Schrödinger Operators and their Spectra

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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

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

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, $j = 1, \ldots, n+1$, 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

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

with a constant $C_f \geq 0$. 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

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

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

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

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*

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

and

$$\lambda_0 \in \sigma_{\mathrm{cont}}(H) \iff E(\cdot) \text{ is strongly continuous at } \lambda_0.$$

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. $\lambda \in \sigma_{\mathrm{ess}}(H) \iff$ *There is a singular sequence for H and λ.*

Proof. We write
$$H = \int_{-\infty}^{\infty} \lambda \,\mathrm{d}E(\lambda)$$
and assume that $\lambda_0 \in \sigma_{\mathrm{ess}}(H)$. 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 $\lambda_0 \in \sigma_{\mathrm{disc}}(H)$ 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. □

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 $\lambda \iff \lambda \in \sigma_{\text{ess}}(H+A)$. □

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 positively oriented 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

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

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. □

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

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

as well as

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

and

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

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

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

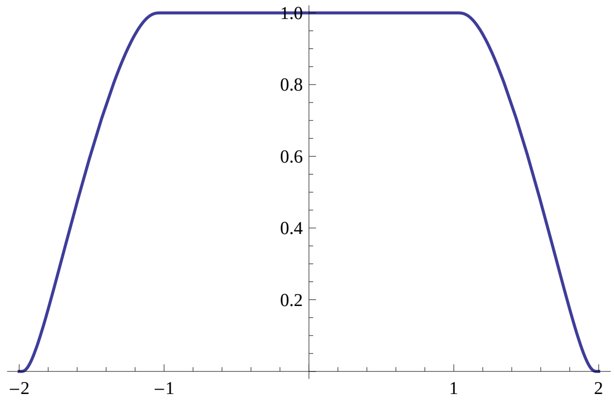
is essentially self-adjoint. The unique self-adjoint extension $H = H_0 + V$ satisfies $D(H) = D(H_0)$.

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. □

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

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

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

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

and that the second term on the right-hand side of (2.3) vanishes for $k \ge K$ 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

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

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

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

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

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

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

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 $u_{n_k} \xrightarrow{\mathrm{w}} u$ 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 $\mathring{\mathcal{H}}_V^1(\mathbb{R}^d)$ 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

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

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

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

and

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

Furthermore, $D(H)$ is dense in $\mathring{\mathcal{H}}_V^1(\mathbb{R}^d)$ 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

$$u_n \coloneqq (H+1)^{-1} f_n.$$

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 $\|u_{n_j}\|^2 < C_2 \varepsilon + \varepsilon$ 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

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

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*

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

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

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

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

(2) *Let $\varphi_n := (A^\dagger)^n \varphi_0$, 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 $(M_x f)(x) := xf(x)$ and $(\partial f)(x) := f'(x)$. 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 $H := (M_{x^2} - \partial^2)\restriction_{\mathscr{S}(\mathbb{R})}$ 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*

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

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 $f_n \xrightarrow{\text{w}} 0$ be given and let $v_n := (H_0 + c)^{-1} f_n$. As in the proof of Theorem 2.3, one shows that

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

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 $\varphi v_n \xrightarrow{\text{w}} 0$ 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

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

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 $V v_n \to 0$ 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

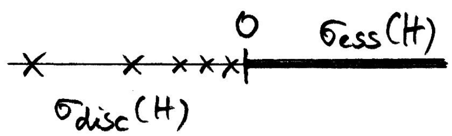
$$\|(H_0-\lambda)u_k\| \leq \|(H-\lambda)u_k\| + \|V\psi_R u_k\| + \|V(1-\psi_R)u_k\|.$$

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.).



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

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

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