal{H} &= \mathcal{H}_{\mathrm{pp}} \oplus \mathcal{H}_{\mathrm{ac}} \oplus \mathcal{H}_{\mathrm{sc}}, \\
T &= T_{\mathrm{pp}} \oplus T_{\mathrm{ac}} \oplus T_{\mathrm{sc}}, \\
\sigma(T) &= \overline{\sigma_{\mathrm{pp}}(T)} \cup \sigma_{\mathrm{ac}}(T) \cup \sigma_{\mathrm{sc}}(T).
\end{aligned}$$

Let us summarize the three decompositions of the spectrum of a self-adjoint operator:

(1) Let T be a closed operator in the Banach space X and define

$$\sigma_{\mathrm{p}}(T) = \{\lambda \in \mathbb{C}; N(T - \lambda) \neq \{0\}\},$$

$$\sigma_{\text{cont}}(T) = \{\lambda \in \mathbb{C}; T - \lambda \text{ injective, } R(T-\lambda) \text{ dense, } R(T-\lambda) \neq X\},$$
$$\sigma_{\text{res}}(T) = \{\lambda \in \mathbb{C}; T - \lambda \text{ injective, } R(T-\lambda) \text{ not dense}\}.$$

Then

$$\boxed{\sigma(T) = \sigma_{\text{p}}(T) \cup \sigma_{\text{cont}}(T) \cup \sigma_{\text{res}}(T).}$$

The subsets $\sigma_{\text{p}}(T), \sigma_{\text{cont}}(T), \sigma_{\text{res}}(T) \subset \sigma(T)$ are disjoint. If X is a Hilbert space and T is self-adjoint, $\sigma(T) \subset \mathbb{R}$ and $\sigma_{\text{res}}(T) = \emptyset$.

(2) Let T be a self-adjoint operator in the Hilbert space $\mathcal{H}$. Then

$$\boxed{\sigma(T) = \sigma_{\text{disc}}(T) \cup \sigma_{\text{ess}}(T).}$$

Here, $\sigma_{\text{disc}}(T)$ is the set of eigenvalues $\lambda \in \sigma_{\text{p}}(T)$ that are isolated points of the spectrum of T and that have finite multiplicity. Moreover,

$$\sigma_{\text{ess}}(T) = \sigma(T) \backslash \sigma_{\text{disc}}(T)$$

contains eigenvalues of infinite multiplicity and accumulation points of the spectrum.

(3) Let T be a self-adjoint operator in the Hilbert space $\mathcal{H}$. Then

$$\boxed{\sigma(T) = \overline{\sigma_{\text{p}}(T)} \cup \sigma_{\text{c}}(T)}$$

with $\sigma_{\text{p}}(T)$ as in (1) but in general $\sigma_{\text{c}}(T) \neq \sigma_{\text{cont}}(T)$. Moreover, $\overline{\sigma_{\text{p}}(T)}$ and $\sigma_{\text{c}}(T)$ are not disjoint in general. Here, $\sigma(T_{\text{pp}}) = \overline{\sigma_{\text{p}}(T)}$ and

$$\boxed{\sigma_{\text{c}}(T) = \sigma_{\text{ac}}(T) \cup \sigma_{\text{sc}}(T),}$$

with $\sigma_{\text{ac}}(T) = \sigma(T_{\text{ac}})$ and $\sigma_{\text{sc}}(T) = \sigma(T_{\text{sc}})$, and T_{ac} and T_{sc} denote the parts of T in the subspaces $\mathcal{H}_{\text{ac}}$ and $\mathcal{H}_{\text{sc}}$ respectively. Finally,

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

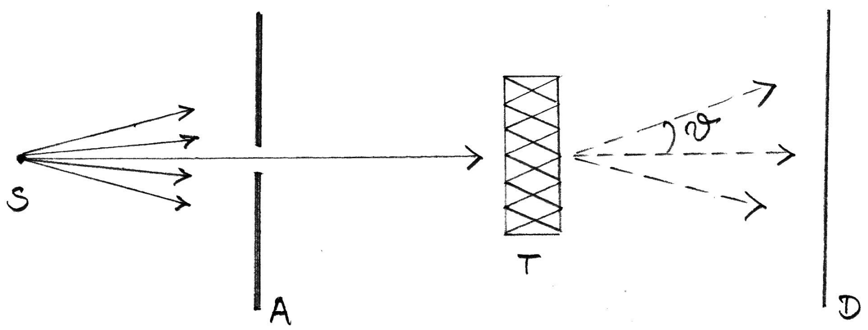
Chapter 5

Outlook: Scattering Theory

5.1 Scattering experiments in physics

One of the main goals in physics is to determine the elementary particles of matter and the forces acting between them. On an atomic or sub-atomic scale, this is only possible using scattering experiments: Examples in the history of physics are, for instance, the discovery of the nucleus, the nuclear fission, the discovery of new particles in a collider and the determination of the structure of crystals. In any of these examples, the length scales are so small (or the energies are so high, respectively) that only a quantum mechanical approach makes sense to come to valuable results. Let us consider some aspects of *quantum mechanical scattering theory* here.

The following setting is typical for scattering experiments: Particles coming from a *source* S move through an *aperture* A and finally reach a *target* T where the scattering takes place. Behind the target there is a *detector* D that measures the intensity as a function of the *angle of deflection* ϑ.



The simplest example for a scattering process is the *elastic 2-particle scattering.* However, in physics, there are more examples like inelastic scattering *(excitation)* or scattering processes in which more than 2 particles are involved *(multi-channel scattering).*

Of particular interest is the determination of the *total* and *differential cross* *section* and more generally of the *scattering operator/scattering matrix*. The main goal is, given a certain potential $V(x)$, to determine the associated cross sections and the scattering operator respectively (which is not easy). Even more difficult is the *inverse scattering problem*: Given certain data of a scattering experiment (cross sections, phase shifts, reflection coefficients etc.) how can one reconstruct the law of force?

5.2 The quantum mechanical two-body problem

We assume that a single particle is shot towards a fixed target (of infinite mass). Then the motion of the particle is described by the Schrödinger equation

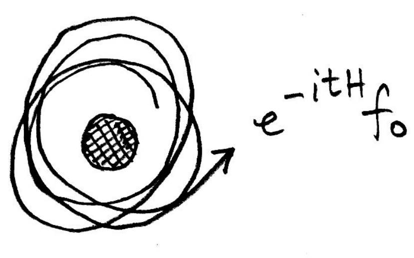
$$\frac{\partial}{\partial t} f(x,t) = \frac{1}{\mathrm{i}} H f(x,t) \tag{5.1}$$

where $H = -\Delta + V$ is a suitable Schrödinger operator in the Hilbert space $L_2(\mathbb{R}^d)$. If the initial state of the particle (at $t=0$) is given by some $f_0 \in L_2$, the solution to (5.1) is given by

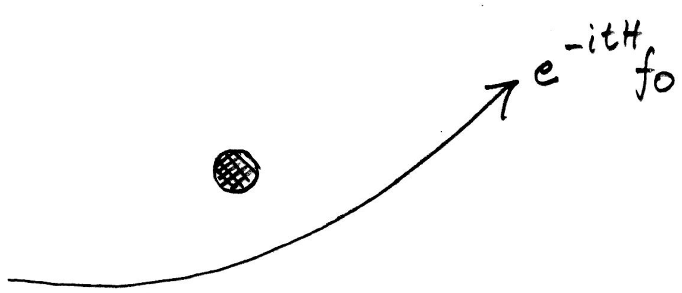
$$f(\cdot,t) = e^{-\mathrm{i}tH} f_0, \quad -\infty < t < \infty.$$

We 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.

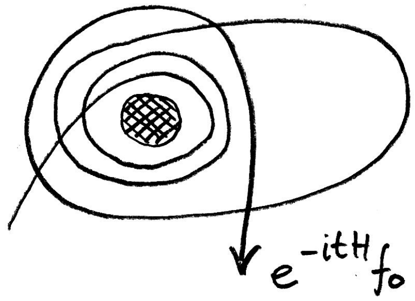
(1) $f_0 \in \mathcal{H}_{\mathrm{pp}}$: *Bound state*. The particle is quasi-localized and moves on some trajectory (not necessarily periodic) within the potential.



(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 $\mathcal{H}_{\mathrm{sc}} = \{0\}$.



Let us shed some more light on the case (2): Let $H = H_0 + V$, $H_0 = -\Delta$, be self-adjoint operators in the Hilbert space $\mathcal{H}$. We assume that

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

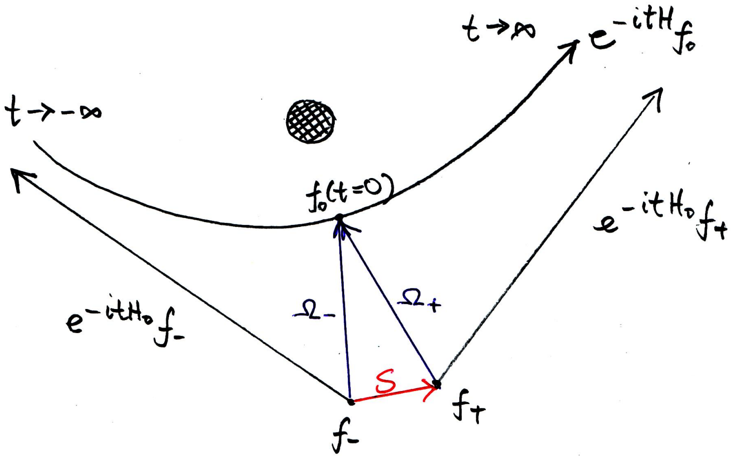
for some $\alpha > 1$. For large $|t|$, we expect that the particle is far away from the scattering center where the potential almost vanishes. Hence the particle should behave like a free particle in these regions. This motivates to look for *asymptotes* to the trajectory as $t \to \infty$ and $t \to -\infty$: Given $f_0 \in \mathcal{H}_{\mathrm{ac}}$, we look for initial values $f_\pm \in \mathcal{H}$ such that $e^{-\mathrm{i}tH_0} f_\pm$ is asymptotic to $e^{-\mathrm{i}tH} f_0$ as $t \to \pm\infty$,

$$\left\| e^{-\mathrm{i}tH} f_0 - e^{-\mathrm{i}tH_0} f_\pm \right\| \to 0, \quad t \to \pm\infty.$$

The wave operators

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

as far as the strong limit exists, interrelate $f_\pm$ and f_0 and $S := \Omega_+^* \Omega_-$ is the scattering operator which figuratively speaking maps the direction of arrival to the direction of deflection. In physics, a scattering matrix is accessible in experiments. A first goal of *time-dependent scattering theory* thus is the construction of the wave operators.



5.3 Mathematical goals

The questions of the existence and completeness ($R(\Omega_-) = R(\Omega_+)$?, $R(\Omega_\pm) = \mathcal{H}_{\mathrm{ac}}$?) of the wave operators is strongly connected with the the spectral properties of the Schrödinger operator $H = -\Delta + V$: Are the absolutely continuous spectra of H and H_0 identical? Is the singularly continuous spectrum of H empty? How many positive eigenvalues can H have? As an example, we cite a theorem of V. Enß.

Theorem 5.1 (Enß, 1978/79). *Let $V\colon \mathbb{R}^3 \to \mathbb{R}$ with $|V(x)| \leq c\rho^{-\alpha}$ be given, with some $\alpha > 1$ and $\rho(x) := \sqrt{1 + |x|^2}$. Then:*

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

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

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

Remark 5.2. The decay property in Theorem 5.1 excludes coulomb potentials. We have to modify the wave operators for potentials that are $\rho(x)^{-1}$-like at ∞ (whereas the singularity of the Coulomb potential at $x = 0$ does not lead to substantial difficulties).

To round this lecture off, we give a very brief overview about some aspects of *time-independent scattering theory*: The Fourier transform $\mathcal{F}$ on L_2 is a unitary operator that diagonalizes $H_0 = -\Delta$:

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

The Fourier transform is built up from the functions $e^{\mathrm{i}k\cdot x}$ that satisfy

$$-\Delta e^{-\mathrm{i}k\cdot x} = k^2 e^{-\mathrm{i}k\cdot x}.$$

As the functions $e^{\mathrm{i}k\cdot x}$ are not in L_2, they are no eigenfunctions in the Hilbert space setting. Nevertheless, they are in strong relation with the operator H_0. We thus call them *generalized eigenfunctions*. The time-independent scattering theory looks for a sufficient number of functions $f(\cdot,k)\colon \mathbb{R}^d \to \mathbb{C}$ such that

$$\begin{aligned}(-\Delta + V)f(\cdot,k) &= k^2 f(\cdot,k), \quad k \in \mathbb{R}^d,\\ f(x,k) &\sim e^{-\mathrm{i}k\cdot x}, \quad |x| \text{ large}.\end{aligned}$$

It is possible to find suitable functions f by solving the *Lippmann-Schwinger equation*. Then one can construct a unitary map (in analogy to the Fourier transform) which diagonalizes H_{ac}, the part of H in $\mathcal{H}_{\mathrm{ac}}$, which leads to an explicit representation of the spectral projections of H_{ac} by integral operators. Furthermore, it is possible to obtain an explicit formula for the scattering matrix.

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