Schrödinger operators and their spectra

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Chapter I

Quantum stability

One of the most striking and important features of quantum mechanics is the fact that classical dynamical systems which exhibit instability have a stable quantum version. A primary example is the stability of the world we live in, *i.e.* the stability of atoms, which cannot be explained by classical physics. In this chapter, on the basis of an elementary spectral analysis, we shall see that the quantum stability is a direct consequence of the mathematical structure of quantum mechanics.

I.1 Introduction

I.1.1 The crisis of classical physics

There is a strong experimental evidence that our world is composed of atoms and that an atom looks like a microscopic planetary system (Rutherford's experiment with α particles). There is a heavy, positively charged nucleus, made of protons and neutrons, which is surrounded by light, negatively charged electrons. Although the proton is much (about 1800 times) heavier than the electron, the gravitational force is negligible on the microscopic level and it is rather the electrostatic, Coulomb force that bound the electrons to orbit around the nucleus.

Now, the following classical paradox arises: According to the laws of classical electrodynamics, an accelerated charged particle emits electromagnetic radiation and loses in this way its total energy. Consequently, the electron particle would move on a spiral trajectory and finally collapse on the nucleus. The atoms should not be stable. (For instance, the lifetime of a hydrogen atom calculated according to the classical electrodynamics is less than 1 nanosecond!)

At the same time, the measured spectra of the radiation absorbed or emitted by an atom consists of discrete frequencies. This suggests that only a discrete set of electron orbits is allowed. Contrary to the laws of classical physics, according to which the energy of a planet varies continuously with the dimension of the orbit, which can be arbitrary.

There are other important experimental facts which cannot be explained on the level of classical physics, like the corpuscular behaviour of light (photoelectric effect), the particle-wave duality of matter (Bragg's experiment), the black-body radiation, *etc.*

These strong disagreements between experimental data and foundations of classical mechanics lead to a crisis of physics in the beginning of the last century. Quantum mechanics was invented on the basis of very practical physical reasons to explain the paradoxes.

I.1.2 The principles of quantum physics

In quantum mechanics, a physical system is not described in a (finite-dimensional) phase space, but in a (usually infinite-dimensional) *Hilbert space* $\mathcal{H}$. It is customary to consider the Hilbert space over the complex field (natural setting for standard quantum mechanics) and to be separable (*i.e.* it has a countable orthonormal basis). The inner product in $\mathcal{H}$ will be denoted by $(\cdot,\cdot)$.

A state of the physical system is not described by a point in the phase space, but rather by a unit vector ψ, called *wavefunction*, in the Hilbert space $\mathcal{H}$. (This explains the separability assumption about the Hilbert space, since countably many observations should be enough to determine a physical state.)

Physical observables are not represented by functions on a phase space, but by *self-adjoint operators* A on the Hilbert space $\mathcal{H}$. The expectation value of a bounded observable A for the system in state represented by the unit vector $\psi \in \mathcal{H}$ is given by the inner product $\langle A\rangle := (\psi, A\psi)$. Moreover, the outcomes of measuring are determined by the spectrum of A, denoted by $\sigma(A)$. (These explain the relevance of self-adjointness, because $\langle A\rangle$ and $\sigma(A)$ are real for self-adjoint A.)

A distinguished observable is the *Hamiltonian* H, *i.e.* the operator corresponding to the total energy of the system, which determines the t-time evolution of the physical system via the *Schrödinger equation*

$$i\hbar\frac{d}{dt}\psi = H\psi\,, \tag{I.1}$$

where $\hbar \approx 10^{-34}\,\mathrm{J\,s}$ is the reduced Planck constant.

For time-independent Hamiltonians, the solution of (I.1) is given by

$$\psi(t) = U(t)\psi_0\,,$$

where ψ_0 is an initial datum of (I.1) and $U(t)$ is the unitary group

$$U(t) := e^{-(i/\hbar)tH} = \int_{\sigma(H)} e^{-(i/\hbar)t\lambda}\, dE_H(\lambda)\,. \tag{I.2}$$

Here the second equality follows by the spectral theorem, E_H being the spectral measure of H. That is, the fundamental equation (I.1) is fully solved by the spectral decomposition of the Hamiltonian H.

I.1.3 Schrödinger operators

For a particle in a position dependent potential field $q \mapsto V(q)$, the classical Hamiltonian is given by the sum of kinetic and potential energies

$$H = \frac{p^2}{2m} + V(q)\,, \tag{I.3}$$

where p is the momentum. It turns out that the quantum counterpart has the same form, with a proper interpretation of the symbols q, p as position and momentum operators, respectively.

Since H is a quadratic function of p, while the dependence on q can be quite complex, it is useful to study (I.1) in the so-called *Schrödinger representation.* In this representation, the Hilbert space is identified with the Lebesgue space

$$\mathcal{H} = L^2(\mathbb{R}^d)\,, \tag{I.4}$$

where d is the dimension of the configuration space of the particle, and the position and momentum operators are represented by the operators

$$(q\psi)(x) = x\psi(x)\,, \qquad (p\psi)(x) = -i\hbar(\nabla\psi)(x)\,, \tag{I.5}$$

respectively. That is, the position is represented by a multiplication operator and the momentum by a differential operator. Consequently,

$$(H\psi)(x) = -\frac{\hbar^2}{2m}(\Delta\psi)(x) + (V\psi)(x)\,. \tag{I.6}$$

The Hamiltonian of the hydrogen atom can be cast just into the form (I.6), if m is interpreted as the reduced mass of the electron-proton couple (*i.e.* $m^{-1} = m_e^{-1} + m_p^{-1}$) and V is the Coulomb interaction

$$V(x) = -\frac{e^2}{|x|}\,,$$

with $e \approx 1.6 \times 10^{-19}\,\mathrm{C}$ being the elementary charge. More generally, for an electron bound to a nucleus of charge Ze, the Coulomb potential is $-Ze^2/|x|$. It is important to stress that (I.6) can be a reasonable Hamiltonian for other many-body systems, too, at least in various approximative regimes (Born-Oppenheimer approximation in molecular dynamics, effective mass approximation in semiconductor physics, *etc*).

Summing up, in view of (I.1), (I.2) and (I.6), many important problems in quantum mechanics can be reduced to the spectral analysis of the second-order elliptic partial differential operator of the form (I.6), called *Schrödinger operator.* The objective of these lectures is to make the reader familiar with some basic methods of spectral analysis of this type of operators.

I.2 Elements of spectral theory

We assume that the reader is familiar with the elements of functional analysis and spectral theory in Hilbert spaces. Here we recall the fundamental notions we shall need in this chapter. Additional topics can be found in Appendix A.

I.2.1 Self-adjointness versus symmetry

Let $\mathcal{H}$ be a separable complex Hilbert space. We adopt the physical convention by always assuming that the inner product $(\cdot,\cdot)$ is linear in the second variable and conjugate linear in the first variable. The corresponding norm will be denoted by $\|\cdot\|$.

A *linear operator* H on $\mathcal{H}$ is, by definition, a linear mapping of a subspace $\mathfrak{D}(H) \subset \mathcal{H}$ into $\mathcal{H}$; $\mathfrak{D}(H)$ is called the *domain* of H.

Any bounded operator can be extended by continuity to a bounded operator in the whole space $\mathcal{H}$. This is no more true for unbounded operators, and different operator domains usually lead to totally different spectra. In any case, it is useful to restrict ourselves to operators which are "continuous" in a generalized sense: we always assume that H is *densely defined* and *closed*.

Furthermore, we assume that H is *self-adjoint*, *i.e.*,

$$H^* = H\,,$$

where H^* is the adjoint of H. For unbounded operators, there is a great difference between self-adjoint and *symmetric* operators. The latter merely means that H^* is an extension of H, *i.e.*,

$$H^* \supset H\,.$$

In other words, a densely defined operator H is symmetric if, and only if,

$$\forall \phi, \psi \in \mathfrak{D}(H), \quad (\phi, H\psi) = (H\phi, \psi)\,, \tag{I.7}$$

while it is self-adjoint if, and only if, it is symmetric and $\mathfrak{D}(H) = \mathfrak{D}(H^*)$.

The symmetry relation (I.7) shows that the inner product $(\psi, H\psi)$ defined for $\psi \in \mathfrak{D}(H)$ is real. A symmetric operator H is said to be *bounded from below* if there exists a real constant c such that

$$\forall \psi \in \mathfrak{D}(H), \qquad (\psi, H\psi) \geq c\,\|\psi\|^2\,. \tag{I.8}$$

In this case we simply write $H \geq c$. The symmetric operator H is said to be *non-negative* if $H \geq 0$.

Both the self-adjointness and boundedness from below of a Hamiltonian H are important in quantum mechanics. The self-adjointness is necessary for the dynamics to be well defined, since, by Stone's theorem [23, Thm. VIII.8], every strongly continuous unitary group arises as the exponential of a self-adjoint operator. (This is probably the strongest justification for the usage of self-adjoint Hamiltonians in quantum physics.) The boundedness from below ensures the stability of the system, since (I.8) implies that the energy is bounded from below.

A given symmetric operator H is not necessarily self-adjoint, and it is important to know whether it possesses any self-adjoint extension $\tilde{H}$. From the general inclusions

$$H \subset \tilde{H} \subset \tilde{H}^* \subset H^*, \tag{I.9}$$

it is clear that the problem reduces to extending H till the central inclusion becomes sharp. This is not easy, however.

I.2.2 Operators defined via sesquilinear forms

An extremely powerful tool for studying Schrödinger operators are sesquilinear forms. A *sesquilinear form* on $\mathcal{H}$ is a mapping $h : \mathfrak{D}(h) \times \mathfrak{D}(h) \to \mathbb{C}$, with $\mathfrak{D}(h) \subset \mathcal{H}$, such that $\psi \mapsto h(\phi, \psi)$ is linear for each fixed $\phi \in \mathfrak{D}(h)$ and $\phi \mapsto h(\phi, \psi)$ is semilinear for each fixed $\psi \in \mathfrak{D}(h)$; $\mathfrak{D}(h)$ is called the domain of h. Many properties of sesquilinear forms are defined in an obvious way as in the case of operators. The mapping from $\mathfrak{D}(h)$ to $\mathbb{C}$ defined by $\psi \mapsto h[\psi] := h(\psi, \psi)$ will be called the *quadratic form* associated with h.

The correspondence between forms and operators

A convenient way how to construct a self-adjoint extension of a symmetric operator is given by a one-to-one correspondence between *closed symmetric sesquilinear forms* h and self-adjoint operators H which are bounded from below. Schematically:

$$H \xleftrightarrow{1-1} h\,.$$

Indeed, if h is a densely defined, closed, symmetric form bounded from below, by the first representation theorem [16, Sec. VI.2.1] (a consequence of the Riesz theorem), there exists a unique self-adjoint operator H bounded from below such that $\mathfrak{D}(H) \subset \mathfrak{D}(h)$ and

$$\forall \phi \in \mathfrak{D}(h),\ \psi \in \mathfrak{D}(H), \qquad h(\phi,\psi) = (\phi, H\psi)\,.$$

On the other hand, if H is a self-adjoint operator satisfying $H \geq c$, by the second representation theorem [16, Sec. VI.2.6], the sesquilinear form h defined by $\mathfrak{D}(h) := \mathfrak{D}\big((H-c)^{1/2}\big)$ and $h(\phi,\psi) := \big((H-c)^{1/2}\phi, (H-c)^{1/2}\psi\big) + c(\phi,\psi)$ is densely defined, closed and symmetric; the operator associated with it via the first representation theorem coincides with H.

Sesquilinear forms are convenient means for constructing self-adjoint Schrödinger operators, for the definition of the closed form associated with (I.6) has to take into account first-order derivatives only. More generally, perhaps the strongest reason for the fact that sesqulinear forms provide an extremely powerful tool for studying second-order differential operators is that many such operators with quite different domains have sesquilinear forms with the same domain.

The Friedrichs extension

We now explain how to find one particular self-adjoint extension of a symmetric operator. Let H be symmetric and bounded from below. Define the sesquilinear form h by $h(\phi,\psi) := (\phi, H\psi)$ for $\phi,\psi \in \mathfrak{D}(h) := \mathfrak{D}(H)$. The form h is clearly symmetric and bounded from below. Consequently, h is closable; let $\tilde{h}$ denote its closure. By the first representation theorem, the operator $\tilde{H}$ associated with $\tilde{h}$ is self-adjoint, bounded from below, and indeed $\tilde{H} \supset H$. It satisfies

$$\begin{aligned} \mathfrak{D}(\tilde{H}) &= \Big\{\psi \in \mathfrak{D}(\tilde{h}) \ \Big| \quad \exists \eta \in \mathcal{H},\ \forall \phi \in \mathfrak{D}(\tilde{h}), \quad \tilde{h}(\phi,\psi) = (\phi,\eta)\Big\}\,, \\ \tilde{H}\psi &= \eta\,. \end{aligned}$$

Moreover, $\mathfrak{D}(h) = \mathfrak{D}(H)$ is a core for $\tilde{h}$. Such a constructed operator $\tilde{H}$ will be called the *Friedrichs extension* of H.

I.2.3 Spectra of self-adjoint operators

The *spectrum* of a self-adjoint operator H on $\mathcal{H}$ is defined by

$$\sigma(H) := \big\{\lambda \in \mathbb{C} \mid \quad H - \lambda \quad \text{is not bijective}\big\}\,.$$

It is easy to see that $\sigma(H) \subset \mathbb{R}$.

We have the following disjoint partition of the spectrum:

$$\sigma(H) = \sigma_{\mathrm{p}}(H) \cup \sigma_{\mathrm{c}}(H)\,,$$

where the set of all eigenvalues of H, *i.e.*,

$$\begin{aligned}\sigma_{\mathrm{p}}(H) &:= \big\{\lambda \in \mathbb{R} \mid \quad H-\lambda \quad \text{is not injective}\big\} \\ &= \big\{\lambda \in \mathbb{R} \mid \quad \exists \psi \subset \mathfrak{D}(H), \quad \|\psi\| = 1, \quad H\psi = \lambda\psi\big\}\end{aligned}$$

is called the *point spectrum* of H, and

$$\sigma_{\mathrm{c}}(H) := \big\{\lambda \in \mathbb{R} \mid \quad H-\lambda \quad \text{is injective but} \quad \mathfrak{R}(H-\lambda) \neq \mathcal{H}\big\}$$

is called the *continuous spectrum* of H. If λ is an eigenvalue of H then the dimension of the kernel of $H-\lambda$ is called the (geometric) *multiplicity* of λ.

We rather use the following, alternative disjoint partition of the spectrum of a self-adjoint operator H:

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

Here the *discrete spectrum* $\sigma_{\mathrm{disc}}(H) \subset \sigma_{\mathrm{p}}(H)$ consists of those eigenvalues of H which are isolated points of $\sigma(H)$ and have finite multiplicity. The complement

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

is called the *essential spectrum* of H and, by definition, it contains either accumulation points of $\sigma(H)$ or isolated eigenvalues of infinite multiplicity.

I.2.4 Basic tools

The *spectral theorem* is by far the most fundamental tool in the spectral theory of self-adjoint operators. It is essentially a generalization of a well known result in finite-dimensional Hilbert spaces that any self-adjoint matrix can be diagonalized.

Theorem I.1 (Spectral theorem)**.** *For every self-adjoint operator H on $\mathcal{H}$ there exists exactly one spectral family E_H for which*

$$H = \int_{\sigma(H)} \lambda \; dE_H(\lambda)\,.$$

(For the notion of spectral family and integration with respect to it, we refer to [29, Sec. 7.2].)

We shall not use much the spectral theorem itself in these lectures. But we shall widely use some of its important consequences.

Weyl's criterion

The following characterization tells us that the points in the (essential) spectrum can be considered as approximate eigenvalues.

Theorem I.2 (Weyl's criterion)**.** *Let H be a self-adjoint operator on $\mathcal{H}$. A point λ belongs to $\sigma(H)$ if, and only if, there exists a sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset \mathfrak{D}(H)$ such that*

1. $\forall n \in \mathbb{N}, \quad \|\psi_n\| = 1\,,$
2. $H\psi_n - \lambda\psi_n \xrightarrow[n\to\infty]{} 0 \quad$ *in* $\quad \mathcal{H}$.

Moreover, λ belongs to $\sigma_{\rm ess}(H)$ if, and only if, in addition to the above properties

3. $\psi_n \xrightarrow[n\to\infty]{w} 0 \quad in \quad \mathcal{H}$.

The fact that the sequence satisfying the items 1 and 2 ensures that λ belongs to the spectrum of H is true for a general (not necessarily self-adjoint) closed operator. It is a consequence of the spectral theorem that the items 1 and 2 represent a necessary condition too. The sequence satisfying the items 1–3 is called a *singular sequence*.

See [29, Sec. 7.4] for a proof of Theorem I.2. An alternative version of Weyl's criterion is stated in Theorem III.4.

The minimax principle

The following theorem (known also as the Rayleigh-Ritz variational principle) provides a variational characterization of eigenvalues below the essential spectrum (*cf* [9, Sec. 4.5]).

Theorem I.3 (Minimax principle)**.** *Let H be a self-adjoint operator on $\mathcal{H}$ that is bounded from below, and let h be the associated sesquilinear form. Let $\{\lambda_n\}_{n=1}^\infty$ be a non-decreasing sequence of numbers defined by*

$$\lambda_n := \inf_{\mathcal{L}^n\subset\mathfrak{D}(H)} \sup_{\psi\in\mathcal{L}^n} \frac{(\psi,H\psi)}{\|\psi\|^2} = \inf_{\mathcal{L}^n\subset\mathfrak{D}(h)} \sup_{\psi\in\mathcal{L}^n} \frac{h[\psi]}{\|\psi\|^2}\,, \tag{I.10}$$

where $\mathcal{L}^n$ is any n-dimensional subspace of the corresponding domain. Then

1. $\lambda_\infty := \lim_{n\to\infty}\lambda_n = \inf\sigma_{\rm ess}(H)$, *with the convention that the essential spectrum is empty if $\lambda_\infty = +\infty$.*
2. $\{\lambda_n\}_{n=1}^\infty\cap(-\infty,\lambda_\infty) = \sigma_{\rm disc}(H)\cap(-\infty,\lambda_\infty)$, *each $\lambda_n\in(-\infty,\lambda_\infty)$ being an eigenvalue of H repeated a number of times equal to its multiplicity.*

Summing up, each λ_n represents either a discrete eigenvalue or the threshold of the essential spectrum of H. Obviously, if the spectrum of H is purely discrete (*i.e.* H is an operator with compact resolvent), all the eigenvalues may be characterized by this variational principle. In any case, the spectral threshold of H always coincides with λ_1:

Corollary I.1. *Under the hypotheses of Theorem I.3,*

$$\inf\sigma(H) = \inf_{\psi\in\mathfrak{D}(H)\setminus\{0\}} \frac{(\psi,H\psi)}{\|\psi\|^2} = \inf_{\psi\in\mathfrak{D}(h)\setminus\{0\}} \frac{h[\psi]}{\|\psi\|^2}\,. \tag{I.11}$$

Theorem I.3 is an extremely useful tool in practical problems in quantum mechanics, (*e.g.*, for computation of eigenvalues of many-body Hamiltonians in quantum chemistry). In these lectures, however, we shall mainly use the variational method to obtain qualitative properties of the spectrum of Schrödinger operators.

Theorem I.3 can be also used to compare the spectra of different operators.

Definition I.1 (Operator inequality)**.** If H_-, H_+ are two self-adjoint operators on $\mathcal{H}$ that are bounded from below, and h_-, h_+ are the associated sesquilinear forms, we write $H_-\leq H_+$ if

1. $\mathfrak{D}(h_-) \supset \mathfrak{D}(h_+)$,
2. $\forall \psi \in \mathfrak{D}(h_+), \quad h_-[\psi] \leq h_+[\psi]$.

We say that the inequality $H_- \leq H_+$ holds *in the sense of quadratic forms.*

Let us write $\lambda_n(H)$ if we want to point out the dependence of the numbers (I.10) on the operator H.

Corollary I.2. *If H_-, H_+ are two self-adjoint operators on $\mathcal{H}$ that are bounded from below and $H_- \leq H_+$, then, for all $n \in \mathbb{N}^*$,*

$$\lambda_n(H_-) \leq \lambda_n(H_+)\,.$$

The KLMN theorem

Finally, let us state a useful criterion for the stability of closedness of a symmetric sesquilinear form (*cf* [16, Sec. VI.1.6]).

Definition I.2 (Relative boundedness of forms)**.** Let h be symmetric and bounded from below in $\mathcal{H}$. A symmetric form h' (which need not be bounded from below) is said to be *relatively bounded* with respect to h if

1. $\mathfrak{D}(h') \supset \mathfrak{D}(h)$,
2. $\forall \psi \in \mathfrak{D}(h), \quad \big|h'[\psi]\big| \;\leq\; a\,h[\psi] + b\,\|\psi\|^2$,

where a, b are non-negative constants. Then we write $h' \prec h$. If the constant a can be chosen less then 1, we write $h' \prec\!\prec h$.

Theorem I.4. *Let h be symmetric and bounded from below in $\mathcal{H}$, and let h' be symmetric and satisfying $h' \prec\!\prec h$. Then $h + h'$ is symmetric and bounded from below. $h + h'$ is closed if, and only if, h is closed.*

Combining this result with the representation theorem, we get the following criterion (an analogue of the Kato-Rellich theorem for forms, called Kato-Lions-Lax-Milgram-Nelson theorem in [24, Thm. X.17]).

Corollary I.3 (KLMN theorem)**.** *Let H be self-adjoint and bounded from below in $\mathcal{H}$, and let h be the associated sesquilinear form. Let h' be a symmetric sesquilinear form satisfying $h' \prec\!\prec h$. Then there exists a unique self-adjoint and bounded from below operator T, associated with the closed symmetric sesquilinear form*

$$t := h + h'\,, \qquad \mathfrak{D}(t) := \mathfrak{D}(h)\,.$$

In particular, if h' is the sesquilinear form associated with a symmetric operator H', the operator T may be regarded as the sum of H and H' in a generalized sense, and we may express this by writing

$$T = H \dot{+} H'\,.$$

In general, $H \dot{+} H' \supset H + H'$, where the latter is the ordinary (operator) sum (*i.e.*, $\mathfrak{D}(H + H') := \mathfrak{D}(H) \cap \mathfrak{D}(H')$).

If h, h' are the sesquilinear form associated with self-adjoint operators H', H and $h' \prec h$, H' is said to be *relatively form-bounded* with respect to H. We write $H' \prec H$ (respectively, $H' \prec\!\prec H$) if $h' \prec h$ (respectively, $h' \prec\!\prec h$).

I.3 The Hamiltonian of a free particle

In this section we are concerned with the self-adjoint operator generated by the Laplacian $-\Delta$ in $\mathbb{R}^d$. Our approach is not the most direct one, but it will enable us to acquire some general techniques in the study of Schrödinger operators.

I.3.1 Definition

It is not at all obvious that the differential expression $-\Delta$ defines a self-adjoint operator H_0 in $\mathcal{H} := L^2(\mathbb{R}^d)$. A function ψ must be rather smooth and sufficiently fast decaying at infinity if $\Delta\psi \in L^2(\mathbb{R}^d)$ is to be meaningful. However, such a restrictive domain may be too small to ensure the self-adjointness, *cf* (I.9). A convenient way how to deal with the problem is the method of sesquilinear forms as described in Section I.2.2.

We begin with the *minimal operator* $\dot{H}_0$ defined by

$$\mathfrak{D}(\dot{H}_0) := C_0^\infty(\mathbb{R}^d)\,, \qquad \dot{H}_0\psi := -\Delta\psi\,.$$

$\dot{H}_0$ is a densely defined linear operator in $L^2(\mathbb{R}^d)$. By an integration by parts, one can easily check the identity (I.7), hence $\dot{H}_0$ is symmetric. Moreover, $\dot{H}_0$ is non-negative because $(\psi, \dot{H}_0\psi) = \|\nabla\psi\|^2 \geq 0$ for all $\psi \in \mathfrak{D}(\dot{H})$.

We define H_0 to be the (self-adjoint) Friedrichs extension of $\dot{H}_0$. That is, H_0 is the operator associated with the closure h_0 of the quadratic form $\dot{h}_0$ defined by

$$\mathfrak{D}(\dot{h}_0) := C_0^\infty(\mathbb{R}^d)\,, \qquad \dot{h}_0[\psi] := (\psi, -\Delta\psi) = \|\nabla\psi\|^2\,.$$

However, from the theory of Sobolev spaces [3], we know the closure explicitly:

$$\mathfrak{D}(h_0) = W_0^{1,2}(\mathbb{R}^d) = W^{1,2}(\mathbb{R}^d)\,, \qquad h_0[\psi] = \|\nabla\psi\|^2\,, \tag{I.12}$$

where ∇ should be interpreted as the distributional gradient.

By the representation theorem, it follows that

$$\mathfrak{D}(H_0) = \left\{\psi \in W^{1,2}(\mathbb{R}^d) \,\middle|\, \exists\eta \in L^2(\mathbb{R}^d),\ \forall\phi \in C_0^\infty(\mathbb{R}^d),\ (\nabla\phi, \nabla\psi) = (\phi, \eta)\right\}\,,$$
$$H_0\psi = \eta\,.$$

Noticing that the identity $(\nabla\phi, \nabla\psi) = (\phi, \eta)$ with $\phi \in C_0^\infty(\mathbb{R}^d)$ is just the definition of the distributional Laplacian $\eta = -\Delta\psi$, we are allowed to write

$$\mathfrak{D}(H_0) = \left\{\psi \in W^{1,2}(\mathbb{R}^d) \,\middle|\, \Delta\psi \in L^2(\mathbb{R}^d)\right\}\,, \qquad H_0\psi = -\Delta\psi\,.$$

Now, we clearly have $W^{2,2}(\mathbb{R}^d) \subset \mathfrak{D}(H_0)$. The opposite inclusion follows by standard elliptic regularity theory [13]. Indeed, the generalized solution $\psi \in W^{1,2}(\mathbb{R}^d)$ to the problem $-\Delta\psi = \eta \in L^2(\mathbb{R}^d)$ is known to belong to $W^{2,2}(\mathbb{R}^d)$. We therefore conclude with

$$\mathfrak{D}(H_0) = W^{2,2}(\mathbb{R}^d)\,, \qquad H_0\psi = -\Delta\psi\,.$$

More generally, it turns out that Sobolev spaces are in a sense optimal when dealing with self-adjoint extensions of symmetric Schrödinger operators.

Remark I.1. By using the Fourier transform [16, Sec. V.5.2], it is possible to show that $\dot{H}_0$ is essentially self-adjoint. Hence, using the uniqueness of self-adjoint extension of an essentially self-adjoint operator [29, Thm. 8.7], we know that the closure of $\dot{H}_0$ coincides with the Friedrichs extension H_0.

I.3.2 Spectrum

Let us consider the eigenvalue problem $H_0\psi = \lambda\psi$. This is equivalent to looking for strong solutions $\psi \in W^{2,2}(\mathbb{R}^d)$ of the Helmholtz equation

$$-\Delta\psi = \lambda\psi \quad \text{in} \quad \mathbb{R}^d\,. \tag{I.13}$$

It follows that we are actually dealing with a classical problem, since any such solution belongs to $C^\infty(\mathbb{R}^d)$ due to standard elliptic regularity theory.

The classical solutions of (I.13) are clearly given by (superpositions of) exponentials

$$e^{ik\cdot x} \quad \text{with} \quad k \in \mathbb{C}^d \quad \text{such that} \quad k^2 := k\cdot k = \lambda\,. \tag{I.14}$$

This suggests that $\sigma(H_0) = \mathbb{C}$, in contradiction with the self-adjointness of H_0. However, (I.14) are not eigenfunctions of H_0 because they even do not belong to $L^2(\mathbb{R}^d)$.

The key observation is that the classical solutions are *bounded* for $k \in \mathbb{R}^d$ (plane waves) and that for such k's $\sigma(H_0) = [0,\infty)$. On the basis of these plane-wave solutions, one can construct the singular sequence of Weyl's theorem (Theorem I.2) and show in this way that the spectrum of H_0 is indeed given by the non-negative semi-axis.

Theorem I.5. $\sigma(H_0) = \sigma_{\text{ess}}(H_0) = [0,\infty)$.

Proof. We divide the proof into three steps.

1. $\sigma(H_0) \subset [0,\infty)$ First of all, notice that H_0 is a non-negative operator because $(\psi, H_0\psi) = \|\nabla\psi\|^2 \geq 0$ for every $\psi \in \mathfrak{D}(H_0)$. It follows from the minimax principle (Corollary I.1) that $\sigma(H_0) \subset [0,\infty)$.

2. $\sigma(H_0) \supset [0,\infty)$ To prove the opposite inclusion, we use Weyl's theorem (Theorem I.2). For any $n \in \mathbb{N}^*$ and $k \in \mathbb{R}^d$, define

$$\psi_n(x) := \varphi_n(x)\, e^{ik\cdot x}\,, \tag{I.15}$$

where $\varphi_n(x) := n^{-d/2}\varphi_1(n^{-1}x)$ and φ_1 is a non-trivial function from $C_0^\infty(\mathbb{R}^d)$, normalized to 1 in $L^2(\mathbb{R}^d)$, *i.e.* $\|\varphi_1\| = 1$. The prefactor of φ_1 is chosen in such a way that also each φ_n is normalized to 1 in $L^2(\mathbb{R}^d)$. In fact, we have

$$\|\varphi_n\| = 1\,, \qquad \|\nabla\varphi_n\| = \frac{\|\nabla\varphi_1\|}{n}\,, \qquad \|\Delta\varphi_n\| = \frac{\|\Delta\varphi_1\|}{n^2}\,. \tag{I.16}$$

We check the hypotheses of Theorem I.2. It is clear that each ψ_n belongs to $\mathfrak{D}(H_0) \supset C_0^\infty(\mathbb{R}^d)$ and that $\|\psi_n\| = 1$. A direct computation yields

$$\begin{aligned} \left|-\Delta\psi_n - k^2\psi_n\right|^2 &= |\Delta\varphi_n|^2 + 4\,|k\cdot\nabla\varphi_n|^2 \\ &\leq |\Delta\varphi_n|^2 + 4\,k^2|\nabla\varphi_n|^2\,. \end{aligned}$$

Using (I.16), we therefore have

$$\left\|-\Delta\psi_n - k^2\psi_n\right\|^2 \leq \|\Delta\varphi_n\|^2 + 4\,k^2\|\nabla\varphi_n\|^2 \xrightarrow[n\to\infty]{} 0\,.$$

Applying Theorem I.2, we conclude that $[0,\infty) \subset \sigma(H_0)$.

3. $\sigma(H_0) = \sigma_{\text{ess}}(H_0)$ Summing up, we have proved $\sigma(H_0) = [0,\infty)$. It is clear that the spectrum is purely essential because (non-degenerate) intervals have no isolated points. □

Hence the spectrum of H_0 is purely essential (*i.e.* there is no discrete component). Furthermore, it follows from the considerations before Theorem I.5 that the point spectrum is empty (there are no embedded eigenvalues).

Remark I.2. It follows from the spectral resolution of H_0 using the Fourier transform (*cf* Remark I.1) that the spectrum of H_0 is in fact purely absolutely continuous (see also Corollary IV.1).

Problem I.1. (It follows from Theorems I.5 and I.2 that the functions (I.15) form a singular sequence, although the item 3 of Theorem I.2 was not established explicitly in the proof of Theorem I.5.) Show "by hand" that the sequence (I.15) is weakly convergent to zero.
Solution: For any $\phi \in C_0^\infty(\mathbb{R}^d)$, we have

$$|(\phi, \psi_n)| \leq n^{-d/2} \, \|\phi\|_{L^1(\mathbb{R}^d)} \, \|\varphi_1\|_{L^\infty(\mathbb{R}^d)} \xrightarrow[n\to\infty]{} 0 \,.$$

Since $C_0^\infty(\mathbb{R}^d)$ is a dense subset of $L^2(\mathbb{R}^d)$, the result extends to all $\phi \in L^2(\mathbb{R}^d)$.

I.4 Definition of Schrödinger operators

In this section we give a meaning to a large class of Schrödinger operators $-\Delta + V$, defined as relatively bounded form perturbation of the free-particle Hamiltonian H_0. Recall that the sum of H_0 with *any* symmetric operator V is well defined through the generalized (form) sum $H_0 \dot{+} V$ whenever $V \prec\!\prec H_0$ (*cf* Definition I.1).

In particular, we show that the Hamiltonian of the hydrogen-type atom, *i.e.* an electron bound to a nucleus of charge $Z \in \mathbb{N}^*$ (putting the physical constants $\hbar$, $2m$ and e equal to one),

$$H_0 + V_Z \,, \qquad \text{where} \qquad V_Z(x) := -\frac{Z}{|x|} \,, \tag{I.17}$$

is well defined, *i.e.* self-adjoint and bounded from below. The latter implies that the system is stable. Indeed, recall that the classical counterpart is unbounded from below and therefore a loss of energy caused by an external perturbation (in this case by emission of electromagnetic radiation) induces transitions to configurations of lower and lower energy and eventually a collapse of the system.

Historically, the stability of the Coulomb problem is probably the most important success of quantum mechanics. However, we would like to stress that this is not a peculiar case: quantum stability is shared by a large class of Hamiltonians, which would otherwise be unbounded from below in the classical case. In fact, it is venerable physical folklore that potentials of the form $V(x) \sim -|x|^{-\alpha}$ produce reasonable quantum mechanics as long as $\alpha < 2$. A mathematical reason for the critical value of the exponent being just 2 is the Hardy inequality we explain now.

I.4.1 The Hardy inequality

The *classical Hardy inequality*, published by Godfrey Harold Hardy in 1920 [15], is the following one-dimensional integral inequality.

Lemma I.1 (Classical 1D Hardy inequality)**.**

$$\forall \psi \in W_0^{1,2}((0,\infty)) \,, \qquad \int_0^\infty |\psi'(x)|^2 \, dx \geq \frac{1}{4} \int_0^\infty \frac{|\psi(x)|^2}{x^2} \, dx \,.$$

Proof. It is enough to prove the inequality for ψ from $C_0^\infty((0,\infty))$, a dense subspace of $W_0^{1,2}((0,\infty))$. Then we have

$$\begin{aligned}\int_0^\infty \frac{|\psi(x)|^2}{x^2}\,dx &= -\int_0^\infty \frac{d}{dx}\left(\frac{1}{x}\right)|\psi(x)|^2\,dx \\ &= \int_0^\infty \frac{1}{x}\,2\,\Re\left\{\overline{\psi(x)}\,\psi'(x)\right\}\,dx \\ &\leq 2\sqrt{\int_0^\infty \frac{|\psi(x)|^2}{x^2}\,dx}\sqrt{\int_0^\infty |\psi'(x)|^2\,dx}\,,\end{aligned}$$

where the second equality follows by an integration by parts and the inequality is due to Schwarz inequality. This is a square-root version of the desired inequality. □

Problem I.2. Show that the Hardy inequality is never achieved (by a non-trivial function).
Solution: For any $\psi \in C_0^\infty((0,\infty))$, it is easy to check that

$$I[\psi] := \int_0^\infty \left(|\psi'(x)|^2 - \frac{1}{4}\frac{|\psi(x)|^2}{x^2}\right)dx = \int_0^\infty \left|\frac{d}{dx}\left(\frac{\psi(x)}{\sqrt{x}}\right)\right|^2 x\,dx \geq 0\,; \tag{I.18}$$

by density the identity extends to all $\psi \in W_0^{1,2}((0,\infty))$ (and represents therefore an alternative proof of Lemma I.1). Assume that there exists $\psi \in W_0^{1,2}((0,\infty))$ such that the Hardy inequality turns into equality, *i.e.*, $I[\psi] = 0$. It follows from the identity (I.18) that $\psi(x) = C\sqrt{x}$ for a.e. $x \in (0,\infty)$, which is an admissible function only if $C = 0$.

Problem I.3. Show that the Hardy inequality is optimal.
Solution: Motivated by the result of the previous problem, we try to construct an optimizing sequence by approximating the function $x \mapsto \sqrt{x}$. For every positive ε, let us define

$$\psi_\epsilon(x) := \sqrt{\varepsilon}\,x^{(\frac{1}{2}+\epsilon)\,\mathrm{sgn}(1-x)}\,.$$

It is easy to check that $\psi_\epsilon \in W_0^{1,2}((0,\infty))$ for every positive ε and that $I[\psi_\varepsilon] \to 0$ as $\varepsilon \to 0$.

An immediate consequence of the one-dimensional Hardy inequality is the following three- and higher-dimensional integral inequality.

Theorem I.6 (Classical Hardy inequality)**.** *Let $d \geq 3$.*

$$\forall \psi \in W^{1,2}(\mathbb{R}^d)\,, \qquad \int_{\mathbb{R}^d} |\nabla\psi(x)|^2\,dx \geq \frac{(d-2)^2}{4}\int_{\mathbb{R}^d}\frac{|\psi(x)|^2}{|x|^2}\,dx\,.$$

Proof. Again, by a density argument, it is enough to prove the inequality for $\psi \in C_0^\infty(\mathbb{R}^d)$. Passing to spherical coordinates $(r,\theta) \in \mathbb{R}_+ \times S^{d-1}$ and neglecting the angular-derivative term, we get the bound

$$\begin{aligned}\int_{\mathbb{R}^d} |\nabla\psi(x)|^2\,dx &= \int_{\mathbb{R}_+\times S^{d-1}} \left(|\partial_r\tilde{\psi}(r,\theta)|^2 + \frac{|\nabla_\theta\tilde{\psi}(r,\theta)|^2}{r^2}\right) r^{d-1}\,dr\,d\theta \\ &\geq \int_{\mathbb{R}_+\times S^{d-1}} |\partial_r\tilde{\psi}(r,\theta)|^2\;r^{d-1}\,dr\,d\theta =: I[\tilde{\psi}]\,,\end{aligned}$$

where $\tilde{\psi}$ is the function ψ expressed in the spherical coordinates. Making the change of trial function

$$\phi(r,\theta) := \sqrt{r^{d-1}}\,\tilde{\psi}(r,\theta)$$

and integrating by parts, we arrive at the identity

$$I[\tilde{\psi}] = \int_{\mathbb{R}_+ \times S^{d-1}} \left\{ |\partial_r \phi(r,\theta)|^2 + \left[\frac{(d-1)^2}{4} - \frac{d-1}{2} \right] \frac{|\phi(r,\theta)|^2}{r^2} \right\} dr\, d\theta \,.$$

For every $\theta \in S^{d-1}$, the function $r \mapsto \phi(r,\theta)$ belongs to $W_0^{1,2}(\mathbb{R}_+)$. Consequently, applying Lemma I.1 with help of Fubini's theorem, we finally get

$$I[\tilde{\psi}] \geq \left[\frac{1}{4} + \frac{(d-1)^2}{4} - \frac{d-1}{2} \right] \int_{\mathbb{R}_+ \times S^{d-1}} \frac{|\phi(r,\theta)|^2}{r^2} \, dr\, d\theta \,,$$

which coincides with the desired inequality after coming back to Cartesian coordinates. □

Remark I.3 (Low dimensions)**.** It is clear that the proof does not extend to $d = 1, 2$. In one dimension, the "spherical" coordinates are trivial, there is no Jacobian leading to vanishing of ϕ at the origin. In two dimensions, $\phi(0,\theta) = 0$ for every $\theta \in S^1$, but the derivative of $r \mapsto \phi(r,\theta)$ does not belong to $L^2(\mathbb{R}_+)$. In the forthcoming chapter we shall see that there is in fact no Hardy inequality of this type in $d = 1, 2$.

The most important application of the Hardy inequality is as a technical tool in more advanced theoretical studies of elliptic partial differential operators. Here we would like to point out its usefulness in the proof of well-posedness of a large class of Schrödinger operators. Indeed, the following result is a direct consequence of Theorem I.6 and Corollary I.3.

Corollary I.4. *Let $d \geq 3$. Let $V : \mathbb{R}^d \to \mathbb{R}$ be a measurable function satisfying*

$$\forall x \in \mathbb{R}^d, \qquad |V(x)| < \frac{(d-2)^2}{4|x|^2} \,.$$

Then the sesquilinear form v defined on $L^2(\mathbb{R}^d)$ by

$$\begin{aligned} \mathfrak{D}(v) &:= \left\{ \psi \in L^2(\mathbb{R}^d) \;\middle|\; \int_{\mathbb{R}^d} V(x)\, |\psi(x)|^2 \, dx < \infty \right\} \,, \\ v(\phi,\psi) &:= \int_{\mathbb{R}^d} V(x)\, \overline{\phi(x)}\, \psi(x) \, dx \,, \end{aligned} \tag{I.19}$$

*satisfies $v \prec\!\prec h_0$ (*cf *Definition* (I.2)*). Consequently, the form*

$$h := h_0 + v \,, \qquad \mathfrak{D}(h) := \mathfrak{D}(h_0) \,,$$

is closed and gives rise to a self-adjoint and bounded from below operator H on $L^2(\mathbb{R}^d)$.

In this way, we give a meaning to the sum "$H_0 + V$".

I.4.2 The stability of matter

Corollary I.4 is obviously not enough to give a meaning to the Coulomb Hamiltonian (I.17), since the decay of V_Z at infinity is slower than that of the Hardy potential. However, this asymptotic behaviour of V_Z can be easily controlled by the term multiplying b in Definition I.2, as we show now.

Let v_Z be the sesquilinear form generated by V_Z in $L^2(\mathbb{R}^3)$, defined in the same way as (I.19). v_Z is clearly symmetric and bounded from above (*i.e.*, $-v_Z$ is bounded from below), since it is in fact non-positive.

It can be shown that v_Z is closed and that it is associated to the maximal operator of multiplication by the function V_Z on $L^2(\mathbb{R}^3)$ (*cf* [16, Sec. VI, Exs. 1.5, 1.15, 1.25, 2.14]), but we will not need these facts.

For any $\psi \in \mathfrak{D}(v_Z)$, we have

$$v_Z[\psi] = \lim_{n\to\infty} v_Z^n[\psi]\,, \qquad \text{where} \qquad v_Z^n[\psi] := -\int_{\mathbb{R}^3} \min\left\{n, \frac{Z}{|x|}\right\} |\psi(x)|^2\, dx\,.$$

However, given any $\varepsilon \in (0,1)$, for any $\psi \in W^{1,2}(\mathbb{R}^3) = \mathfrak{D}(h_0)$ and sufficiently large n, we can write

$$\begin{aligned}
\left|v_Z^n[\psi]\right| &= \int_{B_\varepsilon(0)} \min\left\{n, \frac{Z}{|x|}\right\} |\psi(x)|^2\, dx + \int_{\mathbb{R}^3\setminus B_\varepsilon(0)} \frac{Z}{|x|}\, |\psi(x)|^2\, dx \\
&\leq \int_{B_\varepsilon(0)} \min\left\{n, \frac{Z\varepsilon}{|x|^2}\right\} |\psi(x)|^2\, dx + \frac{Z}{\varepsilon} \int_{\mathbb{R}^3\setminus B_\varepsilon(0)} |\psi(x)|^2\, dx \\
&\leq 4Z\varepsilon\, h_0[\psi] + \frac{Z}{\varepsilon}\, \|\psi\|^2\,.
\end{aligned}$$

Here we have employed the Hardy inequality of Theorem I.6 in the second inequality. It follows that $\mathfrak{D}(v_Z) \supset \mathfrak{D}(h_0)$. Moreover, if $\varepsilon < (4Z)^{-1}$, it is clear that $v_Z \prec\!\prec h_0$ (*cf* Definition I.2).

Consequently, the form

$$h_Z := h_0 + v_Z\,, \qquad \mathfrak{D}(h) := \mathfrak{D}(h_0)\,,$$

is closed and gives rise to a self-adjoint and bounded from below operator H_Z on $L^2(\mathbb{R}^d)$.

In other words, we introduced H_Z as the generalized (form) sum $H_Z = H_0 \dot{+} V_Z$, where V_Z is the (self-adjoint) maximal operator of multiplication by the function V_Z.

We interpret H_Z as the Hamiltonian of the Coulomb system. The latter is stable in the sense that (the ground state energy) $\inf(H_Z) > -\infty$.

Remark I.4 (Uncertainty principle)**.** Probably the deepest reason behind the stability of atoms in quantum mechanics is the non-commutative feature of the theory. It is reflected in the *Heisenberg uncertainty relations* implying an inevitable limitations for the preparation of states with sharper and sharper values of position and momentum. From this point of view, the Hardy inequality of Theorem I.6 can be interpreted as a sort of the *uncertainty principle.* Indeed, the boundedness from below of H_Z is its consequence and $\inf \sigma(H_Z) > -\infty$ is equivalent to

$$\forall \psi \in W^{1,2}(\mathbb{R}^d)\,, \qquad \int_{\mathbb{R}^3} |\nabla\psi(x)|^2\, dx - \int_{\mathbb{R}^3} \frac{Z}{|x|}\, |\psi(x)|^2\, dx > -\infty\,.$$

The classical counterpart of the energy form is unbounded from below because of the singularity of the potential energy at the nucleus position $x = 0$. However, a quantum electron is not allowed to reach the nucleus, because a strict localization close to the nucleus would make the kinetic energy very large.

Problem I.4. Using the Hardy inequality, find an explicit lower bound to $\inf(H_Z)$.
Solution: The problem is readily reduced to the minimization of the function

$$f(r) := \frac{1}{4r^2} - \frac{Z}{r}$$

over $r \in (0, \infty)$. In this way, we obtain $\inf(H_Z) \geq -Z^2$. (Solving the Coulomb problem explicitly, we would get $\inf(H_Z) = -Z^2/4$.)

Remark I.5. The method of the present section clearly enables one to define Schrödinger operators $H_0 + V$ with potentials $V(x) \sim -|x|^{-\alpha}$ for $\alpha \in [0, 2)$.

Chapter II

Ionization and bound states

In the preceding chapter, we saw that a useful functional inequality, called Hardy inequality (Theorem I.6), holds for the Laplacian (*i.e.* the Hamiltonian of a free particle) in three and higher dimensions. We also argued (Remark I.3), but not proved yet, that such an inequality cannot hold in low dimensions (*i.e.*, $d = 1, 2$). In this chapter, *inter alia*, we give a proof of this fact, revealing in this way an important role of the *dimensionality of the Euclidean space*.

It turns out that the existence/non-existence of Hardy inequality is closely related to spectral properties of the free Hamiltonian under potential perturbations. Namely, it has a direct impact on properties of the *spectral threshold* of the perturbed Hamiltonian.

Local potential perturbations do not change the essential spectrum, but may create discrete eigenvalues below it. Such eigenvalues are known under the term *bound states* in quantum mechanics and correspond to stationary solutions of the Schrödinger equation. In potential theory, the question of existence/absence of the bound states is related to the notion of *criticality/subcriticality* of the free Hamiltonian.

On the other hand, the essential spectrum typically corresponds to *ionization* (or *propagating, scattering*) states in quantum physics. This terminology comes from atomic physics where the energy of the highest possible orbital corresponds to the maximal allowed energy under which the electron is still bound to the nucleus; exceeding this energy, the electron is emitted as a free electron.

The first part of this chapter is devoted to a study of the interplay between the absence/existence of the Hardy inequality for the free Hamiltonian and the existence/absence of the bound states of the Hamiltonian under attractive small perturbations. The second part is concerned with a qualitative study of the essential spectrum and bound states.

*

We have seen that potentials with local singularities are physically relevant, the Coulomb potential (I.17) being the primary example. However, to simplify the presentation and focus on the main features of the relationship between the spectrum and the potential perturbation, if not otherwise stated, from now on we restrict ourselves to *bounded potentials* V. The boundedness assumption is actually not so restrictive, since many of the physically relevant (singular) potentials can be approximated by bounded potentials [16, Sec. VIII.3.2].

*

II.1 Subcriticality and Hardy inequality

We start by introducing the notion of criticality/subcriticality of a general self-adjoint bounded from below operator H in $L^2(\mathbb{R}^d)$. Then we generalize the notion of Hardy inequality, introduced for H_0 in the previous chapter (Section I.4.1), to the general case. Finally, we study the relationship between these two notions and the dimension of the Euclidean space for the free Hamiltonian.

First of all, we introduce some useful terminology for potential perturbations of definite sign.

Definition II.1 (Attractive and repulsive potentials)**.** We say that a potential (*i.e.* multiplication operator) V is *attractive* if it is generated by a measurable function (denoted here by the same symbol) $V : \mathbb{R}^d \to \mathbb{R}$ which is non-trivial (*i.e.* $V \neq 0$ on a subset of $\mathbb{R}^d$ of positive measure) and $V \leq 0$. We say that V is *repulsive* if V is non-trivial and $V \geq 0$.

(Obviously, the Coulomb potential (I.17) is attractive.)

II.1.1 Criticality and subcriticality

Note that for a self-adjoint operator H and a bounded potential W on $L^2(\mathbb{R}^d)$, the sum $H + W$ is well defined already as an operator sum (*i.e.* $H + W$ is a self-adjoint operator on $\mathfrak{D}(H + W) := \mathfrak{D}(H)$). If H is bounded from below and W attractive, it follows that $H+W \leq H$. As a consequence of the minimax principle (Corollary I.1), we therefore have $\inf \sigma(H+W) \leq \inf \sigma(H)$. In general, there is no reason for the inequality being strict.

Definition II.2 (Criticality and subcriticality)**.** Let H be a self-adjoint and bounded from below operator on $L^2(\mathbb{R}^d)$. Let $W \in C_0^\infty(\mathbb{R}^d)$ be attractive. We say that

- H is *critical* if: $(\forall W)\ \forall\varepsilon > 0,\ \inf \sigma(H + \varepsilon W) < \inf \sigma(H)$,
- H is *subcritical* if: $(\forall W)\ \exists\varepsilon_0 > 0,\ \forall\varepsilon \in [0, \varepsilon_0],\ \inf \sigma(H + \varepsilon W) = \inf \sigma(H)$.

It is clear that in both the definitions only small values of ε are decisive. One says that $H + \varepsilon W$ is *weakly coupled* if ε is small. The terminology "coupling" comes from quantum physics where ε has the meaning of a parameter controlling the perturbation (*e.g.*, the strength of electric field).

Finally, let us mention that the subcriticality for Schrödinger operators is relevant only in the situation when the spectral threshold is not an eigenvalue:

Proposition II.1. *Let $H = H_0 + V$, where V is bounded. Then*

$$\inf \sigma(H) \in \sigma_{\mathrm{p}}(H) \quad \Longrightarrow \quad H \textit{ is critical}.$$

Proof. Let us assume that the the lowest point in the spectrum of H is an eigenvalue, *i.e.*,

$$\lambda_1 := \inf \sigma(H) \in \sigma_{\mathrm{p}}(H)\,.$$

Let ψ be an eigenfunction of H corresponding to λ_1, normalized to 1 in $L^2(\mathbb{R}^d)$. Let $W \in C_0^\infty(\mathbb{R}^d)$ be attractive and $\varepsilon > 0$. Choosing ψ as a test function for $H+\varepsilon W$ in the variational characterization (Corollary I.1) of the spectral threshold $\inf\sigma(H+\varepsilon W)$, we get

$$\inf\sigma(H+\varepsilon W)\leq\big(\psi,(H+\varepsilon W)\psi\big)=\lambda_1+(\psi,\varepsilon W\psi)\,.$$

Since ψ satisfies the elliptic equation $-\Delta\psi+V\psi=\lambda_1\psi$ in $\mathbb{R}^d$, by unique continuation property (or Harnack's inequality) ψ cannot vanish on an open subset of $\mathbb{R}^d$. Consequently, $(\psi,\varepsilon W\psi)<0$ and $\inf\sigma(H+\varepsilon W)<\lambda_1$. That is, H is critical. □

II.1.2 The Hardy inequality

Recalling Definition I.1, the classical Hardy inequality (Theorem I.6) can be stated as the following inequality for the free Hamiltonian (valid for $d\geq 3$)

$$H_0\geq\frac{(d-2)^2}{4}\,\frac{1}{\delta^2}\,, \tag{II.1}$$

where $\delta(x):=|x|$ is the distance to the origin of $\mathbb{R}^d$ and the right hand side should be interpreted as the operator associated with a form defined as (I.19) (in fact, it coincides with the maximal operator of multiplication by the corresponding function in $L^2(\mathbb{R}^d)$). By Theorem I.5, we know that $\sigma(H_0)=\sigma_{\mathrm{ess}}(H_0)=[0,\infty)$. Hence, although the existence of Hardy inequality for H_0 does not make the operator (strictly) positive, it can be interpreted as some sort of repulsive interaction "sitting at the ground-state energy" $\inf\sigma(H_0)=0$.

Definition II.3 (Hardy inequality)**.** Let H be a self-adjoint and bounded from below operator on $L^2(\mathbb{R}^d)$. We say that there *exists a Hardy inequality* for H if there exists a non-trivial measurable function $\rho:\mathbb{R}^d\to[0,\infty)$ such that

$$H-\inf\sigma(H)\geq\rho \tag{II.2}$$

in the sense of quadratic forms (*cf* Defintion I.1).

It is clear that there can be no $c>0$ such that $\rho(x)\geq c$ for a.e. $x\in\mathbb{R}^d$. (The function ρ is typically vanishing at infinity.)

It turns out that there is always a Hardy inequality for H if it is subcritical.

Proposition II.2. *Let H be a self-adjoint and bounded from below operator on $L^2(\mathbb{R}^d)$. Then*

$$H \text{ is subcritical} \quad\Longrightarrow\quad \exists \text{ Hardy inequality for } H.$$

Proof. Let $W\in C_0^\infty(\mathbb{R}^d)$ be attractive (*i.e.*, $W\leq 0$ and $W\neq 0$). The subcriticality of H together with the minimax principle (Corollary I.1) implies that there exists $\varepsilon_0>0$ such that

$$\inf\sigma(H)=\inf_{\psi\in\mathfrak{D}(h)\setminus\{0\}}\frac{h[\psi]+\varepsilon_0\,(\psi,W\psi)}{\|\psi\|^2}\leq\frac{h[\psi]+\varepsilon_0\,(\psi,W\psi)}{\|\psi\|^2}\,,$$

where the inequality holds for every $\psi\in\mathfrak{D}(h)\setminus\{0\}$. Consequently,

$$H-\inf\sigma(H)\geq-\varepsilon_0\,W\,,$$

where the right hand side represents a non-trivial and non-negative function. □

Problem II.1. Prove the proposition by contraposition.
Solution: Assume that there is no Hardy inequality for H, *i.e.*, for any non-trivial measurable $\rho \geq 0$ either (*cf* Definition I.1)

1. $\mathfrak{D}(h) \not\subset \mathfrak{D}(\rho^{1/2}) := \left\{\psi \in L^2(\mathbb{R}^d) \;\middle|\; \int_{\mathbb{R}^d} \rho(x)\, |\psi(x)|^2\, dx < \infty\right\}$,

or

2. $\exists \psi \in \mathfrak{D}(h), \quad h[\psi] - \inf \sigma(H)\, \|\psi\|^2 < \left\|\rho^{1/2}\psi\right\|^2$,

where h is the sesquilinear form associated with H. We will show that this implies that H is critical. Indeed, for bounded ρ, $\mathfrak{D}(\rho^{1/2}) = L^2(\mathbb{R}^2)$, which excludes the first case. Choosing $\rho := \varepsilon W$ with $W \in C_0^\infty(\mathbb{R}^d)$ and arbitrary $\varepsilon > 0$, the second case yields that H is critical (*cf* Definition II.2).

Finally, as in the case of subcriticality (*cf* Proposition II.1) we mention that $\inf \sigma(H) \notin \sigma_{\mathrm{p}}(H)$ is a necessary condition for the existence of Hardy inequality of a Schrödinger operator H as well.

Theorem II.1. *Let $H = H_0 + V$, where V is bounded. Then*

$$\exists \text{ Hardy inequality for } H \quad \Longrightarrow \quad \inf \sigma(H) \notin \sigma_{\mathrm{p}}(H)\,.$$

Proof. Let $\tilde{\rho} := \min\{\rho, 1\} \leq \rho$. Then the operator $\tilde{H} := H - \tilde{\rho}$ is well defined (self-adjoint and bounded from below on $\mathfrak{D}(\tilde{H}) := \mathfrak{D}(H)$) and (II.2) implies

$$\inf \sigma(\tilde{H}) \geq \inf \sigma(H) =: \lambda_1$$

Assumme, by contradiction, that $\lambda_1 := \inf \sigma(H) \in \sigma_{\mathrm{p}}(H)$. Let ψ be an eigenfunction of H corresponding to λ_1, normalized to 1 in $L^2(\mathbb{R}^d)$. Choosing ψ as a test function for $\tilde{H}$ in the variational characterization of the spectral threshold $\inf \sigma(\tilde{H})$, we can conclude the proof as in the proof of Proposition II.1:

$$\inf \sigma(\tilde{H}) \leq \big(\psi, (H - \tilde{\rho})\psi\big) = \lambda_1 - (\psi, \tilde{\rho}\psi) < \lambda_1\,.$$

Again, it is important that ψ cannot vanish on an open set due to unique continuation property of solutions of elliptic problems. □

II.1.3 The free Hamiltonian

By Theorem I.5, we know that $\sigma(H_0) = \sigma_{\mathrm{ess}}(H_0) = [0, \infty)$. Hence, the question of criticality/subcriticality for the free Hamiltonian H_0 constitutes a non-trivial problem. In other words, H_0 is a non-negative operator and the question is whether a perturbation of H_0 by a small attractive potential W will make $H_0 + W$ negative. It turns out that the answer depends on the dimension of the Euclidean space $\mathbb{R}^d$.

Theorem II.2 (The role of the dimension of $\mathbb{R}^d$)**.**

$$H_0 \text{ is } \begin{cases} \text{critical} & \text{if} \quad d = 1, 2\,, \\ \text{subcritical} & \text{if} \quad d \geq 3\,. \end{cases}$$

Proof. The subcriticality of H_0 for $d \geq 3$ follows from the existence of Hardy inequality (II.1). Indeed, given any $W \in C_0^\infty(\mathbb{R}^d)$,

$$H_0 + \varepsilon W \geq \frac{(d-2)^2}{4} \frac{1}{\delta^2} + \varepsilon W > 0$$

for sufficiently small ε. It remains to show that H_0 is critical for $d = 1, 2$.

Given an attractive potential W as in Definition II.2, we want to show that $H_0 + \varepsilon W$ is negative for arbitrarily small $\varepsilon > 0$. The strategy is to construct a trial function $\psi \in \mathfrak{D}(h_0) = W^{1,2}(\mathbb{R}^d)$ such that

$$h_\varepsilon[\psi] := h_0[\psi] + \varepsilon\,(\psi, W\psi) = \|\nabla\psi\|^2 + \varepsilon\,(\psi, W\psi) < 0\,. \tag{II.3}$$

Then, indeed, $\inf\sigma(H_0 + \varepsilon W) < 0$ due to the minimax principle (Corollary I.1).

Formally, $h_\varepsilon[1] = \varepsilon \int_{\mathbb{R}^d} W(x)\,dx < 0$, because $\nabla 1 = 0$. Hence, the idea is to use a sequence $\{\psi_n\}_{n=1}^{\infty} \subset W^{1,2}(\mathbb{R}^d)$ such that

1. $\forall x \in \mathbb{R}^d, \quad \psi_n(x) \xrightarrow[n\to\infty]{} 1,$
2. $\|\nabla\psi_n\| \xrightarrow[n\to\infty]{} 0.$

Then, for any fixed $\varepsilon > 0$, there obviously exists $n \in \mathbb{N}^*$ such that $h_\varepsilon[\psi_n] < 0$. Such a sequence exists only in low dimensions $d = 1, 2$.

We set

$$\psi_n(x) := \varphi_n(|x|) \qquad \text{with} \qquad \varphi_n(r) := \begin{cases} 1 & \text{if} \quad r < n\,, \\ \dfrac{\log n^2 - \log r}{\log n^2 - \log n} & \text{if} \quad n < r < n^2, \\ 0 & \text{otherwise}\,. \end{cases}$$

It is easy to check that $\psi_n \in W^{1,2}(\mathbb{R}^d)$ for every $n \in \mathbb{N}^*$ and that the items 1 and 2 hold true (the latter only if $d \leq 2$). Consequently, H_0 is critical if $d \leq 2$. □

Remark II.1. For $d = 1$, it is enough to take linear functions instead of the logarithms in the definition of φ_n.

Remark II.2. Note that the second part of the proof establishes a stronger result: $\inf\sigma(H_0 + \varepsilon W) < 0$ for *any attractive* $W \prec\!\prec H_0$.

Recall that, by Proposition II.2, the existence of Hardy inequality for a general operator H in $L^2(\mathbb{R}^d)$ is implied by its subcriticality. It follows from the second part of the proof of Theorem II.2 that the two notions are in fact equivalent for the free Hamiltonian H_0:

$$H_0 \text{ is subcritical} \quad \Longleftrightarrow \quad \exists \text{ Hardy inequality for } H_0.$$

Indeed, assuming the criticality of H_0 and the existence of Hardy inequality for H_0 at the same time, the former implies $d = 1$ or 2 by Theorem II.2, while the latter yields

$$\forall\psi \in W^{1,2}(\mathbb{R}^d), \qquad h[\psi] := \|\nabla\psi\|^2 - (\psi, \rho\psi) \geq 0\,.$$

However, for $d = 1, 2$ the expression $h[\psi_n]$ can be made negative by choosing ψ_n as in the proof of Theorem II.2 (*cf* Remark II.2).

II.1.4 Positive perturbations

Let us study the relationship between the subcriticality and the existence of Hardy inequality for Schrödinger operators arising from *repulsive* perturbations of H_0. Let

$$H := H_0 \dot{+} V \qquad \text{with} \qquad V \prec\prec H_0\,.$$

We assume that V is a non-negative potential such that $\inf \sigma(H) = 0$.

If V is non-trivial, then H satisfies the Hardy inequality $H \geq V$. We say that the Hardy inequality $H \geq V$ is *local* if $V = 0$ on a set of positive measure. On the other hand, if V is almost everywhere positive, then the Hardy inequality is said to be *global*, and this implies that H is subcritical. At the same time, H is subcritical for $d \geq 3$ even if $V = 0$, because $H \geq H_0$ and H_0 satisfies the global Hardy inequality (II.1). The question remains whether a local Hardy inequality $H \geq V$ implies that H is subcritical for $d = 1, 2$. The following result shows that the answer is affirmative if V is positive on an open set, because then the local Hardy inequality implies a global one.

Theorem II.3 (Local HI $\Rightarrow$ global HI)**.** *Let $H := H_0 \dot{+} V$, where $V \prec\prec H_0$ satisfies*

1. $V \geq 0$,

2. $\inf \sigma(H) = 0$,

3. $\exists x_0 \in \mathbb{R}^d, R > 0, V_0 > 0, \forall x \in B_R(x_0),\ V(x) \geq V_0$.

Then a global Hardy inequality holds for H. More precisely, there exists a continuous function $\rho : \mathbb{R}^d \to (0, \infty)$, depending on R, V_0 and x_0, such that $H \geq \rho$. Consequently, H is subcritical.

Proof. We distinguish three situation depending on the dimension.

$\boxed{d \geq 3}$ The theorem clearly holds for $d \geq 3$ (even without the assumption 3) because of (II.1).

$\boxed{d = 1}$ Let $\psi \in C_0^\infty(\mathbb{R})$. Let $\eta : \mathbb{R} \to \mathbb{R}$ be a Lipschitz function defined by

$$\eta(x) := \begin{cases} \dfrac{|x - x_0|}{R} & \text{if} \quad |x - x_0| < R\,, \\ 1 & \text{if} \quad |x - x_0| \geq R\,. \end{cases}$$

Then $\eta\psi \in W_0^{1,2}(\mathbb{R} \setminus \{0\})$. Writing $\psi = \eta\psi + (1 - \eta)\psi$, we obtain the following chain of inequalities:

$$\begin{aligned}
&\int_{\mathbb{R}} \frac{|\psi(x)|^2}{1+(x-x_0)^2}\,dx \\
&\quad \leq 2\int_{\mathbb{R}} \frac{|\eta(x)\psi(x)|^2}{(x-x_0)^2}\,dx + 2\int_{\mathbb{R}} \big|[1-\eta(x)]\psi(x)\big|^2\,dx \\
&\quad \leq 8\int_{\mathbb{R}} \big|(\eta\psi)'(x)\big|^2\,dx + 2\int_{B_R(x_0)} |\psi(x)|^2\,dx \\
&\quad \leq 16\int_{\mathbb{R}} |\psi'(x)|^2\,dx + \big(16\,\|\eta'\|_{L^\infty(\mathbb{R})}+2\big)\int_{B_R(x_0)} |\psi(x)|^2\,dx \\
&\quad \leq 16\int_{\mathbb{R}} |\psi'(x)|^2\,dx + \frac{16\,\|\eta'\|_{L^\infty(\mathbb{R})}+2}{V_0}\int_{B_R(x_0)} V(x)\,|\psi(x)|^2\,dx \\
&\quad \leq \max\left\{16, \frac{16\,\|\eta'\|_{L^\infty(\mathbb{R})}+2}{V_0}\right\}\int_{\mathbb{R}} \Big(|\psi'(x)|^2 + V(x)\,|\psi(x)|^2\Big)\,dx\,.
\end{aligned}$$

Here the second inequality follows by the classical one-dimensional Hardy inequality (Lemma I.1) using the fact that $(\eta\psi)(x_0)=0$, and the last but one employs the hypothesis 3. Since $C_0^\infty(\mathbb{R})$ is a dense subset of $W^{1,2}(\mathbb{R})=\mathfrak{D}(h)$, the last inequality establishes

$$H \geq \frac{c(R,V_0)}{1+(\cdot-x_0)^2} \tag{II.4}$$

with (noticing that $\|\eta'\|_{L^\infty(\mathbb{R})}=1/R$)

$$c(R,V_0) := \min\left\{\frac{1}{16}, \frac{RV_0}{2R+16}\right\}\,. \tag{II.5}$$

$\boxed{d=2}$ We extend the definition of the constant (II.5) for $R=0$ or $V_0=0$ by putting it equal to zero. Then, combining the one-dimensional global Hardy inequality (II.4) with Fubini's theorem, we get, for all $\psi\in C_0^\infty(\mathbb{R}^2)$,

$$h[\psi] \geq \int_{\mathbb{R}}\int_{\mathbb{R}} \left\{|\partial_2\psi(x)|^2 + \frac{c(R_{x^2},V_0)}{1+(x^1-x_0^1)^2}\,\chi_{[x_0^2-R,x_0^2+R]}(x^2)\right\} dx^2\,dx^1\,,$$

where $R_{x^2} := \sqrt{R^2-(x^2-x_0^2)^2}$ is the half of the length of the chord of the disc $B_R(x_0)$ corresponding to the secant line $\mathbb{R}\times\{x^2\}$. Since $R\mapsto c(R,V_0)$ is a non-decreasing function, we may further estimate

$$h[\psi] \geq \int_{\mathbb{R}}\int_{\mathbb{R}} \left\{|\partial_2\psi(x)|^2 + \frac{c(R/2,V_0)}{1+(x^1-x_0^1)^2}\,\chi_{[x_0^2-R/2,x_0^2+R/2]}(x^2)\right\} dx^2\,dx^1\,,$$

so that we get, for each fixed $x^1\in\mathbb{R}$, a characteristic function of x^2 in the integral on the right hand side. Applying once again the one-dimensional global Hardy inequality (II.4), we conclude with

$$H \geq \rho \qquad \text{with} \qquad \rho(x) := \frac{c\left(R/2, \frac{c(R/2,V_0)}{1+(x^1-x_0^1)^2}\right)}{1+(x^2-x_0^2)^2}\,. \tag{II.6}$$

□

Remark II.3 (More about $d = 2$)**.** It follows from the proof of the theorem that the global Hardy weight satisfies

$$\rho(x) \sim \frac{1}{|x|^2} \qquad \text{as} \qquad |x| \to \infty \qquad \text{if} \qquad d \neq 2\,.$$

On the other hand, although the Hardy weight in (II.6) can be replaced by the more symmetric version

$$\max\{\rho(x^1, x^2), \rho(x^2, x^1)\}\,,$$

we only get

$$\rho(x) \sim \frac{1}{(x^1)^2(x^2)^2} \qquad \text{as} \qquad |x| \to \infty \qquad \text{if} \qquad d = 2\,.$$

This does not seem to be optimal. *Open problem:* How to get the quadratic asymptotic behaviour in $d = 2$ as well?

Let us also comment on why the proof used in $d = 1$ cannot be extended to two dimensions. Let $\psi \in C_0^\infty(\mathbb{R}^2)$. Let η be such that $\eta(r) = r$ for $r < R$ and $\eta(r) = 1$ for $r \geq R$. Passing to polar coordinates $(r, \theta) \in \mathbb{R}_+ \times S^1$ centered at the point x_0, the quadratic form associated with the function (without the constant c) on the right hand side of (II.4) can be written as

$$\int_{\mathbb{R}^2} \frac{|\psi(x)|^2}{1 + |x - x_0|^2}\, dx = \int_{\mathbb{R}_+ \times S^1} \frac{|\tilde{\psi}(r,\theta)|^2}{1 + r^2}\, r\, dr\, d\theta\,,$$

where $\tilde{\psi}$ is the function ψ expressed in the polar coordinates. For any fixed $\theta \in S^1$, we abbreviate $f := \psi(\cdot, \theta)$ and write $f = \eta f + (1 - \eta)f$. Then

$$\begin{aligned}\int_0^\infty \frac{|f(r)|^2}{1 + r^2}\, r\, dr &\leq 2 \int_0^\infty \frac{|\eta(r) f(r)|^2}{r^2}\, r\, dr + 2 \int_0^\infty \big|[1 - \eta(r)] f(r)\big|^2\, r\, dr \\ &\leq 2 \int_0^\infty \frac{\big|r^{1/2}\eta(r) f(r)\big|^2}{r^2}\, dr + 2 \int_0^R |f(r)|^2\, r\, dr\,.\end{aligned}$$

Using the fact that $(\eta f)(0) = 0$, we can apply the classical one-dimensional Hardy inequality (Lemma I.1) to the first term on the right hand side:

$$\begin{aligned}\int_0^\infty \frac{\big|r^{1/2}\eta(r) f(r)\big|^2}{r^2}\, dr &\leq 4 \int_0^\infty \left| \frac{d}{dr}\big[r^{1/2}\eta(r) f(r)\big] \right|^2 dr \\ &= 4 \int_0^\infty \left| \frac{d}{dr}\big[\eta(r) f(r)\big] \right|^2 r\, dr + \int_0^\infty \frac{\big|r^{1/2}\eta(r) f(r)\big|^2}{r^2}\, dr\,.\end{aligned}$$

Here the equality follows by an integration by parts. But this is not good! (This inequality does not give anything.)

The problem is essentially the following one. How to show that

$$\forall f \in W_0^{1,2}(\mathbb{R}_+), \qquad \int_0^\infty \left[|f'(r)|^2 - \frac{|f(r)|^2}{4r^2} + V_0 \chi_{[0,R]}(r) |f(r)|^2 - \frac{\epsilon}{1 + r^2} |f(r)|^2 \right] dr \geq 0$$

for sufficiently small ϵ*?*

II.2 Qualitative analysis

Let $H := H_0 \dot{+} V$ with a relatively form-bounded potential V, *i.e.* $V \prec\prec H_0$. In low dimensions, *i.e.* $d = 1, 2$, we know that H_0 is critical (Theorem II.2). Recalling that $\sigma(H_0) = [0, \infty)$ (Theorem I.5), it follows that (*cf* Remark II.2)

$$\lambda_1 := \inf \sigma(H) < \inf \sigma(H_0) = 0 \qquad \text{whenever } V \text{ is attractive.}$$

Furthermore, if V is such that $\sigma_{\text{ess}}(H) \subset [0, \infty)$, then $\lambda_1 \in \sigma_{\text{disc}}(H)$ and the corresponding eigenfunction ψ is called a *ground state* of H in quantum physics. More generally, we say that H possesses a *bound state* if $\sigma_{\text{disc}}(H) \neq \varnothing$. Recall that eigenfunctions of H correspond to stationary solutions of the Schrödinger equation generated by H.

The goal of this section is twofold. Firstly, we establish a sufficient condition about the potential V which guarantees that the essential spectra of H and H_0 coincide. Secondly, we use variational methods to state some basic qualitative properties about eigenvalues below the essential spectrum. We begin with introducing an extremely powerful technique in the study of Schrödinger operators.

II.2.1 Dirichlet and Neumann bracketings

The method of Dirichlet-Neumann bracketing is explained in [25, Sec. XIII.15].

Let Σ be a closed subset of $\mathbb{R}^d$ of measure zero. Let H^D and H^N be the self-adjoint operators on $L^2(\mathbb{R}^d \setminus \Sigma)$ associated respectively with the quadratic forms h^D and h^N which both act as

$$\psi \mapsto \int_{\mathbb{R}^d\setminus\Sigma} |\nabla\psi(x)|^2\, dx + \int_{\mathbb{R}^d\setminus\Sigma} V(x)\, |\psi(x)|^2\, dx \tag{II.7}$$

but differ by their domains

$$\mathfrak{D}(h^D) := W_0^{1,2}(\mathbb{R}^d \setminus \Sigma)\,, \qquad \mathfrak{D}(h^N) := W^{1,2}(\mathbb{R}^d \setminus \Sigma)\,.$$

Note that for $V = 0$ the forms are closed by definition of Sobolev spaces, while for arbitrary $V \prec\prec H_0$ the closedness follow by the fact that $|\Sigma| = 0$.

Clearly,

$$\mathfrak{D}(h^D) \subset \mathfrak{D}(h) \subset \mathfrak{D}(h^N)\,,$$

where h is the form associated with H, and the identification

$$L^2(\mathbb{R}^d \setminus \Sigma) \simeq L^2(\mathbb{R}^d)\,,$$

by setting any $\psi \in L^2(\mathbb{R}^d \setminus \Sigma)$ equal to zero on Σ, is adopted. Moreover, since the measure of Σ is zero, h^D and h^N act as h, *i.e.*,

$$\forall \psi \in \mathfrak{D}(h^D), \qquad h^D[\psi] = h[\psi] = h^N[\psi]\,.$$

Consequently,

$$H^N \le H \le H^D\,, \tag{II.8}$$

and the same inequalities hold for the "eigenvalues" defined by the minimax principle (*cf* Corollary I.2).

H^D is called the operator H *with additional Dirichlet condition imposed on* Σ. Similarly, H^N is called the operator H *with additional Neumann condition imposed on* Σ. The reason for this terminology being that, if Σ is a smooth hypersurface, the functions ψ from $\mathfrak{D}(H^D)$ (respectively, from $\mathfrak{D}(H^N)$) satisfy $\psi = 0$ on Σ (respectively, $\partial\psi/\partial n = 0$ on Σ, where n is a normal vector to Σ). Then (II.8) can be interpreted as that adding the Dirichlet condition raise energies, and adding the Neumann condition lower energies.

Assume now that Σ divides $\mathbb{R}^d$ into two disjoint open subsets Ω_1, Ω_2 in the following sense:

1. $\Omega_1 \cap \Omega_2 = \varnothing$,
2. $\overline{\Omega_1 \cup \Omega_2} = \mathbb{R}^d$,
3. $\left|\mathbb{R}^d \setminus (\Omega_1 \cup \Omega_2)\right| = 0$.

Then the Hilbert space admits a direct sum decomposition

$$L^2(\mathbb{R}^d) = L^2(\Omega_1) \oplus L^2(\Omega_2)\,.$$

Let h_i^D and h_i^N be the quadratic forms on $L^2(\Omega_i)$ which both act as (II.7), with the range of integration being replaced by Ω_i, and have domains

$$\mathfrak{D}(h_i^D) := W_0^{1,2}(\Omega_i)\,, \qquad \mathfrak{D}(h_i^N) := W^{1,2}(\Omega_i)\,.$$

The forms h_i^D are closed because $V \prec\prec H_0$ immediately yields that the form v_i on $L^2(\Omega_i)$ defined by

$$\mathfrak{D}(v_i) := \left\{ \psi \in L^2(\Omega) \;\middle|\; \int_{\Omega_i} V(x)\,|\psi(x)|^2\,dx < \infty \right\}\,,$$
$$v_i[\psi] := \int_{\Omega_i} V(x)\,|\psi(x)|^2\,dx\,,$$

is relatively bounded with respect to the form $h_{0,i}^D$ defined by

$$\mathfrak{D}(h_{0,i}^D) := W_0^{1,2}(\Omega_i)\,, \qquad h_{0,i}^D[\psi] := \int_{\Omega_i} |\nabla\psi(x)|^2\,dx\,.$$

To see it, one only needs to notice that any $\psi \in W_0^{1,2}(\Omega_i)$ extended to $\mathbb{R}^d$ by setting it equal to zero outside Ω_i belongs to $W^{1,2}(\mathbb{R}^d)$. Hence the operator H_i^D associated with h_i^D is self-adjoint and bounded from below and we can write

$$H^D = H_1^D \oplus H_2^D\,.$$

On the other hand, it is not clear that h_i^N are closed. It will be the case if $v_i \prec\prec h_{0,i}^N$, where $h_{0,i}^N$ is defined by

$$\mathfrak{D}(h_{0,i}^N) := W^{1,2}(\Omega_i)\,, \qquad h_{0,i}^N[\psi] := \int_{\Omega_i} |\nabla\psi(x)|^2\,dx\,.$$

Under this assumption, the operator H_i^N associated with h_i^N is self-adjoint and bounded from below and we can also write

$$H^N = H_1^N \oplus H_2^N\,.$$

Finally, let us mention that the advantage of an operator H admitting the direct sum decomposition

$$H = H_1 \oplus H_2$$

consists in that the (separate components of the) spectrum satisfies the simple relations (*cf* [10, Sec. IX.5])

$$\begin{aligned} \sigma(H) &= \sigma(H_1) \cup \sigma(H_2)\,, \\ \sigma_{\mathrm{p}}(H) &= \sigma_{\mathrm{p}}(H_1) \cup \sigma_{\mathrm{p}}(H_2)\,, \\ \sigma_{\mathrm{ess}}(H) &= \sigma_{\mathrm{ess}}(H_1) \cup \sigma_{\mathrm{ess}}(H_2)\,. \end{aligned} \tag{II.9}$$

Problem II.2. Such an identity is not available for the discrete spectra in general. Find a counterexample.
Solution: For instance, $\sigma(H_1) = \{-1\} \cup [0,\infty)$, $\sigma(H_2) = (-\infty, 0]$. Then $\sigma(H) = \sigma_{\mathrm{ess}}(H) = \mathbb{R}$, *i.e.* $\sigma_{\mathrm{disc}}(H) = \varnothing$, but $\sigma_{\mathrm{disc}}(H_1) \cup \sigma_{\mathrm{disc}}(H_2) = \{-1\}$.

II.2.2 Stability of the essential spectrum

It is a common knowledge that the essential spectrum is stable under *local* perturbations. For Schrödinger operators it means that the essential spectrum of $H_0 + V$ is determined by the asymptotic behaviour of the potential V at the space infinity only. This principle is justified as follows.

For simplicity, let us assume that the potential is bounded, *i.e.*, $V \in L^\infty(\mathbb{R}^d)$.

Definition II.4 (Potentials vanishing at infinity)**.** We say that a bounded potential V *vanishes at infinity* if

$$\lim_{R\to\infty} \|V\|_{L^\infty(\mathbb{R}^d\setminus B_R(0))} = 0\,.$$

In symbols we write $V \overset{\infty}{\longrightarrow} 0$.

Theorem II.4 (Stability of $\sigma_{\rm ess}$ under asymptotically vanishing perturbation)**.** *Let $H := H_0 + V$, where V is bounded. If $V \overset{\infty}{\longrightarrow} 0$, then*

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

Proof. The proof is divided into two parts.

1. $\sigma_{\rm ess}(H) \subset [0,\infty)$ Let $R > 0$ and abbreviate $B_R := B_R(0)$. We impose an additional Neumann condition (in the sense of Section II.2.1) on the sphere ∂B_R. Then

$$H \geq H^N := H^N_{\rm int} \oplus H^N_{\rm ext}\,,$$

where $H^N_{\rm int}$ is the operator on $L^2(B_R)$ associated with the quadratic form

$$\mathfrak{D}(h^N_{\rm int}) := W^{1,2}(B_R)\,, \qquad h^N_{\rm int}[\psi] := \int_{B_R} |\nabla\psi(x)|^2\,dx + \int_{B_R} V(x)\,|\psi(x)|^2\,dx\,,$$

and $H^N_{\rm ext}$ is the operator defined analogously on $L^2(\mathbb{R}^d\setminus B_R)$. It follows from (II.9) and the minimax principle (Theorem I.3) that

$$\inf \sigma_{\rm ess}(H) \geq \min\big\{\inf\sigma_{\rm ess}(H_{\rm int}), \inf\sigma_{\rm ess}(H_{\rm ext})\big\}\,.$$

However, since the embedding $W^{1,2}(B_R) \hookrightarrow L^2(B_R)$ is compact, the essential spectrum of $H_{\rm int}$ is empty and we have

$$\inf\sigma_{\rm ess}(H) \geq \inf\sigma_{\rm ess}(H_{\rm ext})\,.$$

For every $\psi \in W^{1,2}(\mathbb{R}^d \setminus B_R)$, we have

$$h^N_{\rm ext}[\psi] \geq \int_{\mathbb{R}^d\setminus B_R} V(x)\,|\psi(x)|^2\,dx \geq -\|V\|_{L^\infty(\mathbb{R}\setminus B_R)}\|\psi\|^2_{L^2(\mathbb{R}\setminus B_R)}\,.$$

Consequently,

$$\inf\sigma_{\rm ess}(H) \geq \inf\sigma_{\rm ess}(H_{\rm ext}) \geq \inf\sigma(H_{\rm ext}) \geq -\|V\|_{L^\infty(\mathbb{R}\setminus B_R)}\,.$$

Since R can be made arbitrarily large and and the right hand side tends to zero as $R \to \infty$ by assumption, while H is independent of R, it follows that $\inf\sigma_{\rm ess}(H) \geq 0$.

2. $\sigma_{\mathrm{ess}}(H) \supset [0,\infty)$ The proof of this inclusion is very similar to the second part of the proof of Theorem I.5. The only modification is that the the singular sequence has to be chosen "localized at infinity", to make the contribution of V negligible. That is, for any $n \in \mathbb{N}^*$ and $k \in \mathbb{R}^d$, we again define

$$\psi_n(x) := \varphi_n(x)\, e^{ik\cdot x}\,,$$

but now $\varphi_n(x) := n^{-d/2}\varphi_1(n^{-1}x - n)$ and φ_1 is a non-trivial function from $C_0^\infty(\mathbb{R}_+^d)$, normalized to 1 in $L^2(\mathbb{R}^d)$. The localization at infinity is reflected in that

$$\operatorname{supp}\varphi_n \subset (n,\infty)^d\,.$$

Now the desired inclusion follows by Weyl's criterion (Theorem I.2). Indeed, it is again easy to verify that $\psi_n \in \mathfrak{D}(H) = W^{2,2}(\mathbb{R}^d)$ and $\|\psi_n\| = \|\varphi_n\| = \|\varphi_1\| = 1$. Writing

$$\big\|-\Delta\psi_n + V\psi_n - k^2\psi_n\big\| \le \big\|-\Delta\psi_n - k^2\psi_n\big\| + \|V\|_{L^\infty(\operatorname{supp}\varphi_n)}\|\varphi_n\|$$

and recalling that the first two terms on the right hand side tend to zero as $n \to \infty$ by properties (I.16) of φ_n, it remains to realize that the last term vanishes by the hypothesis about V. □

Remark II.4. It follows from the (suitably modified) second part of the proof that the inclusion $[0,\infty) \subset \sigma_{\mathrm{ess}}(H)$ is implied by merely assuming that there exists a sequence of balls $B_n := B_{R_n}(a_n) \subset \mathbb{R}^d$ (with centres $a_n \in \mathbb{R}^d$ and radii $R_n \in \mathbb{R}_+$) such that

$$\lim_{n\to\infty} |B_n| = \infty \qquad \text{and} \qquad \lim_{n\to\infty} \|V\|_{L^\infty(B_n)} = 0\,.$$

This also explains why this conditions is not enough to guarantee the other inclusion, *i.e.* $\inf\sigma_{\mathrm{ess}}(H) \ge 0$. (Indeed, for V such that $V = -1$ on $\mathbb{R}_- \times \mathbb{R}^{d-1}$ and zero elsewhere, $\sigma(H) = [-1,\infty)$.)

II.2.3 Basic properties of the discrete spectrum

In the preceding subsection, we have seen that the essential spectrum of $H_0 + V$ is stable under bounded potential perturbations V that vanish at infinity. That is, the latter guarantees that $\sigma_{\mathrm{ess}}(H_0 + V) = [0,\infty)$. From this perspective, the non-negative spectrum is easily determined. What can we say in general about the negative part of the spectrum, namely about the possibly existing discrete eigenvalues?

First of all, we discuss the very question of existence. Recall that for $d = 1, 2$ the negative bound states always exist if the potential V is (vanishing at infinity and) attractive. This follows from the criticality of H_0 in the low dimensions (Theorem II.2, *cf* also Remark II.2). The proof of the respective part of Theorem II.2 can be easily modified to include sign-changing perturbations.

Theorem II.5 (Existence of bound states in low dimensions)**.** *Let* $d = 1$ *or* 2. *Let* $H := H_0 + V$ *where* $V \in L^\infty(\mathbb{R}^d) \cap L^1(\mathbb{R}^d)$. *Then*

$$\langle V\rangle := \int_{\mathbb{R}^d} V(x)\, dx < 0 \qquad \Longrightarrow \qquad \inf\sigma(H) < 0\,.$$

Proof. Taking the sequence $\{\psi_n\}_{n\in\mathbb{N}^*}$ from the proof of Theorem II.2 as a test function for the form h associated with H, we readily gets

$$h[\psi_n] = \|\nabla\psi_n\|^2 + (\psi_n, V\psi_n) \xrightarrow[n\to\infty]{} \langle V\rangle \,,$$

where the right hand side is negative by assumption. Hence, $h[\psi_n]$ can be made negative by taking n sufficiently large, and a usage of the minimax principle (Corollary I.1) concludes the proof. □

The theorem says that it is enough that the potential V is "attractive in the mean" to generate a negative spectrum. Consequently, H possesses a bound state, *i.e.* $\sigma_{\mathrm{disc}}(H) \neq \varnothing$, if in addition $V \overset{\infty}{\longrightarrow} 0$. The critical case $\langle V\rangle = 0$ will be considered in the following chapter.

In three and higher dimensions, on the other hand, one cannot make the kinetic energy represented by $\|\nabla\psi\|^2$ negligible; there is in fact a substantial interplay between the kinetic and potential energies. Indeed, it follows from the subcriticality of H_0 (Theorem II.2) that there is no negative spectrum if V is small in the supremum norm. On the other hand, it is easily seen that there are always negative bound states if the potential is sufficiently attractive on a measurable set.

Theorem II.6 (Existence of bound states for highly attractive potentials)**.** *Let $H := H_0 + V$ where $V \in L^\infty(\mathbb{R}^d)$. Assume that there exist $x_0 \in \mathbb{R}^d$, $R > 0$ and $V_0 < 0$ such that*

$$\forall x \in B_R(x_0), \qquad V(x) \leq V_0 < 0.$$

Then there exists a dimensional constant $c_d > 0$ such that

$$R^2\,|V_0| > c_d \qquad \Longrightarrow \qquad \inf\sigma(H) < 0\,.$$

Proof. Let ψ be an eigenfunction of the Dirichlet Laplacian in the ball $B_R := B_R(x_0)$ corresponding to its lowest eigenvalue $\mu_1(R)$, *i.e.*,

$$\begin{cases} -\Delta\psi = \mu_1(R)\,\psi & \text{in} \quad B_R(x_0)\,, \\ \quad \psi = 0 & \text{on} \quad \partial B_R(x_0)\,. \end{cases}$$

It is well known that $\mu_1(R) = \mu_1(1)/R^2$, where $\mu_1(1)$ depends exclusively on the dimension d (it is determined as a zero of a Bessel function). Using ψ as a test function for the form h associated with H, we get

$$\begin{aligned} h[\psi] &= \|\nabla\psi\|^2_{L^2(B_R)} + (\psi, V\psi)_{L^2(B_R)} \\ &\leq \|\nabla\psi\|^2_{L^2(B_R)} + V_0\,\|\psi\|^2_{L^2(B_R)} \\ &= \left(\frac{\mu_1(1)}{R^2} + V_0\right)\|\psi\|^2\,. \end{aligned}$$

This proves the sufficient condition for the existence of negative spectrum by virtue of the minimax principle (Corollary I.1). □

The theorem says that, regardless of the dimension, a negative spectrum is always generated by potentials V which are either "sufficiently negative" on an open subset of $\mathbb{R}^d$ or the negativeness is "well spread" across $\mathbb{R}^d$. Again, it follows that H possesses a bound state, *i.e.* $\sigma_{\mathrm{disc}}(H) \neq \varnothing$, if in addition $V \overset{\infty}{\longrightarrow} 0$.

The proofs of the two theorems above show that the variational argument of test functions is a powerful technique for the study of bound states. In addition to the existence, a good choice of test function can even provide optimal quantitative estimates of eigenvalues. The variational methods are also of highly important in numerical computations.

Summing up, we have seen that the spectrum of a Schrödinger operator $H_0 + V$ with the potential V vanishing at infinity typically consists of a non-negative essential spectrum and negative eigenvalues:

$$\{\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_N\} \cup [0, \infty) \tag{II.10}$$

Here the natural number N can be either finite or equal to $+\infty$.

This is a characteristic spectrum of atomic Hamiltonians as well, where the discrete eigenvalues correspond to *bound-state energies* of electron orbits and the zero represents the *ionization energy* after which the electron is not bound to the nucleus any more (it becomes free).

It is customary in spectral theory to arrange the eigenvalues in a non-decreasing order and to repeat them according to their multiplicities (*cf* Theorem I.3). That is why the inequalities in (II.10) are not strict in general, since the eigenvalues can be degenerate. However, it is a general fact that the first eigenvalue is always simple.

Theorem II.7 (Uniqueness and positivity of the ground state)**.** *Let* $H := H_0+V$ *where* $V \in L^\infty(\mathbb{R}^d)$*. Assume that* $\lambda_1 := \inf \sigma(H)$ *is a discrete eigenvalue. Then the eigenvalue is simple and the corresponding eigenfunction is nowhere zero (it can be chosen to be positive).*

Proof. We adapt the proof of [13, Thm. 8.38]. If ψ is an eigenfunction of H corresponding to λ_1, then it follows from the Rayleigh-Ritz formula (Corollary I.1)

$$\lambda_1 = \frac{\|\nabla\psi\|^2 + (\psi, V\psi)}{\|\psi\|^2}$$

that $|\psi| \geq 0$ is one also. But then, by the unique continuation principle (or Harnack's inequality), we must have $|\psi| > 0$ a.e. in $\mathbb{R}^d$. Hence, using the polar decomposition $\psi = |\psi| e^{i \arg \psi}$, ψ cannot be equal to zero on a measurable subset of $\mathbb{R}^d$ (and $|\psi|$ represents a positive eigenfunction corresponding to λ_1). This argument also shows that it is impossible that two eigenfunctions corresponding to λ_1 are orthogonal. Indeed, if ϕ is another eigenfunction of H corresponding to λ_1, then $(\phi, \psi) = \int |\phi||\psi| e^{i \arg(\psi - \phi)} \neq 0$. Consequently, the corresponding eigenspace must be one-dimensional and λ_1 simple. □

Chapter III

Weak and strong couplings

In the preceding chapter, we saw that the spectrum of a Schrödinger operator $H_0 + V$ (with the potential V vanishing at infinity) typically consists of a (non-negative) essential spectrum and of some eigenvalues (called bound states) below it (*cf* (II.10)). Variational methods are particularly useful to find sufficient conditions which guarantee the existence of bound states and to derive their basic properties.

To say more about the bound states, however, more precise methods have to be used. In this chapter we use perturbation methods to analyse two asymptotic regimes: *weak coupling* when V is small in the supremum norm and *strong coupling* when V is on the contrary large in the supremum norm.

In the end of this chapter, we discuss interesting spectral bounds, called *Lieb-Thirring inequalities*, which are uniform and optimal in the strong-coupling regime.

III.1 Leitmotif: quantum square well

To illustrate the characteristic behaviour of the spectrum of Schrödinger operators in the weak and strong couplings, we first analyse the quantum-mechanical text-book example of the square-well potential.

III.1.1 The model

In the Hilbert space $L^2(\mathbb{R}^d)$, consider the Schrödinger operator

$$H_\varepsilon := H_0 + \varepsilon V \,, \tag{III.1}$$

where $\varepsilon \geq 0$ is a (not necessarily small!) parameter and the potential is assumed to have the piece-wise constant form

$$V(x) := \begin{cases} -1 & \text{if} \quad |x| < R \,, \\ 0 & \text{if} \quad |x| \geq R \,, \end{cases} \tag{III.2}$$

where R is a given positive number (radius of the well).

III.1.2 The essential spectrum

Since V is compactly supported, it is obviously vanishing at infinity and, by Theorem II.4, we have

$$\sigma_{\text{ess}}(H_\varepsilon) = [0, \infty)$$

for every $\varepsilon \geq 0$.

III.1.3 The discrete spectrum

By virtue of the trivial bounds

$$H_0 - \varepsilon \leq H_\varepsilon \leq H_0 \,,$$

it follows that the possible discrete eigenvalues are squeezed between $-\varepsilon$ and 0, *i.e.*,

$$\sigma_{\text{disc}}(H_\varepsilon) \subset (-\varepsilon, 0) \,.$$

To see it, it is enough to realize that $\sigma(H - \varepsilon) = [-\varepsilon, \infty)$ for every $\varepsilon \geq 0$, which gives the inclusion with a semi-closed interval. Indeed, 0 cannot be a discrete(!) eigenvalue by definition. At the same time, $-\varepsilon$ is excluded by the following argument. Let us assume, by contradiction, that $-\varepsilon$ is an eigenvalue and let ψ be the corresponding eigenfunction. Then the identity $h_\varepsilon[\psi] = -\varepsilon\|\psi\|^2$, where h_ε is the form associated with H_ε, can be rewritten as follows

$$\|\nabla\psi\|^2 + \varepsilon \, \|\psi\|^2_{L^2(\mathbb{R}^d \setminus B_R)} = 0 \,,$$

where $B_R := B_R(0)$. Consequently, ψ is constant almost everywhere in $\mathbb{R}^d$, which contradicts $\psi \in L^2(\mathbb{R}^d)$, unless ψ is trivial.

III.1.4 Dirichlet-Neumann bracketing

Let us now demonstrate the powerfulness of the Dirichlet-Neumann bracketing (*cf* Section II.2.1) on this model. Let H_ε^D and H_ε^N denote the operator H_ε, subject to the additional Dirichlet and Neumann condition on the sphere ∂B_R, respectively. We have

$$H^N_{\varepsilon,\text{int}} \oplus H^N_{\text{ext}} \leq H^N_\varepsilon \leq H_\varepsilon \leq H^D_\varepsilon \leq H^D_{\varepsilon,\text{int}} \oplus H^D_{\text{ext}} \,.$$

Here $H^N_{\varepsilon,\text{int}}$ and $H^D_{\varepsilon,\text{int}}$ are the operators on $L^2(B_R)$ associated with the quadratic form

$$\psi \mapsto \int_{B_R} |\nabla\psi(x)|^2 \, dx - \varepsilon \int_{B_R} |\psi(x)|^2 \, dx \,,$$

with domain $W^{1,2}(B_R)$ and $W^{1,2}_0(B_R)$, respectively, and H^N_{ext} and H^D_{ext} are the operators on $L^2(\mathbb{R}^d \setminus B_R)$ associated with the quadratic form

$$\psi \mapsto \int_{\mathbb{R}^d \setminus B_R} |\nabla\psi(x)|^2 \, dx \,,$$

with domain $W^{1,2}(\mathbb{R}^d \setminus B_R)$ and $W^{1,2}_0(\mathbb{R}^d \setminus B_R)$, respectively.

It is easy to see that

$$\sigma(H^\iota_{\text{ext}}) = \sigma_{\text{ess}}(H^\iota_{\text{ext}}) = [0, \infty) \,, \qquad \sigma(H^\iota_{\varepsilon,\text{int}}) = \sigma_{\text{disc}}(H^\iota_{\varepsilon,\text{int}}) =: \{\lambda^\iota_n(\varepsilon)\}_{n=1}^\infty \,,$$

with $\iota \in \{N, D\}$, where the eigenvalues $\lambda_n^\iota(\varepsilon)$ are, as usual, sorted in a non-decreasing order and repeated according to their multiplicities. Hence, denoting by $\{\lambda_n(\varepsilon)\}_{n=1}^\infty$ the analogous set of "eigenvalues" of H_ε as defined by the minimax principle (Theorem I.3), we arrive at

$$\min\left\{\lambda_n^N(\varepsilon), 0\right\} \leq \lambda_n(\varepsilon) \leq \min\left\{\lambda_n^D(\varepsilon), 0\right\} . \tag{III.3}$$

This provides quite explicit bounds on the discrete spectrum of H_ε, since $\lambda_n^\iota(\varepsilon)$ are well known eigenvalues of the Laplacian in the ball B_R, subject to Neumann or Dirichlet boundary condition.

For instance, for $d = 1$ we have

$$\lambda_n^N(\varepsilon) = \left(\frac{(n-1)\pi}{2R}\right)^2 - \varepsilon\,, \qquad \lambda_n^D(\varepsilon) = \left(\frac{n\pi}{2R}\right)^2 - \varepsilon\,.$$

III.1.5 The number of bound states

The method of Dirichlet-Neumann bracketing can be also used to estimate the *number of negative eigenvalues* of H_ε. Let us define

$$N_\varepsilon := \max_n\{\lambda_n(\varepsilon) < 0\}\,, \qquad N_\varepsilon^\iota := \max_n\{\lambda_n^\iota(\varepsilon) < 0\}\,.$$

Here we adopt the convention that $N_\varepsilon^D = 0$ if there is no $n \geq 1$ such that $\lambda_n^D(\varepsilon) < 0$, which is always the case if ε is small enough, because $\lambda_1^D(0) > 0$. On the other hand, $N_\varepsilon^N \geq 1$ whenever $\varepsilon > 0$, because $\lambda_1^N(\varepsilon) = -\varepsilon < 0$. As a consequence of (III.3), we get

$$N_\varepsilon^D \leq N_\varepsilon \leq N_\varepsilon^N\,.$$

Since $H_{\varepsilon,\mathrm{int}}^\iota$ are operators with compact resolvents, their eigenvalues $\lambda_n^\iota(\varepsilon)$ accumulate at $+\infty$ for any fixed ε and we have

$$\lim_{\varepsilon\to\infty} N_\varepsilon = +\infty\,.$$

Concerning the opposite limit, using $\lambda_1^D(0) > 0$, $\lambda_2^N(0) > 0$ and $\lambda_1^N(\varepsilon) = 0$, we have

$$\lim_{\varepsilon\to 0} N_\varepsilon \leq 1\,.$$

This is trivially true for $d \geq 3$, where we know that H_ε has no discrete spectrum for sufficiently small ε (hence $\lim_{\varepsilon\to 0} N_\varepsilon = 0$), because H_0 is subcritical (*cf* Theorem II.2). On the other hand, H_0 is critical for $d = 1, 2$ and this together with the asymptotic inequality tells us that H_ε possesses *exactly one* negative eigenvalue for all sufficiently small ε.

III.1.6 One dimension

In general, the eigenvalue problem $H_\varepsilon\psi = \lambda\psi$ can be solved by gluing together the general solutions on B_R and $\mathbb{R}^d \setminus B_R$, where the differential equation admits explicit solution in terms of Bessel functions. Let us demonstrate the procedure for $d = 1$.

Let $\lambda \in (-\varepsilon, 0)$ be an eigenvalue of H_ε. The corresponding eigenfunction $\psi \in \mathfrak{D}(H_\varepsilon) = H^2(\mathbb{R})$ is a solution of the differential equation

$$-\psi'' = \begin{cases} (\lambda+\varepsilon)\psi & \text{if} \quad |x| < R\,, \\ \lambda\psi & \text{if} \quad |x| \geq R\,. \end{cases} \tag{III.4}$$

In view of the mirror symmetry $x \mapsto -x$, the solutions are either even or odd functions; in other words, the eigenfunctions satisfy either Neumann or Dirichlet conditions at the origin, respectively. We are particularly interested in the ground state which, as the eigenfunction of the lowest eigenvalue, must be even due to the Dirichlet-Neumann bracketing. Hence, we consider only even solutions of (III.4) in the sequel, but odd solutions can be determined analogously.

Even solutions of (III.4) are given by

$$\psi(x) = \begin{cases} A\,\cos\left(\sqrt{\lambda+\varepsilon}\,x\right) & \text{if} \quad |x| < R\,, \\ B\,e^{-\sqrt{-\lambda}\,x} & \text{if} \quad |x| \geq R\,, \end{cases}$$

(odd solutions have sinus instead of the cosinus). The eigenvalue $\lambda \in (-\varepsilon, 0)$ and the (complex) constants A and B are determined in such a way that ψ and ψ' are continuous at 0, for any function in $H^2(\mathbb{R}) \hookrightarrow C^1(\mathbb{R})$ must satisfy these conditions, and by the normalization condition $\|\psi\| = 1$. The formers lead to the following implicit equation

$$\sqrt{-\lambda}\,\cos\left(\sqrt{\lambda+\varepsilon}\,x\right) = \sqrt{\lambda+\varepsilon}\,\sin\left(\sqrt{\lambda+\varepsilon}\,x\right).$$

A straightforward analysis of the implicit equation leads to to the following asymptotic formulae for the lowest eigenvalue

$$\lambda_1(\varepsilon) = -\varepsilon^2 R^2 + \mathcal{O}(\varepsilon^3) \qquad = -\varepsilon^2 \frac{\langle V\rangle^2}{4} + \mathcal{O}(\varepsilon^3) \qquad \text{as} \quad \varepsilon \to 0+\,, \tag{III.5}$$

$$\lambda_1(\varepsilon) = -\varepsilon + o(\varepsilon) \qquad = \varepsilon\,\min V + o(\varepsilon) \qquad \text{as} \quad \varepsilon \to +\infty\,. \tag{III.6}$$

The first line represents a weak-coupling expansions for the ground-state energy; it turns out that the expression after the second equality holds for general potentials V. The second line represents a strong-coupling expansions for the ground-state energy; it turns out that the expression after second equality holds for general potentials V and also for all eigenvalues $\lambda_n(\varepsilon)$ (uniformly in n).

III.2 Weak coupling

In this section we give a proof of the second equality in (III.5) for a general potential. First we point out where the difficulty lies.

III.2.1 Perturbations of discrete versus essential spectra

Let $H_\varepsilon := H + \varepsilon V$, where H is a self-adjoint and bounded from below operator (one can think about a Schrödinger operator $H = H_0 + W$ on $L^2(\mathbb{R}^d)$ with $W \prec\prec H_0$), $V \prec\prec H$ and ε is a real parameter. Then H_ε forms a holomorphic family of operators (of type (B), *cf* [16, Sec. VII.4]).

Consequently, by analytic perturbation theory [16, Sec. VII], *isolated eigenvalues of finite multiplicity* behave with respect to ε as in the finite-dimensional case. For instance, if λ is a simple isolated eigenvalue of H and ψ the corresponding eigenfunction, then the eigenvalue $\lambda(\varepsilon)$ of H_ε is analytic in ε near $\varepsilon = 0$ and it satisfies the well known perturbation formula

$$\lambda(\varepsilon) = \lambda + \frac{(\psi, V\psi)}{\|\psi\|^2}\,\varepsilon + \mathcal{O}(\varepsilon^2) \qquad \text{as} \quad \varepsilon \to 0\,. \tag{III.7}$$

This explains the relevance of definition of the discrete spectrum.

However, the situation is very different if λ is a point of the essential spectrum of H. For instance, the square-well Hamiltonian (III.1) clearly forms a holomorphic family of operators (here we have even a bounded perturbation since the potential (III.2) is bounded), but $\lambda = 0$ is not an eigenvalue and the perturbation formula (III.7) does not make any sense. Still, however, the discrete eigenvalue created at the essential spectral threshold possesses a quite nice analytic expansion (III.5) in $\varepsilon > 0$ near $\varepsilon = 0$. How to derive it for a general potential?

III.2.2 Birman-Schwinger principle

A powerful approach to study singular perturbation problems is represented by the so-called *Birman-Schwinger principle*. (For more facts and applications, we refer to [26].)

Let $H := H_0 + V$, where V is bounded. Assume that λ is a *negative* eigenvalue of H with eigenfunction ψ, *i.e.*, $H\psi = \lambda\psi$. We rewrite the eigenvalue equation as follows

$$(H_0 - \lambda)\psi = -V\psi = -V^{1/2}|V|^{1/2}\psi\,,$$

where we have denoted $V^{1/2} := |V|^{1/2}\operatorname{sgn}(V)$. Now, let us *formally* multiply the identity by $V^{-1/2}$ and *formally* decompose $1 = |V|^{-1/2}|V|^{1/2}$, which gives

$$V^{-1/2}(H_0 - \lambda)|V|^{-1/2}|V|^{1/2}\psi = -|V|^{1/2}\psi\,.$$

Introducing $\phi := |V|^{1/2}\psi$ and *formally* inverting the operator on the left hand side, we finally arrive at

$$-\phi = \left[V^{-1/2}(H_0 - \lambda)|V|^{-1/2}\right]^{-1}\phi = |V|^{1/2}(H_0 - \lambda)^{-1}V^{1/2}\phi =: K_\lambda\phi\,.$$

That is, the operator K_λ has eigenvalue -1.

Notice that, while the derivation of the eigenvalue equation for K_λ has been formal, the ultimate equation does not pose any problems, since K_λ is a well defined bounded operator on $L^2(\mathbb{R}^d)$. Indeed, $|V|^{1/2}$ and $V^{1/2}$ are operators of multiplication by bounded functions, and the inverse $(H_0 - \lambda)^{-1}$ exists and is bounded because $\sigma(H_0) = [0, \infty)$. This suggests:

Proposition III.1 (Birman-Schwinger principle). *Let V be bounded and $\lambda < 0$. Then*

$$\lambda \in \sigma_\mathrm{p}(H_0 + V) \qquad \Longleftrightarrow \qquad -1 \in \sigma_\mathrm{p}(K_\lambda)\,,$$

where $K_\lambda := |V|^{1/2}(H_0 - \lambda)^{-1}V^{1/2}$ with $V^{1/2} := |V|^{1/2}\operatorname{sgn}(V)$.

Proof. $\boxed{\Rightarrow}$ If $(H_0+V)\psi=\lambda\psi$, we have $\psi\in W^{2,2}(\mathbb{R}^d)$, so $\phi:=|V|^{1/2}\psi$ is in $L^2(\mathbb{R}^d)$ and

$$K_\lambda\phi\equiv|V|^{1/2}(H_0-\lambda)^{-1}V\psi=-|V|^{1/2}(H_0-\lambda)^{-1}(H_0-\lambda)\psi=-|V|^{1/2}\psi\equiv-\phi\,.$$

$\boxed{\Leftarrow}$ Conversely, if $K_\lambda\phi=-\phi$, then we define $\psi:=-(H_0-\lambda)^{-1}V^{1/2}\phi\in\mathfrak{D}(H)$ and get

$$(H_0-\lambda)\psi=-V^{1/2}\phi=V^{1/2}K_\lambda\phi=V(H_0-\lambda)^{-1}V^{1/2}\phi\equiv-V\psi\,.$$

□

The *free resolvent* $R_z:=(H_0-z)^{-1}$ for $z\in\mathbb{C}\setminus[0,\infty)$ is an integral operator (*i.e.*, $(R_z\psi)(x)=\int_{\mathbb{R}^d}G_z(x,x')\psi(x')dx'$) with explicit kernel (Green's function)

$$G_z(x,x'):=\begin{cases}\dfrac{e^{-\sqrt{-z}\,|x-x'|}}{2\sqrt{-z}} & \text{if}\quad d=1\,,\\[2mm] \dfrac{K_0\big(\sqrt{-z}\,|x-x'|\big)}{2\pi} & \text{if}\quad d=2\,,\\[2mm] \dfrac{e^{-\sqrt{-z}\,|x-x'|}}{4\pi\,|x-x'|} & \text{if}\quad d=3\,,\end{cases}\tag{III.8}$$

where K_0 is Macdonald's function [1, Sec. 9.6.4] (for higher dimensions, the kernel can be expressed in terms of Bessel functions).

Consequently, K_λ for $\lambda<0$ is an integral operator with kernel

$$K_\lambda(x,x')=|V(x)|^{1/2}G_\lambda(x,x')V(x')^{1/2}$$

(with an abuse of notation, we keep the same letter for the kernel of an integral operator). Hence, the idea of the Birman-Schwinger principle is that a partial differential equation is replaced by an integral one. The latter is more suitable for the analysis of the singular limit $\lambda\to0-$.

Let $x\neq x'$. We note that

$$G_\lambda(x,x')\sim\begin{cases}\dfrac{1}{2\sqrt{-\lambda}} & \text{if}\quad d=1\,,\\[2mm] \dfrac{-\log\sqrt{-\lambda}}{2\pi} & \text{if}\quad d=2\,,\end{cases}\qquad\text{as}\quad\lambda\to0-$$

while the limit of $G_\lambda(x,x')$ as $\lambda\to0-$ exists for $d=3$ (and also for higher dimensions). This singularity of the Green function in one and two dimensions is in fact responsible for the criticality of H_0.

III.2.3 Weak-coupling analysis in one dimension

Now we are in a position to justify the weakly coupled asymptotics (III.5) for *any* potential V "attractive in the mean", *i.e.* $\langle V\rangle<0$. For simplicity, we restrict ourselves to the one-dimensional case. The analysis in two dimensions is analogous, one only needs to take into account the different type of singularity of the free resolvent. We follow [27].

Consider the Schrödinger operator $H_\varepsilon:=H_0+\varepsilon V$ on $L^2(\mathbb{R})$, where ε is a small positive parameter and V is bounded (further assumptions about the potential will be imposed later). According to the Birman-Schwinger principle

(Proposition III.1), $\lambda = \lambda(\varepsilon)$ is a *negative* eigenvalue of H_ε if, and only if, -1 is an eigenvalue of the integral operator εK_λ, where

$$K_\lambda(x,x') = |V(x)|^{1/2}\,\frac{e^{-\sqrt{-\lambda}\,|x-x'|}}{2\sqrt{-\lambda}}\,V(x')^{1/2}\,.$$

The key idea is that K_λ has a well behaved limit as $\lambda \to 0-$ except for a divergent rank-one piece. The singularity can be singled out by decomposing the operator K_λ as follows

$$K_\lambda = L_\lambda + M_\lambda\,,$$

where L_λ and M_λ are integral operators with kernels

$$L_\lambda(x,x') := |V(x)|^{1/2}\,\frac{1}{2\sqrt{-\lambda}}\,V(x')^{1/2}\,,$$

$$M_\lambda(x,x') := |V(x)|^{1/2}\,\frac{e^{-\sqrt{-\lambda}\,|x-x'|}-1}{2\sqrt{-\lambda}}\,V(x')^{1/2}\,.$$

The operator M_λ is well behaved in the limit $\lambda \to 0-$. Indeed, it is easy to see that its kernel converges pointwise to the kernel

$$M_0(x,x') := -|V(x)|^{1/2}\,\frac{|x-x'|}{2}\,V(x')^{1/2}$$

as $\lambda \to 0-$. Furthermore, it can be shown that the convergence holds in the operator norm.

Lemma III.1. *Assume* $V \in L^1(\mathbb{R}, (1+x^2)\,dx)$. *Then*

$$\lim_{\lambda\to 0-} \|M_\lambda - M_0\| = 0\,,$$

where $\|\cdot\|$ *denotes the operator norm on* $L^2(\mathbb{R})$.

Proof. We actually prove the convergence in a stronger topology of *Hilbert-Schmidt* operators. We have

$$\begin{aligned}
\|M_0\|_{\mathrm{HS}}^2 &\equiv \int_{\mathbb{R}\times\mathbb{R}} |M_0(x,x')|^2\,dx\,dx' \\
&\le \frac{1}{4}\int_{\mathbb{R}\times\mathbb{R}} |V(x)|(x^2+x'^2)|V(x')|\,dx\,dx' \\
&= \frac{1}{2}\int_{\mathbb{R}} |V(x)|\,x^2\,dx \int_{\mathbb{R}} |V(x')|\,dx' \\
&\le \frac{1}{2}\left(\int_{\mathbb{R}} |V(x)|\,(1+x^2)\,dx\right)^2 .
\end{aligned}$$

Hence, under the stated assumptions, M_0 is a Hilbert-Schmidt operator (therefore bounded because $\|A\| \le \|A\|_{\mathrm{HS}}$ holds for any Hilbert-Schmidt operator as a consequence of the Schwarz inequality). Since $M_\lambda(x,x')$ converges to $M_0(x,x')$ pointwise (*i.e.*, for every $x,x' \in \mathbb{R}$) as $\lambda \to 0-$ and $|M_\lambda(x,x')| \le |M_0(x,x')|$ for every $x,x' \in \mathbb{R}$ and all $\lambda < 0$, the dominated convergence theorem yields

$$\lim_{\lambda\to 0-} \|M_\lambda - M_0\|_{\mathrm{HS}} = 0\,.$$

In particular, M_λ converges to M_0 in the operator norm. ∎

It is clear from the proof of the preceding lemma that $\|M_\lambda\| \leq \|M_0\|_{\mathrm{HS}} < \infty$. Thus $\|\varepsilon M_\lambda\| < 1$ holds for sufficiently small ε; namely for such that

$$\varepsilon \int_{\mathbb{R}} |V(x)|\,(1+x^2)\,dx < \sqrt{2}\,. \tag{III.9}$$

Then $I + \varepsilon M_\lambda$ is invertible and we may write

$$\begin{aligned}(I+\varepsilon K_\lambda)^{-1} &= \Big\{(I+\varepsilon M_\lambda)\left[I+(I+\varepsilon M_\lambda)^{-1}\varepsilon L_\lambda\right]\Big\}^{-1} \\ &= \left[I+(I+\varepsilon M_\lambda)^{-1}\varepsilon L_\lambda\right]^{-1}(I+\varepsilon M_\lambda)^{-1}\,.\end{aligned}$$

It follows that εK_λ has eigenvalue -1 if, and only if, the same is true for the operator

$$P_\lambda^\varepsilon := (I+\varepsilon M_\lambda)^{-1}\varepsilon L_\lambda\,.$$

Since L_λ is a rank-one operator by definition, we can write

$$P_\lambda^\varepsilon = \phi\,(\psi,\cdot)\,,$$

with

$$\psi := \varepsilon\,\frac{1}{2\sqrt{-\lambda}}\,V^{1/2}\,, \qquad \phi := (I+\varepsilon M_\lambda)^{-1}|V|^{1/2}\,.$$

Then it is clear that P_λ^ε has just one eigenvalue, namely (ψ,ϕ). Putting it equal to -1, we get the following condition.

Theorem III.1 (Basic criterion for the existence of bound state)**.** *Assume $V \in L^1(\mathbb{R},(1+x^2)\,dx)$. Let ε be so small that* (III.9) *holds. Let $\lambda < 0$. Then*

$$\lambda \in \sigma_{\mathrm{p}}(H_\varepsilon) \qquad \Longleftrightarrow \qquad \sqrt{-\lambda} = -\frac{\varepsilon}{2}\left(V^{1/2},(I+\varepsilon M_\lambda)^{-1}|V|^{1/2}\right)\,. \tag{III.10}$$

In this way the integral equation $K_\lambda\phi = -\phi$ has been reduced to solving an algebraic equation.

Finally, inserting the identity

$$(I+\varepsilon M_\lambda)^{-1} = I - \varepsilon M_\lambda(I+\varepsilon M_\lambda)^{-1}$$

into the implicit equation in (III.10) and employing (the proof of) Lemma III.1, we get the following sufficient condition for the existence of negative bound state.

Corollary III.1 (Sufficient condition for the existence of bound state)**.** *Assume $V \in L^1(\mathbb{R},(1+x^2)\,dx)$. Let ε be so small that* (III.9) *holds. If $\langle V\rangle < 0$, then H_ε possesses a negative eigenvalue $\lambda = \lambda(\varepsilon)$. The following asymptotic expansion*

$$\sqrt{-\lambda(\varepsilon)} = -\frac{\varepsilon}{2}\,\langle V\rangle + \mathcal{O}(\varepsilon^2) \qquad \text{as} \quad \varepsilon \to 0+ \tag{III.11}$$

holds.

This asymptotic expansion coincides with (III.5) in the special case of square-well potential.

III.2.4 Addenda to Section III.2.3

The analysis of the preceding section is incomplete from several respects.

The essential spectrum

Notice that we did not say a word about the essential spectrum of H_ε. The potential V was not assumed to be vanishing at infinity, so it is not clear that $\inf \sigma_{\text{ess}}(H_\varepsilon) \geq 0$ and that the negative eigenvalue of Corollary III.1 belongs to the discrete spectrum of H_ε. However, this is true under the hypotheses of Theorem III.1 and Corollary III.1.

Proposition III.2 (Stability of σ_{ess} under relatively compact perturbation)**.** *Let $H := H_0 + V$ on $L^2(\mathbb{R})$, where $V \in L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$. Then*

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

Proof. Since V is bounded, we obviously have $z \in \rho(H_0) \cap \rho(H)$ for sufficiently negative $z \in \mathbb{R}$. Then the *second resolvent identity* yields

$$\begin{aligned}
(H - z)^{-1} &- (H_0 - z)^{-1} \\
&= -(H - z)^{-1} V (H_0 - z)^{-1} \\
&= -\underbrace{(H - z)^{-1} V^{1/2}}_{\text{bounded}} \; \underbrace{|V|^{1/2}(H_0 - z)^{-1/2}}_{\text{compact}} \; \underbrace{(H_0 - z)^{-1/2}}_{\text{bounded}} .
\end{aligned}$$

To see that $A := |V|^{1/2}(H_0 - z)^{-1/2}$ is compact, it is enough to notice that

$$AA^* = |V|^{1/2}(H_0 - z)^{-1}|V|^{1/2}$$

is compact, since it is in fact Hilbert-Schmidt if $V \in L^1(\mathbb{R})$ (*cf* the proof of Lemma III.1). Hence, the resolvent difference is a compact operator and it follows (from *Weyl's theorem* [25, Thm. XIII.14], different from Theorem I.2!) that H and H_0 have the same essential spectrum. □

Problem III.1. Find an example of $V \in L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$ that does not vanish at infinity.
Solution. For instance,

$$V(x) := \sum_{n=1}^{\infty} \chi_{[n-n^{-2}, n+n^{-2}]}(x) .$$

The uniqueness of the bound state

It is not clear from Corollary III.1 that there are no additional negative eigenvalues (in addition to λ) provided that ε is small enough. However, this is true under the stated assumptions about V.

Indeed, it is obvious for compactly supported potentials, since then

$$H_\varepsilon \geq H_0 + \varepsilon V_0 \qquad \text{with} \qquad V_0(x) := (\operatorname{ess\,inf} V)\; \chi_{[\inf \operatorname{supp} V, \sup \operatorname{supp} V]}(x) .$$

(Note that necessarily $\operatorname{ess\,inf} V < 0$ because $\langle V \rangle < 0$.) Hence, the number of negative eigenvalues of H_ε is bounded from above by the number of negative eigenvalues of the square-well Hamiltonian $H_0 + \varepsilon V_0$. However, from the analysis in Section III.1.5, we know that the latter tends to 1 as $\varepsilon \to 0+$.

For a general $V \in L^1(\mathbb{R}, (1 + x^2)\, dx)$, the uniqueness of $\lambda(\varepsilon)$ for sufficiently small ε can be established by a careful analysis of the implicit equation in (III.10), *cf* [27].

On the other hand, if an attractive V is vanishing very slowly at infinity, H_ε can have an infinite number of negative eigenvalues for arbitrarily small positive ε.

The sufficient and necessary condition for the bound state

Using the uniqueness of the bound state corresponding to the expansion (III.11), it is easy to see that the discrete spectrum of H_ε is empty if $\langle V\rangle > 0$ and $\varepsilon > 0$ is sufficiently small. It remains to analyse the critical situation $\langle V\rangle = 0$.

Employing Theorem III.1, it is not difficult to compute the next term in the asymptotic expansion of the bound state:

$$\sqrt{-\lambda(\varepsilon)} = -\frac{\varepsilon}{2}\,\langle V\rangle - \frac{\varepsilon^2}{4}\int_{\mathbb{R}\times\mathbb{R}} V(x)|x-x'|V(x')\,dx\,dx' + \mathcal{O}(\varepsilon^3)\,. \qquad \text{(III.12)}$$

as $\varepsilon \to 0+$. If $\langle V\rangle = 0$, the leading-order term vanishes and one has to check the sign of the quadratic term. It turns out that it is positive whenever $\langle V\rangle = 0$ and $V \neq 0$. Indeed,

$$\begin{aligned}
-\int_{\mathbb{R}\times\mathbb{R}} V(x)|x-x'|V(x')\,dx\,dx' &= \lim_{\epsilon\to 0}\int_{\mathbb{R}\times\mathbb{R}} V(x)\,\frac{e^{-\epsilon|x-x'|}-1}{2\epsilon}\,V(x')\,dx\,dx' \\
&= \lim_{\epsilon\to 0} 2\int_{\mathbb{R}\times\mathbb{R}} V(x)\,\frac{e^{-\epsilon|x-x'|}}{2\epsilon}\,V(x')\,dx\,dx' \\
&\equiv \lim_{\epsilon\to 0} 2\,\big(V, G_{-\epsilon^2} * V\big) \\
&= \lim_{\epsilon\to 0} 2\,\big(\widehat{V}, \widehat{G_{-\epsilon^2} * V}\big) \\
&= \lim_{\epsilon\to 0} 2\,\big(\widehat{V}, \widehat{G_{-\epsilon^2}}\widehat{V}\big) \\
&= \lim_{\epsilon\to 0} 2\int_{\mathbb{R}} \frac{|\widehat{V}(k)|^2}{k^2+\epsilon^2}\,dk \\
&= 2\int_{\mathbb{R}} \frac{|\widehat{V}(k)|^2}{k^2}\,dk > 0\,.
\end{aligned}$$

Summing up, we have:

Theorem III.2 (Weakly coupled ground state)**.** *Let* $V \in L^1(\mathbb{R},(1+x^2)\,dx)$ *and* $V \neq 0$*. Then* H_ε *has an eigenvalue* $\lambda(\varepsilon) < 0$ *for all small* $\varepsilon > 0$ *if, and only if,* $\langle V\rangle \leq 0$*. In such a case, the eigenvalue is is unique, simple and obeys* (III.12).

Of course, this does not prevent H_ε from possessing negative eigenvalues for some large ε even if $\langle V\rangle \geq 0$. Actually, as we shall se in the following section, the number of negative eigenvalues of H_ε overpasses any given number as $\varepsilon \to \infty$ provided that V is negative on a measurable set.

Two dimensions

In two dimensions, under suitable assumption about the decay of V at infinity, $\langle V\rangle \leq 0$ is again a sufficient and necessary condition for the existence of a negative eigenvalue $\lambda(\varepsilon)$ of H_ε for all small $\varepsilon > 0$, and the eigenvalue is again simple and unique if ε is sufficiently small. The main difference with respect to the one-dimensional case is that the weakly coupled bound state is *much weaklier coupled*, in the sense that the eigenvalue has an exponential decay as $\varepsilon \to 0+$. Indeed, the eigenvalue can be expressed as

$$\lambda(\varepsilon) = -e^{2w(\varepsilon)^{-1}}\,,$$

where $w(\varepsilon)$ has the following asymptotic expansion

$$w(\varepsilon) = \frac{\varepsilon}{2\pi}\,\langle V\rangle + \left(\frac{\varepsilon}{2\pi}\right)^2 \int_{\mathbb{R}^2\times\mathbb{R}^2} V(x)\left(\gamma_{\mathrm{E}} + \log\frac{|x-x'|}{2}\right) V(x')\,dx\,dx' + \mathcal{O}(\varepsilon^3)$$

as $\varepsilon \to 0+$. Here γ_{E} denotes Euler's constant.

III.3 Strong coupling

In this section $H_\varepsilon := H_0 + \varepsilon V$ on $L^2(\mathbb{R}^d)$, where V is bounded and $\varepsilon > 0$. The potential V may be non-vanishing at infinity. We are interested in the behaviour of the spectrum of H_ε in the limit when $\varepsilon \to +\infty$. We follow [11, App. A].

III.3.1 The result

For every non-negative ε, we consider the non-decreasing sequence of numbers $\{\lambda_n(\varepsilon)\}_{n=1}^\infty$ as defined for H_ε by the minimax principle (Theorem I.3).

Theorem III.3 (Strong-coupling asymptotics)**.** *Let $H_\varepsilon := H_0 + \varepsilon V$, where V is bounded. Then*

$$\forall n \in \mathbb{N}^*, \qquad \lim_{\varepsilon\to+\infty} \frac{\lambda_n(\varepsilon)}{\varepsilon} = V_{\min} := \operatorname{ess\,inf} V\,.$$

In other words, for every $n \in \mathbb{N}^*$, we have the asymptotic expansion

$$\lambda_n(\varepsilon) = \varepsilon V_{\min} + o(\varepsilon) \qquad \text{as} \quad \varepsilon \to +\infty\,. \tag{III.13}$$

In particular, if V is vanishing at infinity, $\sigma_{\mathrm{ess}}(H_\varepsilon) = [0,\infty)$ and the numbers $\lambda_n(\varepsilon) < 0$ (if any) represent negative eigenvalues of H_ε. Then the theorem extends the asymptotic formula (III.6) for the strongly coupled negative ground state of the square-well Hamiltonian to general potentials and to *all* negative eigenvalues.

Theorem III.3 is proved in two steps: by establishing a lower bound for $\lambda_n(\varepsilon)$ and then an asymptotic upper bound as $\varepsilon \to +\infty$.

III.3.2 A lower bound

For every $\psi \in \mathfrak{D}(h_\varepsilon) = W^{1,2}(\mathbb{R}^d)$, where h_ε is the form associated with H_ε, we have

$$h_\varepsilon[\psi] \equiv \|\nabla\psi\|^2 + \varepsilon\,(\psi, V\psi) \geq \varepsilon V_{\min}\,\|\psi\|^2\,.$$

Then the minimax principle implies

$$\lambda_n(\varepsilon) \geq \varepsilon V_{\min} \tag{III.14}$$

for every $\varepsilon > 0$ and all $n \in \mathbb{N}^*$. (This also shows that the remainder $o(\varepsilon)$ becomes non-negative as $\varepsilon \to +\infty$.)

III.3.3 Auxiliary results

Before proving an opposite estimate, we need some auxiliary results from elementary spectral theory.

First, we need to recall some basic facts about multiplication operators. To clarify the exposition, in this subsection we consistently distinguish between a multiplication operator and its generating function.

Let $V : \mathbb{R}^d \to \mathbb{R}$ be a measurable function (not necessarily bounded). We denote by $\hat{V}$ the maximal operator of multiplication by V on $L^2(\mathbb{R}^d)$, *i.e.*,

$$\mathfrak{D}(\hat{V}) := \left\{\psi \in L^2(\mathbb{R}^d) \mid V\psi \in L^2(\mathbb{R}^d)\right\}, \qquad \hat{V}\psi := V\psi\,.$$

Since V is real-valued, the operator $\hat{V}$ is self-adjoint (*cf* [29, Sec. 5.1, Ex. 2]). $\hat{V}$ is bounded if, and only if, $V \in L^\infty(\mathbb{R}^d)$. If $V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d)$, then $C_0^\infty(\mathbb{R}^d)$ is a core of $\hat{V}$ (*cf* [29, Sec. 5.1, Ex. 2]).

Every eigenvalue of $\hat{V}$ has infinite multiplicity (*cf* [29, Exe. 5.23]), hence the spectrum of $\hat{V}$ is purely essential. In general, the spectrum of $\hat{V}$ is equal to the essential range of the function V (*cf* [6, Ex. 4.3.7]). Summing up,

$$\sigma(\hat{V}) = \sigma_{\mathrm{ess}}(\hat{V}) = \mathfrak{R}_{\mathrm{ess}}(V) := \left\{\lambda \in \mathbb{R} \,\middle|\, \forall\delta > 0,\ |V^{-1}((\lambda-\delta, \lambda+\delta))| > 0\right\}.$$

In particular, if V is continuous, then $\sigma(\hat{V}) = \overline{\mathfrak{R}(V)}$.

We shall also need the following general characterization of the spectrum of a self-adjoint operator H. It resembles Weyl's criterion (Theorem I.2), except for the fact that the singular sequence of the latter is not required to be orthogonal. This makes Weyl's criterion more suitable for determining the essential spectrum, but less explicit if the essential spectrum is known and one wants to exploit the orthogonality of the singular sequence.

Theorem III.4 (Improved Weyl's criterion)**.** *Let H be a self-adjoint operator on $\mathcal{H}$. A point λ belongs to $\sigma_{\mathrm{ess}}(H)$ if, and only if, there exists a sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset \mathfrak{D}(H)$ such that*

1. $\forall n, m \in \mathbb{N}, \quad (\psi_n, \psi_m) = \delta_{nm}$,
2. $H\psi_n - \lambda\psi_n \xrightarrow[n\to\infty]{} 0$.

Proof. $\boxed{\Leftarrow}$ Every orthonormal sequence weakly converges to zero. This follows from the Bessel inequality

$$\forall\psi \in \mathcal{H}, \qquad \|\psi\|^2 \geq \sum_{n\in\mathbb{N}} |(\psi_n, \psi)|^2\,.$$

Hence, $\{\psi_n\}_{n\in\mathbb{N}}$ is a singular sequence of H and Weyl's criterion yields $\lambda \in \sigma_{\mathrm{ess}}(H)$.

$\boxed{\Rightarrow}$ To prove the converse implication, we mimic the proof of Weyl's criterion based on spectral theorem in [29, proof of Thm. 7.2.4]. There are two alternatives for a point λ to be in the essential spectrum of a self-adjoint H. First, if λ is an eigenvalue of infinite multiplicity, then there exists an orthonormal sequence $\{\psi_n\}_{n\in\mathbb{N}}$ in the kernel of $H - \lambda$; this sequence trivially satisfies item 2. Second, if λ is an accumulation point of of $\sigma(H)$, then there exists a sequence $\{\lambda_n\}_{n\in\mathbb{N}}$ such that, for all $n, m \in \mathbb{N}$,

$$\lambda_n \neq \lambda\,, \qquad \lambda_n = \lambda_m \Rightarrow n = m\,, \qquad \lambda_n \xrightarrow[n\to\infty]{} \lambda\,.$$

Let now choose $\epsilon_n > 0$ so small that the intervals $(\lambda_n - \epsilon_n, \lambda_n + \epsilon_n)$ be mutually disjoint. Since $\lambda_n \in \sigma(H)$, we have

$$E(\lambda_n + \epsilon_n) - E(\lambda_n - \epsilon_n) \neq 0\,,$$

where E is the spectral family of H. Let us choose a normed element

$$\psi_n \in \mathfrak{R}\big(E(\lambda_n + \epsilon_n) - E(\lambda_n - \epsilon_n)\big)\,.$$

Then we obviously have that such a constructed sequence $\{\psi_n\}_{n\in\mathbb{N}}$ is a subset of $\mathfrak{D}(H)$ and satisfy items 1 and 2. □

III.3.4 An upper bound

Now we continue with the proof of Theorem III.3. To obtain an upper bound to $\lambda_n(\varepsilon)$, we construct a suitable "test function" based on the singular sequence of $\hat{V}$ corresponding to $V_{\min}$.

Since $V_{\min} \in \sigma_{\mathrm{ess}}(\hat{V})$, by Theorem III.4, there exists a sequence $\{\psi_i\}_{i\in\mathbb{N}^*} \subset \mathfrak{D}(\hat{V})$ orthonormalized in $L^2(\mathbb{R}^d)$ such that

$$\|V\psi_i - V_{\min}\psi_i\| \xrightarrow[i\to\infty]{} 0\,.$$

Since $C_0^\infty(\mathbb{R}^d)$ is a core of $\hat{V}$ and V is bounded, it follows that there is also a sequence $\{\phi_i\}_{i\in\mathbb{N}^*} \subset C_0^\infty(\mathbb{R}^d)$ satisfying the double limits

$$(\phi_i, \phi_j) - \delta_{ij} \xrightarrow[i,j\to\infty]{} 0\,, \qquad (\phi_i, V\phi_j - V_{\min}\phi_j) \xrightarrow[i,j\to\infty]{} 0\,.$$

For $k, N \in \mathbb{N}^*$, define $N \times N$ symmetric matrices $A_N(k)$ and $B_N(k)$ by

$$A_N(k) := \big\{(\phi_{i+k}, V\phi_{j+k})\big\}_{i,j=1}^N\,, \qquad B_N(k) := \big\{(\phi_{i+k}, \phi_{j+k})\big\}_{i,j=1}^N\,.$$

Given any $N \in \mathbb{N}^*$, choose $k = k(N) \in \mathbb{N}^*$ sufficiently large so that

$$A_N(k(N)) - V_{\min}\, I_N \leq N^{-1}\, I_N\,, \qquad B_N(k(N)) \geq \tfrac{1}{2}\, I_N\,, \tag{III.15}$$

in the sense of matrices, where I_N denotes the $N \times N$ identity matrix.

In view of the second inequality of (III.15), $\mathrm{span}\{\phi_{i+k}\}_{i=1}^N$ is an N-dimensional subspace of $\mathfrak{D}(h_\varepsilon) \supset C_0^\infty(\mathbb{R}^d)$. Thus, the minimax principle (Theorem I.3) yields

$$\forall n \in \{1, \dots, N\}, \qquad \lambda_n(\varepsilon) \leq c_n(\varepsilon, N)\,,$$

where $\{c_n(\varepsilon, N)\}_{n=1}^N$ are the eigenvalues (written in increasing order and repeated according to multiplicity) of the matrix, with $k = k(N)$,

$$C_N(\varepsilon) := \big\{h_\varepsilon(\phi_{i+k}, \phi_{j+k})\big\}_{i,j=1}^N\,.$$

However, (III.15) implies

$$\begin{aligned} C_N(\varepsilon) &= \big\{(\nabla\phi_{i+k}, \nabla\phi_{j+k})\big\}_{i,j=1}^N + \varepsilon A_N(k(N)) \\ &\leq d(N)\, I_N + \varepsilon\,(V_{\min} + N^{-1})\, I_N\,, \end{aligned}$$

where $d(N)$ denotes the maximal eigenvalue of the matrix $\left\{(\nabla\phi_{i+k}, \nabla\phi_{j+k})\right\}_{i,j=1}^{N}$. Consequently,

$$\forall n \in \{1, \dots, N\}, \qquad \lim_{\varepsilon\to+\infty} \frac{\lambda_n(\varepsilon)}{\varepsilon} \leq V_{\min} + N^{-1} .$$

Since N can be chosen arbitrarily large, we eventually have

$$\forall n \in \mathbb{N}^*, \qquad \lim_{\varepsilon\to+\infty} \frac{\lambda_n(\varepsilon)}{\varepsilon} \leq V_{\min} .$$

This together with (III.14) concludes the proof of Theorem III.3.

III.3.5 A relation to semiclassical limit

Recall that, already in Chapter I, we put Planck's constant, $\hbar$, and twice the particle mass, $2m$, equal to one. Recovering the physical constants, the Hamiltonian a quantum particle of mass m subjected to potential energy V reads

$$H_\alpha^{\text{phys}} = \alpha H_0 + V , \qquad \text{with} \qquad \alpha := \frac{\hbar^2}{2m} ,$$

where we keep the notation H_0 for the self-adjoint realization of the Laplacian on $L^2(\mathbb{R}^d)$. The *semiclassical limit* usually referres to taking $\alpha \to 0+$ (small Planck's constant or large particle mass).

Writing

$$H_\alpha^{\text{phys}} = \alpha\left(H_0 + \alpha^{-1} V\right) ,$$

we have

$$\sigma(H_\alpha^{\text{phys}}) = \alpha\, \sigma(H_{\alpha^{-1}}) ,$$

where, in accordance with our previous notation, $H_\varepsilon := H_0 + \varepsilon V$. Hence, as a consequence of the strong-coupling asymptotics (Theorem III.3),

$$\inf \sigma(H_\alpha^{\text{phys}}) = V_{\min} + o(1) \qquad \text{as} \quad \alpha \to 0+ .$$

This result can be interpreted as that quantum physics reduces to classical physics on large scales (*i.e.*, small Planck's constant or large mass). Indeed, the equilibrium of a classical particle is achieved at the minimum of the potential energy (in quantum physics, however, the situation is not that simple).

III.4 Lieb-Thirring inequalities

We conclude this chapter by saying a few words of one type of bounds on a sum of powers of eigenvalues, known as *Lieb-Thirring inequalities*. These estimates are particularly interesting from two points of view. Firstly, as uniform estimates, they hold globally, regardless of the coupling regime. Secondly, they become sharp in the semiclassical/strong-coupling limit. We rely on [21, 5, 20].

Let $H := H_0 + V$ on $L^2(\mathbb{R}^d)$, where $V = V_+ - V_-$ is a bounded potential ($V_\pm := \max\{\pm V, 0\}$). For simplicity, in this section we assume $V \in C_0(\mathbb{R}^d)$. Since the potential is bounded and of compact support, it follows that $\sigma_{\text{ess}}(H) = [0, \infty)$ and that the number N (counting multiplicities) of negative eigenvalues (if any)

$$-\infty < \lambda_1 < \lambda_2 \leq \cdots \leq \lambda_N < 0$$

is finite (*i.e.* $0 \leq N < \infty$).

Put $\gamma \geq 0$. A *Lieb-Thirring (LT) inequality* is the following bound on the sum of momenta of the discrete eigenvalues

$$\sum_{n=1}^{N} |\lambda_n|^\gamma \leq L_{\gamma,d} \int_{\mathbb{R}_d} V_-(x)^{\gamma+\frac{d}{2}}\, dx\,. \tag{III.16}$$

Here, for appropriate pairs γ and d, $L_{\gamma,d}$ is a finite constant, which is independent of V.

An interesting feature of such type of estimates consists in that the integral on the right hand side appears in the semiclassical/strong-coupling asymptotics for such a sum. Indeed, it is proportional to the phase-space integral

$$\int_{\mathbb{R}_d} \int_{\mathbb{R}_d} \left\{|p|^2 + V(x)\right\}_-^\gamma \frac{dx\, dp}{(2\pi)^d}$$

of the corresponding classical system. Hence the inequalities allow one to extract hard information on the negative spectrum of Schrödinger operators from their classical counterparts, uniformly, in the non-asymptotical regime as well.

It is important to stress that (III.16) cannot hold for arbitrary values of γ and d. Indeed, it follows from our weak coupling analysis in one dimension (*cf* Corollary III.1) that any arbitrarily small potential V such that $V_+ = 0$ and $V_- > 0$ generate at least one bound state. Hence the left hand side of (III.16) for $\gamma = 0$, being the counting function of the negative spectrum, is a positive integer for any such potential. On the other hand, the phase-space integral on the right hand side of (III.16) can be arbitrarily small. This contradicts (III.16) for $\gamma = 0$ and $d = 1$. The same argument applies in $d = 2$ (*cf* the last paragraph of Section III.2.4). This shows that the validity of LT inequalities is far from being trivial (without speaking about the issue of optimal constant $L_{\gamma,d}$ in (III.16)).

Theorem III.5 (Validity of LT inequalities)**.** *Let* $V \in C_0(\mathbb{R}^d)$*. Then* (III.16) *holds if, and only if,*

$$\begin{aligned} &\gamma \geq 1/2 && \textit{for} \quad d = 1\,,\\ &\gamma > 0 && \textit{for} \quad d = 2\,,\\ &\gamma \geq 0 && \textit{for} \quad d \geq 3\,. \end{aligned}$$

The proof of the theorem is based on 'trace identities' (for a proof in $d \leq 3$, see [21, Thm. 12.4]). We shall not prove the theorem here, but we would like to present an alternative, beautiful proof of R. Benguria and M. Loss [5], employing 'commutation method', for the special case $\gamma = 3/2$ and $d = 1$:

$$\sum_{n=1}^{N} |\lambda_n|^{3/2} \leq \frac{3}{16} \int_{\mathbb{R}} V_-(x)^2\, dx\,. \tag{III.17}$$

Here the constant $L_{3/2,1} = 3/16$ is best possible, as it can be seen from Weyl's law on the distribution of eigenvalues.

Proof for $\gamma = 3/2$ *and* $d = 1$. First of all, we see from the minimax principle that the effect of V_+ is only to increase the eigenvalues λ_n and, since V_+ does not appear on the right hand side of (III.17), we may as well set $V_+ = 0$ (so that $V = -V_- \le 0$). (This reasoning applies to the proof of any of the LT inequalities (III.16).)

Recall that H has N negative eigenvalues

$$\lambda_1 < \lambda_2 \le \cdots \le \lambda_N .$$

It is well known that the lowest eigenvalue λ_1 is not degenerate and that the corresponding eigenfunction ψ_1 can be chosen to be positive (*cf* Theorem II.7). Moreover, outside the range of the potential, we have

$$\psi_1(x) = \begin{cases} C_- e^{\sqrt{|\lambda_1|}x} & \text{if} \quad x < \inf \operatorname{supp}(V)\,, \\ C_+ e^{-\sqrt{|\lambda_1|}x} & \text{if} \quad x > \sup \operatorname{supp}(V)\,, \end{cases} \tag{III.18}$$

where $C_\pm$ are some positive constants. Thus the function

$$F := \frac{\psi_1'}{\psi_1}$$

is well defined on $\mathbb{R}$ and satisfies the Riccati equation

$$F' + F^2 = V - \lambda_1\,, \tag{III.19}$$

together with the conditions

$$F(x) = \begin{cases} \sqrt{|\lambda_1|} & \text{if} \quad x < \inf \operatorname{supp}(V)\,, \\ -\sqrt{|\lambda_1|} & \text{if} \quad x > \sup \operatorname{supp}(V)\,. \end{cases} \tag{III.20}$$

A simple computation shows that the operator H can be written as

$$H = D^* D + \lambda_1\,,$$

where

$$D := \nabla - F\,, \qquad D^* := -\nabla - F\,, \qquad \mathfrak{D}(D) := W^{1,2}(\mathbb{R}) =: \mathfrak{D}(D^*)\,.$$

It is a general fact [1] that the operators D^*D and DD^* on $L^2(\mathbb{R})$ have the same spectrum, with the possible exception of the zero eigenvalue. Obviously, D^*D *has* a zero eigenvalue which corresponds to the ground state ψ_1 of H. On the other hand, DD^* *does not have* a zero eigenvalue. It follows from the fact that the corresponding eigenfunction ϕ satisfies $\phi' = -F\phi$ (because $D^*\phi = 0$), and hence $\phi(x) = C/\psi_1(x)$ which grows exponentially due to (III.18) and is not therefore normalizable.

Thus the new Schrödinger operator

$$\tilde{H} := DD^* + \lambda_1 = -\Delta - F' + F^2 + \lambda_1 = -\Delta + V - 2F'$$

has, except for the eigenvalue λ_1, precisely the same negative eigenvalues as H. Also note that the potential $V - 2F'$ is continuous and has support in the same interval as V due to (III.20).

[1] Check conditions. Is $V \in C_0(\mathbb{R})$ enough?

Next, we compute using the Riccati equation (III.19)

$$\int_{\mathbb{R}} [V(x) - 2F'(x)]^2 \, dx = \int_{\mathbb{R}} V(x)^2 \, dx - 4 \int_{\mathbb{R}} [\lambda_1 + F(x)^2] F'(x) \, dx \, .$$

The last term can be computed explicitly using (III.20) and we obtain

$$\int_{\mathbb{R}} [V(x) - 2F'(x)]^2 \, dx = \int_{\mathbb{R}} V(x)^2 \, dx - \frac{16}{3} \, |\lambda_1|^{3/2} \, .$$

Thus

$$\sum_{n=1}^{N} |\lambda_n|^{3/2} - \frac{3}{16} \int_{\mathbb{R}} V(x)^2 \, dx = \sum_{n=2}^{N} |\lambda_n|^{3/2} - \frac{3}{16} \int_{\mathbb{R}} [V(x) - 2F'(x)]^2 \, dx$$

and the Schrödinger operator $\tilde{H}$ with the potential $V - 2F'$ has precisely the negative eigenvalues

$$\lambda_2 < \lambda_3 \leq \cdots \leq \lambda_N \, .$$

Continuing this process we remove one eigenvalue after another. After the last one is removed, a manifestly negative quantity is left over, and this proves (III.17).

□

Chapter IV

The nature of essential spectrum

Up to now we have been interested only in qualitative properties of the essential spectrum of Schrödinger operators. Our study has been restricted to locating the essential spectrum as a set (which coincides with the non-negative semi-axis for potentials vanishing at infinity) and then we have been mainly concerned with bound states corresponding to discrete (negative) eigenvalues. However, the information coming from the discrete spectrum is far from being satisfactory for the full understanding of spectral properties.

In atomic physics, the discrete spectrum corresponds to energies of electron orbits, while the essential spectrum is referred to as the ionization energies for which the electron typically propagates as a free particle. However, the latter is still to be proved, since, by definition, the essential spectrum may contain "singular" components, such as embedded eigenvalues, and it is just its specific part which indeed corresponds to "freely propagating states".

In this chapter we therefore focus on the *nature* of the essential spectrum and present methods which enables one to state properties (or even prove the absence) of the singular components of the essential spectrum.

IV.1 Preliminaries

IV.1.1 Singular and continuous spectra

Up to now we have considered the partition of the spectrum of a self-adjoint operator into discrete and essential spectra. In this chapter another partition of the spectrum will be useful. (We refer to [16, Sec. X.1.2], [29, Sec. 7.4] or [23, Sec. 7.2] for more details.)

By the spectral theorem (Theorem I.1), to every self-adjoint operator H on a Hilbert space $\mathcal{H}$ there exists exactly one (right-continuous) *spectral family* $E_H : \mathbb{R} \to \mathcal{B}(\mathcal{H})$ for which

$$H = \int_{\sigma(H)} \lambda \, dE_H(\lambda) .$$

The spectral family $\{E_H(\lambda)\}_{\lambda\in\mathbb{R}}$ determines a projection-valued function $E_H(\Omega)$ defined for all Borel sets $\Omega \in \mathbb{R}$ via

$$E_H((a,b]) := E_H(b) - E_H(a)\,, \qquad E_H([a,b]) := E_H(b) - E_H(a-)\,,$$
$$E_H([a,b)) := E_H(b-) - E_H(a-)\,, \qquad E_H((a,b)) := E_H(b-) - E_H(a)\,,$$

where $a < b$. For any fixed $\psi \in \mathcal{H}$, this in turn defines a (non-negative, countably additive) *spectral measure* associated with H, for all Borel sets $\Omega \in \mathbb{R}$, via

$$\mu_\psi(\Omega) := \big(\psi, E_H(\Omega)\psi\big)\,. \tag{IV.1}$$

By the Lebesgue decomposition theorem, any measure μ on $\mathbb{R}$ can be uniquely decomposed into

$$\mu = \mu_{\rm pp} + \mu_{\rm ac} + \mu_{\rm sc}\,,$$

where $\mu_{\rm pp}$ is a pure point measure, $\mu_{\rm ac}$ is an absolutely continuous measure and $\mu_{\rm sc}$ is a singularly continuous measure (with respect to Lebesgue measure). Then the Hilbert space $\mathcal{H}$ admits the decomposition

$$\mathcal{H} = \mathcal{H}_{\rm pp} \oplus \mathcal{H}_{\rm ac} \oplus \mathcal{H}_{\rm sc}\,, \tag{IV.2}$$

where

$$\mathcal{H}_{\rm pp} := \{\psi \in \mathcal{H} \mid \mu_\psi \text{ is pure point}\}\,,$$
$$\mathcal{H}_{\rm ac} := \{\psi \in \mathcal{H} \mid \mu_\psi \text{ is absolutely continuous}\}\,,$$
$$\mathcal{H}_{\rm sc} := \{\psi \in \mathcal{H} \mid \mu_\psi \text{ is singularly continuous}\}\,.$$

The sets

$$\sigma_{\rm pp}(H) := \sigma(H \restriction \mathcal{H}_{\rm pp})\,, \quad \sigma_{\rm ac}(H) := \sigma(H \restriction \mathcal{H}_{\rm ac})\,, \quad \sigma_{\rm sc}(H) := \sigma(H \restriction \mathcal{H}_{\rm sc})\,,$$

are called the *pure point*, *absolutely continuous* and *singularly continuous* spectrum of H, respectively. We obviously have

$$\sigma(H) = \sigma_{\rm pp}(H) \cup \sigma_{\rm ac}(H) \cup \sigma_{\rm sc}(H)\,.$$

Attention,

$$\sigma_{\rm pp}(H) \neq \sigma_{\rm p}(H)\,, \qquad \text{but} \qquad \sigma_{\rm pp}(H) = \overline{\sigma_{\rm p}(H)}\,,$$

where $\sigma_{\rm p}(H)$ denotes the set of eigenvalues of H, in accordance with our previous notation. Finally, the sets

$$\sigma_{\rm c}(H) := \sigma_{\rm ac}(H) \cup \sigma_{\rm sc}(H)\,, \qquad \sigma_{\rm s}(H) := \sigma_{\rm sc}(H) \cup \sigma_{\rm pp}(H)$$

are called the *continuous* and *singular* spectrum of H.

In the quantum-mechanical context, the decomposition (IV.2) means that any quantum state is a sum of bound states (correspodning to not necessarily discrete eigenvalues), scattering states and states with no physical interpretation. One goal of this chapter is to show that this last type of states does not occur, *i.e.* $\sigma_{\rm sc}(H) = \varnothing$, for a class of physically interesting potentials. Another objective is to possibly exclude eigenvalues embedded in the essential spectrum.

There exist examples of Schrödinger operators possessing singularly continuous spectrum, or even having purely(!) singularly continuous spectrum. The potentials are typically random or almost periodic functions [7].

IV.1.2 Two examples of embedded eigenvalues

At the same time, it is not difficult to construct examples of Schrödinger operators possessing eigenvalues embedded in the essential spectrum.

Example IV.1 (Tensor product of operators)**.** Let us consider

$$H_1 := H_0 + V \qquad \text{on} \qquad L^2(\mathbb{R}),$$

where the potential V is such that $\sigma_{\mathrm{ess}}(H_1) = [0, \infty)$ and H_1 possesses a (finite or infinite) number of negative eigenvalues λ_n, *i.e.*,

$$\sigma(H_1) = \{\lambda_1 < \lambda_2 \leq \lambda_3 \leq \dots\} \cup [0, \infty).$$

We know that the essential spectrum coincides with the non-negative semi-axis if $V \xrightarrow{\infty} 0$ (Theorem II.4) and that there exists at least one negative eigenvalue if in addition $\langle V \rangle < 0$ (Theorem II.5). Moreover, in the strong-coupling limit (*cf* Theorem III.3), the number of negative eigenvalues can be made arbitrarily large and they are all located close to $V_{\min} < 0$. In particular, recalling the simplicity of the ground state and the continuous dependence of the eigenvalues on the coupling parameter, there clearly exists a potential V for which

$$\frac{\lambda_1}{2} < \lambda_2 < 0$$

(and/or other negative eigenvalues λ_n satisfy this inequality). That is, the second eigenvalue λ_2 (and/or another excited eigenvalue) is closer to the threshold of the essential spectrum 0 than to the threshold of the spectrum λ_1.

We define the decomposed operator

$$H := \overline{H_1 \otimes I + I \otimes H_1} \qquad \text{on} \qquad L^2(\mathbb{R}) \otimes L^2(\mathbb{R}),$$

where I denotes the identity operator on $L^2(\mathbb{R})$ and $\otimes$ stands for the tensor product of operators (*cf* [23, Sec. VIII.10]). Since

$$\sigma(H) = \overline{\sigma(H_1) + \sigma(H_1)},$$

the essential spectrum of H is $[\lambda_1, \infty)$, H possesses discrete eigenvalues in the interval $[2\lambda_1, \lambda_1)$ (at least $2\lambda_1$ and doubly degenerated $\lambda_1 + \lambda_2$) but also at least one embedded eigenvalue $2\lambda_2 > \lambda_1$. Schematically,

$$\begin{aligned}\sigma(H) = \{2\lambda_1 < \lambda_1 + \lambda_2 \leq \lambda_1 + \lambda_2 \leq \lambda_1 + \lambda_3 \leq \dots\} &\cup [\lambda_1, \infty) \\ &\ni \{2\lambda_2 \leq \lambda_2 + \lambda_3 \leq \dots\}.\end{aligned}$$

Clearly, H is a Schrödinger operator (indeed, it can be identified with the Schrödinger operator on $L^2(\mathbb{R}^2)$ determined by the potential $x \mapsto V(x_1) + V(x_2)$) and the generalization to higher dimensions is straightforward. □

A more sophisticated example is the following.

Example IV.2 (Zero eigenvalue for a quantum square well)**.** Let us consider the square-well Hamiltonian (III.1)

$$H_\varepsilon := H_0 - \varepsilon \chi_{B_R},$$

where $\varepsilon \geq 0$ and χ_{B_R} denotes the (operator of multiplication by the) characteristic function of the ball B_R of radius $R > 0$ centered at the origin of $\mathbb{R}^d$. We derive a sufficient condition which guarantees that the threshold of the essential spectrum, *i.e.* $\inf \sigma_{\mathrm{ess}}(H_\varepsilon) = 0$, is at the same time an eigenvalue of H_ε.

A $\psi \in \mathfrak{D}(H_\varepsilon) = W^{2,2}(\mathbb{R}^d)$ is an eigenfunction of H_ε corresponding to zero eigenvalue if, and only if,

$$-\Delta\psi = \begin{cases} \varepsilon\psi & \text{in} \quad B_R\,, \\ 0 & \text{in} \quad \mathbb{R}^d \setminus B_R\,. \end{cases} \tag{IV.3}$$

The second equation does not admit a non-trivial radially symmetric solution $\psi \in L^2(\mathbb{R}^d \setminus B_R)$ unless $d \geq 5$ when

$$\psi(x) := |x|^{-(d-2)} \qquad \text{for} \qquad |x| \geq R$$

is easily checked to be harmonic and square-integrable in $\mathbb{R}^d \setminus B_R$. To satisfy the first equation, we consider the eigenfunction ϕ_1 corresponding to the lowest eigenvalue λ_1 of the Robin problem

$$\begin{cases} -\Delta\phi = \lambda\phi & \text{in} \quad B_R\,, \\ \dfrac{\partial\phi}{\partial n} + \alpha\phi = 0 & \text{on} \quad \partial B_R\,, \end{cases}$$

where $\alpha \in \mathbb{R}$ and n denotes the outward-pointing unit normal to the boundary ∂B_R. ϕ_1 is radially symmetric and can be chosen to be positive; we normalize it in such a way that

$$\phi_1 = R^{-(d-2)} \qquad \text{on} \qquad \partial B_R\,.$$

This ensures that, defining

$$\psi(x) := \phi_1(x) \qquad \text{for} \qquad |x| < R\,,$$

we get a continuous function ψ on $\mathbb{R}^d$. It satisfies (IV.3) provided that we choose $\varepsilon := \lambda_1$. It remains to ensure that $\lambda_1 > 0$ and that the radial derivative ψ is continuous on ∂B_R, so that $\psi \in W^{2,2}(\mathbb{R}^d)$ (the trace must exist). The latter requires

$$-\alpha R^{-(d-2)} = -\alpha\phi_1\big|_{|x|\to R-} = \frac{\partial\psi}{\partial n}\bigg|_{|x|\to R-} = \frac{\partial\psi}{\partial n}\bigg|_{|x|\to R+} = -(d-2)R^{-(d-1)}\,,$$

which is verified by taking $\alpha R = d - 2$. This relation yields $\alpha > 0$, which in turn implies $\lambda_1 > 0$.

Summing up,

$$\left.\begin{array}{r} d \geq 5 \\ \alpha R = d-2 \\ \varepsilon = \lambda_1 \end{array}\right\} \quad \Longrightarrow \quad 0 = \inf \sigma_{\mathrm{ess}}(H_\varepsilon) \in \sigma_{\mathrm{p}}(H_\varepsilon)\,.$$

A characteristic feature of this example is that the dimension has to be sufficiently large (obviously, 0 is never an eigenvalue of H_ε if $d = 1$ [1]). □

[1] $d = 2, 3, 4$? (non-radial solutions?)

IV.2 The limiting absorption principle

IV.2.1 An abstract setting

Let H be a self-adjoint operator in a Hilbert space $\mathcal{H}$. The resolvent operator $R_z := (H - z)^{-1}$ is a holomorphic function (with values in $\mathcal{B}(\mathcal{H})$) for every $z \in \mathbb{C} \setminus \sigma(H)$. Since

$$\|R_z\|_{\mathcal{B}(\mathcal{H})} = \frac{1}{\operatorname{dist}\big(z, \sigma(H)\big)} ,$$

it is clear that R_z cannot have a limit in $\mathcal{B}(\mathcal{H})$ as $z \to \lambda \in \sigma(H)$. In other words, $z \mapsto R_z$ cannot be continued up to the spectrum of H. However, it might happen that such a limit can be achieved in a *weaker topology*, and this can be used to infer results on the spectral properties of H.

Definition IV.1 (Limiting absorption principle)**.** We say that the *limiting absorption principle* (LAP) holds for H on an open interval $J \subset \mathbb{R}$ if there exists another Hilbert space $\mathcal{K}$ such that

$$\mathcal{K} \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{K}^* \qquad \text{(continuously and densely)}$$

and

$$\forall \lambda \in J, \qquad \lim_{\varepsilon \to 0+} R_{\lambda \pm i\varepsilon} =: R_{\lambda \pm i0} \qquad \text{exists in} \qquad \mathcal{B}(\mathcal{K}, \mathcal{K}^*) . \tag{IV.4}$$

(The two respective limits from the upper and lower half-plane will be different in general.)

Clearly, the trivial LAP (*i.e.*, with $\mathcal{K} = \mathcal{H}$) holds for H on $\mathbb{R} \setminus \sigma(H)$. On the other hand, it is easy to see (*cf* Problem IV.1) that the limits (IV.4) cannot hold for any dense subspace $\mathcal{K} \subset \mathcal{H}$ if $\lambda \in \sigma_{\mathrm{p}}(H)$. Moreover, it turns out that the LAP excludes singularly continuous spectrum too. This can be seen as follows. There exists a formula giving directly the spectral measure E_H of H in terms of its resolvent (*cf* [29, Thm. 7.17]):

$$\big(\phi, [E_H(b) - E_H(a)]\psi\big) = \frac{1}{2\pi i} \lim_{\delta \to 0+} \lim_{\varepsilon \to 0+} \int_{a+\delta}^{b+\delta} \big(\phi, [R_{\lambda+i\varepsilon} - R_{\lambda-i\varepsilon}]\psi\big)\, d\lambda$$

for all $\phi, \psi \in \mathcal{H}$ and $-\infty < a \leq b < +\infty$. If the LAP holds for H in J, this gives

$$\big(\phi, [E_H(b) - E_H(a)]\psi\big) = \frac{1}{2\pi i} \int_a^b \big(\phi, [R_{\lambda+i0} - R_{\lambda-i0}]\psi\big)\, d\lambda \tag{IV.5}$$

for all bounded $[a, b] \subset J$. As a consequence, we get

Proposition IV.1. *Let H be a self-adjoint operator for which the LAP holds on J. Then H has purely absolutely continuous spectrum in J,* i.e.,

$$J \cap \sigma(H) = J \cap \sigma_{\mathrm{ac}}(H) .$$

Proof. We follow the proof of [7, Prop. 4.1]. By (IV.5),

$$\mu_\psi((a,b)) \equiv \big(\psi, E_H((a,b))\psi\big) \leq C_{a,b}\, \|\psi\|_{\mathcal{K}}^2 \int_a^b d\lambda = C_{a,b}\, \|\psi\|_{\mathcal{K}}^2\, |b - a|$$

for every $\psi \in \mathcal{K}$, where

$$C_{a,b} := \frac{1}{2\pi} \sup_{\lambda \in [a,b]} \Big(\|R_{\lambda+i0}\|_{\mathcal{B}(\mathcal{K},\mathcal{K}^*)} + \|R_{\lambda-i0}\|_{\mathcal{B}(\mathcal{K},\mathcal{K}^*)} \Big) .$$

This implies

$$\mu_\psi(\Omega) \equiv \big(\psi, E_H(\Omega)\psi\big) \leq C_{a,b} \, \|\psi\|_{\mathcal{K}}^2 \, |\Omega|$$

for every Borel set $\Omega \subset (a,b)$, which means that the spectral measures (IV.1) are absolutely continuous (indeed, $\mu_\psi(\Omega) = 0$ for every Borel set Ω of Lebesgue measure zero). That is, $E_H((a,b))\psi \in \mathcal{H}_{\mathrm{ac}}$ for every $\psi \in \mathcal{K}$. Since the set $\mathcal{K}$ is assumed to be dense in $\mathcal{H}$ and $\mathcal{H}_{\mathrm{ac}}$ is a closed subspace of $\mathcal{H}$, the spectrum is purely absolutely continuous. □

Problem IV.1. Show (by an elementary argument) that if the LAP holds for H on an open interval $J \subset \mathbb{R}$, then $J \cap \sigma_{\mathrm{p}}(H) = \varnothing$.
Solution: ...[2]

IV.2.2 The free Hamiltonian

In this section we establish the LAP for the free Hamiltonian H_0 on $L^2(\mathbb{R}^d)$. Although our proof does not apply to higher dimensions (*i.e.* $d \geq 4$) and the result is far from being optimal, the proof is rather elementary.

We state the LAP in the weighted spaces

$$\mathcal{K}_s := L^2\big(\mathbb{R}^d, \langle x \rangle^s dx\big) , \qquad \text{where} \qquad \langle x \rangle := \sqrt{1+|x|^2} \,, \quad s \in \mathbb{R} .$$

Clearly, $\mathcal{K}_s \hookrightarrow \mathcal{K}_0 \equiv L^2(\mathbb{R}^d)$ for every $s > 0$, continuously and densely.

Theorem IV.1 (LAP for the free Hamiltonian)**.** *For every $z \in \mathbb{C} \setminus [0,\infty)$, let us set $R_z := (H_0 - z)^{-1}$. Then*

$$\forall \lambda \in (0,\infty), \qquad \lim_{\varepsilon \to 0+} R_{\lambda \pm i\varepsilon} =: R_{\lambda \pm i0} \qquad \textit{exists in} \qquad \mathcal{B}(\mathcal{K}_s, \mathcal{K}_{-s}) \qquad \text{(IV.6)}$$

with $s > d$. That is, the LAP holds for H_0 on $(0,\infty)$.

Proof. Let $\lambda \in (0,\infty)$. For every $s > 0$, we have

$$\|R_{\lambda \pm i\varepsilon}\|_{\mathcal{B}(\mathcal{K}_s,\mathcal{K}_{-s})} = \sup_{\phi,\psi \in \mathcal{K}_s \setminus \{0\}} \frac{|(\phi, R_{\lambda \pm i\varepsilon}\psi)|}{\|\phi\|_{\mathcal{K}_s} \|\psi\|_{\mathcal{K}_s}} \leq \|K_{\pm\varepsilon}\|_{\mathcal{B}(\mathcal{K}_0)} ,$$

where $K_{\pm\varepsilon}$ is an integral operator on $\mathcal{K}_0$ with the kernel

$$K_{\pm\varepsilon}(x,x') := \langle x \rangle^{-s/2} \, G_{\lambda \pm i\varepsilon}(x,x') \, \langle x' \rangle^{-s/2} ,$$

with G_z denoting Green's function of the free Hamiltonian (given explicitly by (III.8) for $d \leq 3$). It is enough to prove that $K_{\pm\varepsilon}$ converges to $K_{\pm 0}$ in $\mathcal{K}_0$ as $\varepsilon \to 0+$, where

$$K_{\pm 0}(x,x') := \langle x \rangle^{-s/2} \, G_{\lambda \pm i0}(x,x') \, \langle x' \rangle^{-s/2} ,$$

with (pointwise limit)

$$G_{\lambda \pm i0}(x,x') := \lim_{\varepsilon \to 0+} G_{\lambda \pm i\varepsilon}(x,x') .$$

[2] ???

We give a proof for $d \leq 3$ only, when we can estimate the operator norm by the Hilbert-Schmidt norm. Note that

$$G_{\lambda \pm i0}(x,x') := \begin{cases} \dfrac{e^{\pm i\sqrt{\lambda}\,|x-x'|}}{\mp 2\,i\,\sqrt{\lambda}} & \text{if} \quad d=1\,, \\ \dfrac{K_0\big(\mp i\sqrt{\lambda}\,|x-x'|\big)}{2\pi} & \text{if} \quad d=2\,, \\ \dfrac{e^{\pm i\sqrt{\lambda}\,|x-x'|}}{4\pi\,|x-x'|} & \text{if} \quad d=3\,. \end{cases} \tag{IV.7}$$

This is easily seen by writing the square root in (III.8) as a sum of its real and imaginary parts:

$$\sqrt{-(\lambda \pm i\varepsilon)} = \sqrt{\frac{1}{2}\left(-\lambda + \sqrt{\lambda^2+\varepsilon^2}\right)} \mp i\varepsilon\sqrt{\frac{1}{2}\left(\lambda + \sqrt{\lambda^2+\varepsilon^2}\right)} =: \alpha + i\beta\,.$$

$\boxed{d=1}$ We readily have

$$\|K_{\pm 0}\|_{\mathrm{HS}} = \frac{1}{2\sqrt{\lambda}} \int_{\mathbb{R}} \langle x\rangle^{-s}\,dx\,,$$

where the integral is finite as long as $s > 1$. At the same time, we have the uniform bound

$$|G_{\lambda \pm i\varepsilon}(x,x')| = \frac{e^{-\alpha|x-x'|}}{2\sqrt[4]{\lambda^2+\varepsilon^2}} \leq \frac{1}{2\sqrt{\lambda}} = |G_{\lambda\pm i0}(x,x')|$$

for every $x,x' \in \mathbb{R}$ and $\varepsilon \geq 0$. Hence, taking into account that $K_{\pm\varepsilon}(x,x')$ converges to $K_{\pm 0}(x,x')$ pointwise for $x,x' \in \mathbb{R}$ as $\varepsilon \to 0$, the dominated convergence theorem yields

$$\|K_{\pm\varepsilon} - K_{\pm 0}\|_{\mathrm{HS}} \xrightarrow[\varepsilon\to 0+]{} 0\,. \tag{IV.8}$$

$\boxed{d=3}$ The problem with higher dimensions is that Green's function has a singularity at $x = x'$. Nevertheless, the singularity is square-integrable as long as $d < 4$. Indeed, for $d = 3$, we have

$$\|K_{\pm 0}\|_{\mathrm{HS}}^2 = \frac{1}{(4\pi)^2} \int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\langle x\rangle^{-s}\langle x'\rangle^{-s}}{|x-x'|^2}\,dx\,dx' \leq C\left(\int_{\mathbb{R}^3} \langle x\rangle^{-3s/2} dx\right)^{4/3},$$

where the inequality follows by the Hardy-Littlewood-Sobolev inequality [21, Thm. 4.3] (also referred to as the weak Young inequality) and the last integral is finite as long as $s > 2$ (note that we have got a better lower bound to the exponent than announced in the theorem for $d = 3$). At the same time, we have the uniform bound

$$|G_{\lambda\pm i\varepsilon}(x,x')| = \frac{e^{-\alpha|x-x'|}}{4\pi|x-x'|} \leq \frac{1}{4\pi|x-x'|} = |G_{\lambda\pm i0}(x,x')|$$

for every $x,x' \in \mathbb{R}$, $x \neq x'$, and $\varepsilon \geq 0$. Hence, in the same way as above, we conclude with (IV.8).

$\boxed{d=2}$ The additional problem with dimensions $d \neq 1, 3$ is that the Green's function is not so explicit. Nevertheless, using the asymptotics (*cf* [1, 9.6.8, 9.7.2])

$$K_0(\xi) \sim -\log \xi \qquad \text{as} \quad \xi \to 0\,,$$
$$K_0(\xi) \sim \sqrt{\frac{\pi}{2\xi}}\, e^{-\xi} \qquad \text{as} \quad |\xi| \to \infty,\ |\arg \xi| < 3\pi/2\,,$$

it follows that there exists a positive constant C such that

$$|K_0(\xi)| \leq C\rho(\xi)\,, \qquad \text{where} \qquad \rho(\xi) := \begin{cases} |\log|\xi|| & \text{if} \quad |\xi| < 1\,, \\ 1 & \text{if} \quad |\xi| \geq 1\,. \end{cases}$$

This enables us to estimate the Green's function as follows

$$|G_{\lambda \pm i\varepsilon}(x,x')| \leq C\rho\big(\sqrt{\lambda^2+\varepsilon^2}\,|x-x'|\big) \leq C\rho\big(\lambda\,|x-x'|\big)$$

for every $x, x' \in \mathbb{R}$, $x \neq x'$, and $\varepsilon \geq 0$. Such a logarithmic singularity is square-integrable for $d = 2$. Indeed, dividing the integration of the bound to the Hilbert-Schmidt norm of $K_{\pm\varepsilon}$ into two regions where $\lambda|x-x'| \geq 1$, respectively $\lambda|x-x'| < 1$, we can estimate

$$\int_{\{\lambda|x-x'|\geq 1\}} \langle x\rangle^{-s}\, \rho\big(\lambda\,|x-x'|\big)^2\, \langle x'\rangle^{-s}\, dx\, dx' \leq \left(\int_{\mathbb{R}^2} \langle x\rangle^{-s} dx\right)^2\,,$$

respectively

$$\begin{aligned}\int_{\{\lambda|x-x'|<1\}} \langle x\rangle^{-s}\, \rho\big(\lambda\,|x-x'|\big)^2\, \langle x'\rangle^{-s}\, dx\, dx' &\leq \int_{\{\lambda|x-x'|<1\}} \frac{\langle x\rangle^{-s}\,\langle x'\rangle^{-s}}{\lambda\,|x-x'|}\, dx\, dx' \\ &\leq \frac{C}{\lambda} \left(\int_{\mathbb{R}^3} \langle x\rangle^{-4s/3} dx\right)^{3/2}\,.\end{aligned}$$

Here the last inequality follows again by the Hardy-Littlewood-Sobolev inequality. In both the estimates, the integrals are finite as long as $s > 2$. This enables us to conclude as above with (IV.8). □

Remark IV.1. Note that the proof for $d = 3$ actually shows that the limits (IV.6) hold also for $\lambda = 0$. This reflects the subcriticality of H_0 as long as $d \geq 3$.

Remark IV.2 (Proof for higher dimensions)**.** It can be shown that the singularity of the Green function behaves for $d \geq 3$ as

$$G_z(\xi) \sim \frac{c_d}{|\xi|^{d-2}} \qquad \text{as} \qquad |\xi| \to 0\,.$$

Clearly, such a singularity is not locally square-integrable if $d \geq 4$. For higher dimensions, the estimate of the operator norm via the Hilbert-Schmidt norm is not good, since the latter becomes infinite. However, even for $d \geq 4$, the singularity is locally integrable. This suggests that it should be possible to apply the Schur-Holmgren bound instead. [3]

[3] To be done.

As a consequence of Theorem IV.1, we get

Corollary IV.1. $\sigma(H_0) = \sigma_{\rm ac}(H_0) = [0,\infty)$.

Proof. We already know from Theorem I.5 that $\sigma(H_0) = [0,\infty)$. It follows from Theorem IV.1 that the spectrum in the open interval $(0,\infty)$ is absolutely continuous. Hence, $\sigma_{\rm sc}(H_0) = \varnothing$. It remains to exclude the possibility that $0 \in \sigma_{\rm p}(H_0)$. If ψ were an eigenfunction of H_0 corresponding to the eigenvalue 0, then $\|\nabla\psi\| = 0$. Consequently, ψ would have to be a non-zero constant, which contradicts $\psi \in L^2(\mathbb{R}^d)$. □

IV.3 The conjugate operator method

Since the method we are going to explain now is rather technical, and we shall not provide proofs of all the presented results, it is useful to get a physical insight first.

IV.3.1 Heuristic considerations

Recall that a quantum state $\psi \in \mathcal{H}$ evolves according to the Schrödinger equation (*cf* (I.1))

$$i\frac{d}{dt}\psi = H\psi\,, \tag{IV.9}$$

where H is the Hamiltonian (total energy operator) of the system. Let A be some other self-adjoint operator on $\mathcal{H}$, representing a physical observable. The expectation value of A for the system in the state ψ is given by the inner product (we do not care about operator domains in these heuristic considerations)

$$\langle A\rangle := (\psi, A\psi)\,.$$

Differentiating it with respect to time t and using (IV.9), we (formally) get

$$\begin{aligned}\frac{d}{dt}\langle A\rangle &= \left(\frac{d}{dt}\psi, A\psi\right) + \left(\psi, A\frac{d}{dt}\psi\right)\\ &= \big(-iH\psi, A\psi\big) + \big(\psi, A(-iH\psi)\big)\\ &= i\big(\psi, HA\psi\big) - i\big(\psi, AH\psi\big)\\ &= \big(\psi, i[H,A]\psi\big)\\ &= \big\langle i[H,A]\big\rangle\,. \end{aligned}\tag{IV.10}$$

Hence the evolution of the expectation value of A is given by the expectation value of the commutator with H.

Now, let $H = p^2 + V(q)$ be a one-particle Schrödinger operator and A be the quantum counterpart of the radial momentum

$$A := \frac{q\cdot p + p\cdot q}{2}\,,$$

where q and p are the position and momentum operators, respectively. (In the Schrödinger representation, the Hilbert space is $L^2(\mathbb{R}^d)$ and $p\psi = -i\nabla\psi$, $(q\psi)(x) = x\psi(x)$, *cf* (I.5).) Note that we had to take a symmetrized version of $q\cdot p$ in A, since the observables do not commute in quantum mechanics.

Assume that the commutator with H is *positive* in the sense that there exists a positive number a such that

$$i[H, A] \geq a\,I\,. \tag{IV.11}$$

Then it follows from (IV.10) (assuming $\|\psi\| = 1$) that the differential inequality

$$\frac{d}{dt}\langle A\rangle > a$$

holds, which in turn implies

$$\langle A\rangle(t) > \langle A\rangle(0) + at$$

for all times $t \geq 0$. Consequently,

$$\lim_{t\to+\infty}\langle A\rangle(t) = +\infty\,.$$

This can be interpreted in physical terms as that the particle escapes to infinity of $\mathbb{R}^d$ for large times. That is, it is not bound, it propagates. Recalling that it is the absolutely continuous spectrum which corresponds to propagating states, this suggests that the positivity of $i[H, A]$ can be used to deduce the absence of the singular spectrum of H. Schematically,

$$\text{“ } i[H, A] \geq a\,I \quad \Longrightarrow \quad \sigma_{\mathrm{s}}(H) = \varnothing \text{ ”}\,. \tag{IV.12}$$

Problem IV.2. Show that (IV.11) is impossible for bounded H and A.
Solution: For any $z \in \rho(H)$, (IV.11) yields

$$\begin{aligned}\|R_z\psi\|^2 = (R_z\psi, R_z\psi) &\leq a^{-1}\big(R_z\psi, i[H, A]R_z\psi\big)\\ &= ia^{-1}\left\{\big(zR_z\psi, A\psi\big) - \big(A\psi, zR_z\psi\big)\right\}\\ &\leq 2\,|z|\,a^{-1}\,\|R_z\psi\|\,\|A\|\,\|\psi\|\,.\end{aligned}$$

Consequently, $\|R_z\| \leq 2\,|z|\,a^{-1}\,\|A\|$. This implies that R_z is bounded for all $z \in \mathbb{C}$, *i.e.* that H has no spectrum.

IV.3.2 The Mourre estimate: an abstract setting

The above considerations are behind *local commutator estimates*. (The main references for these methods are the books [4] and [7].) To explain their relevance, let us comment on some problems with the positivity requirement (IV.11).

Weakening of the commutator estimate

First of all, in view of (IV.12), the requirement (IV.11) is unnecessarily too strict, since many physically interesting Hamiltonians (*e.g.*, atomic Hamiltonians) possess singular spectra represented by the eigenvalues outside the essential spectrum. For scattering, it is more relevant to study the singular spectrum inside the essential spectrum. This problem can be solved by replacing (IV.11) by an estimate “localized in the spectrum” of H:

$$E_H(J)\;i[H, A]\;E_H(J) \;\geq\; a\;E_H(J)\,, \tag{IV.13}$$

where $J \subset \mathbb{R}$ is an open interval (reasonably taken inside the essential spectrum).

Moreover, we have seen (Section IV.1.2) that it is not unusual that there do exist embedded eigenvalues inside the essential spectrum. In order to deal even with such situations (*i.e.*, relaxing the proof of absence of embedded eigenvalues, but still proving the absence of singularly continuous spectrum), the localized estimate can be considerably weaken by allowing an additional compact operator K on the right hand side of (IV.13):

$$E_H(J)\ i[H,A]\ E_H(J)\ \geq\ a\ E_H(J) + K\,. \tag{IV.14}$$

The estimates (IV.13) and (IV.14) are usually associated with the name of E. Mourre who introduced, in his 1981 paper [22], the concept of weaken commutator estimates for the study of Schrödinger operators. For an account of the general theory, we refer to the books [4] and [7].

Defining the commutator

Finally, we have to give a meaning to the commutator operator $i[H,A]$. It is not easy to extend the usual definition of commutator to unbounded operators because of the difficulty related to the domains. Usually this extension is done partly, by assuming that one of the operators is bounded (*cf* [16, Sec. III.5.6]).

An elegant way how to introduce $i[H,A]$ is as follows. Let H and A be a pair of self-adjoint operators in a Hilbert space $\mathcal{H}$. Let R_z denote the resolvent of H for some $z \in \rho(H)$. Let $\{e^{iAt}\}_{t\in\mathbb{R}}$ be the unitary group generated by A.

Definition IV.2 (C^1-regularity class)**.** We say that H is of class $C^1(A)$ if the map

$$\left\{t \mapsto e^{iAt} R_z e^{-iAt}\right\} : \mathbb{R} \to \mathcal{B}(\mathcal{H}) \tag{IV.15}$$

is of class C^1 for the strong topology of $\mathcal{B}(\mathcal{H})$.

Under this condition, the derivative at zero defines a bounded operator on $\mathcal{H}$:

$$i[A,R_z] := \text{s-}\lim_{t\to 0} \frac{e^{iAt}R_z e^{-iAt} - R_z}{t}\,. \tag{IV.16}$$

Then the formula

$$i[H,A] := (H-z)\, i[A,R_z]\, (H-z) \tag{IV.17}$$

defines a bounded operator in $\mathcal{B}(D(H), D(H)^*)$, which can be shown to be independent of z.

There exists an alternative definition of $i[H,A]$, using the following characterization of C^1-regular operators:

Theorem IV.2 ([4, Thm. 6.2.10])**.** *$H \in C^1(A)$ if, and only if, the following two conditions are satisfied:*

1. *$\exists C > 0$, $\forall \psi \in \mathfrak{D}(A) \cap \mathfrak{D}(H)$,*

$$\left|(H\psi, A\psi) - (A\psi, H\psi)\right| \leq C\left(\|H\psi\|^2 + \|\psi\|^2\right)\,, \tag{IV.18}$$

2. *$\exists z \in \rho(H)$,*

$$\left\{\psi \in \mathfrak{D}(A) \mid R_z\psi \in \mathfrak{D}(A)\ \wedge\ R_{\bar z}\psi \in \mathfrak{D}(A)\right\} \quad \textit{is a core for} \quad A\,.$$

We first observe that the set $R_z\mathfrak{D}(A)$ is a core for H. Indeed, R_z is a homeomorphism of $\mathcal{H}$ onto $\mathfrak{D}(H)$ and $\mathfrak{D}(A)$ is dense in $\mathcal{H}$; so $R_z\mathfrak{D}(A)$ is dense in $\mathfrak{D}(H)$ (equipped with the graph topology defined by H). Let us now assume $H \in C^1(A)$. Then it follows from the second condition of the theorem that $R_z\mathfrak{D}(A) \subset \mathfrak{D}(H)\cap\mathfrak{D}(A)$, whence we infer that the intersection $\mathfrak{D}(H)\cap\mathfrak{D}(A)$ is a core for H. Consequently, taking into account also the first condition of the theorem, the symmetric sesquilinear form

$$l(\phi,\psi) := i(H\phi, A\psi) - i(A\phi, H\psi)\,, \qquad \mathfrak{D}(l) := \mathfrak{D}(H)\cap\mathfrak{D}(A)\,.$$

has a bounded extension $\tilde{l}$ to $\mathfrak{D}(H)$. By the Riesz lemma, there is a bounded operator $\tilde{L} : \mathfrak{D}(H) \to \mathfrak{D}(H)^*$ such that $(\phi, \tilde{L}\psi) = \tilde{l}(\phi,\psi)$ (the brackets on the left hand side means anti-duality between $\mathfrak{D}(H)$ and $\mathfrak{D}(H)^*$) for all $\phi,\psi \in \mathfrak{D}(H)$. It is straightforward to check that $\tilde{L} = i[H,A]$ and (IV.17) can be written as

$$i[A,R_z] := R_z\, i[H,A]\, R_z\,. \tag{IV.19}$$

Formal definitions

As before, A and H are two self-adjoint operators on a Hilbert space $\mathcal{H}$. Let $J \subset \mathbb{R}$ be an open interval.

Definition IV.3 (Mourre's estimate)**.**

- We say that A is *conjugate* to H on J, or that the *Mourre estimate holds* for H on J, if there is a positive number a and a compact operator K such that (IV.14) holds.
- If this inequality holds with $K = 0$ (*i.e.* (IV.13) holds), we say that A is *strictly conjugate* to H on J, or that the *strict Mourre estimate holds* for H on J.
- Finally, we say that A is (strictly) conjugate to H at a point $\lambda \in \mathbb{R}$, or that the (strictly) Mourre estimate holds for H at λ, if there exists an interval $J \ni \lambda$ such that (strictly) Mourre estimate holds for H on J.

We conclude this section by another useful characterization of C^1-regular operators:

Theorem IV.3 ([4, Thm. 6.3.4])**.** *Assume that the unitary one-parameter group* $\{e^{iAt}\}_{t\in\mathbb{R}}$ *leaves the domain* $\mathfrak{D}(H)$ *invariant,* i.e., $e^{iAt}\,\mathfrak{D}(H) \subset \mathfrak{D}(H)$. *Then*

$$H \in C^1(A) \quad\Longleftrightarrow\quad i[H,A] \in \mathcal{B}\big(\mathfrak{D}(H), \mathfrak{D}(H)^*\big)\,.$$

IV.3.3 The Mourre estimate: Schrödinger operators

Now we find sufficient conditions which guarantee that a Mourre estimate holds for the Schrödinger operator

$$H := H_0 + V \qquad \text{on} \qquad L^2(\mathbb{R}^d)\,,$$

where V is a bounded potential. Recall that the boundedness implies $\mathfrak{D}(H) = \mathfrak{D}(H_0) = W^{2,2}(\mathbb{R}^d)$.

The dilation operator

Motivated by the considerations in Section IV.3.1, we introduce the operator

$$A := -\frac{i}{2}\big(x\cdot\nabla+\nabla\cdot x\big) = -i\,x\cdot\nabla - i\,\frac{d}{2}\,, \qquad \mathfrak{D}(A) := C_0^\infty(\mathbb{R}^d)\,. \tag{IV.20}$$

Using the fact that the closure of A is just the infinitesimal generator of the (strongly continuous unitary one-parameter) *dilation group* $\{W_t\}_{t\in\mathbb{R}}$ defined on $L^2(\mathbb{R}^d)$ by

$$(W_t\psi)(x) := e^{td/2}\psi(e^t x)\,, \tag{IV.21}$$

it can be shown [4] that A is essentially self-adjoint (*cf* [4, Prop. 4.2.3]). We denote the self-adjoint extension by the same symbol A.

The C^1-regularity

We observe that W_t leaves $\mathfrak{D}(H)$ invariant (*cf* [4, Prop. 4.2.4]). Hence, in view of Theorem IV.3, it remains to check the continuity of $i[H,A]$ considered as an operator between $\mathfrak{D}(H)$ and its dual $\mathfrak{D}(H)^*$.

Recall that the space $C_0^\infty(\mathbb{R}^d)$ is a core for both the operators H and A, whence we get that it is also a dense subspace of $\mathfrak{D}(H)\cap\mathfrak{D}(A)$. For all $\psi\in C_0^\infty(\mathbb{R}^d)$, an integration by parts gives the identity

$$l[\psi] = \big(\psi,(2H_0 - x\cdot\nabla V)\psi\big)\,.$$

Consequently,

$$\begin{aligned}\big|l[\psi]\big| &= \big|2\big(\psi,2H_0\psi\big) - \big((H_0+1)\psi,(H_0+1)^{-1}(x\cdot\nabla V)(H_0+1)^{-1}(H_0+1)\psi\big)\big|\\ &\le 2\|\psi\|\|H_0\psi\| + \|(H_0+1)\psi\|^2\big\|(H_0+1)^{-1}(x\cdot\nabla V)(H_0+1)^{-1}\big\|\,,\end{aligned}$$

which can be cast into the inequality (IV.18) after writing

$$\|H_0\psi\| = \big\|H_0(H+i)^{-1}(H+i)\psi\big\| \le \big\|H_0(H+i)^{-1}\big\|\,\|(H+i)\psi\|\,,$$

where $H_0(H+i)^{-1}$ is a bounded operator on $L^2(\mathbb{R}^d)$, and assuming

$$(H_0+1)^{-1}(x\cdot\nabla V)(H_0+1)^{-1}\in\mathcal{B}\big(L^2(\mathbb{R}^d)\big)\,. \tag{IV.22}$$

Under this condition, l extends to a bounded form on $\mathfrak{D}(H)$ and we can write

$$i[H,A] = 2H_0 - x\cdot\nabla V \tag{IV.23}$$

as an operator identity in $\mathcal{B}(\mathfrak{D}(H),\mathfrak{D}(H)^*)$. This proves that $H\in C^1(A)$.

The Mourre estimate

We rewrite (IV.23) as follows

$$i[H,A] = 2H+\tilde V\,, \qquad \text{where} \qquad \tilde V := -2V - x\cdot\nabla V\,,$$

and sandwich the both sides between the spectral projections $E_H(J)$,

$$E_H(J)\ i[H,A]\ E_H(J) \ = \ 2E_H(J)\,H\,E_H(J) + E_H(J)\,\tilde V\,E_H(J)\,.$$

[4] To be done.

Strengthening the condition (IV.22) to

$$(H_0+1)^{-1}(x\cdot\nabla V)(H_0+1)^{-1}\in\mathcal{B}_\infty\big(L^2(\mathbb{R}^d)\big) \tag{IV.24}$$

and assuming also

$$V(H_0+1)^{-1}\in\mathcal{B}_\infty\big(L^2(\mathbb{R}^d)\big)\,, \tag{IV.25}$$

it follows that $E_H(J)\,\tilde V\,E_H(J)$ is compact for any finite interval J. Note that (IV.25) means that V is a relatively compact perturbation of H_0, which implies the stability of the essential spectrum

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

If J lies below 0 (the threshold of the essential spectrum), then $E_H(J)$ and $E_H(J)\,H\,E_H(J)$ are also compact, so the Mourre estimate (IV.14) is trivially satisfied. If $J=(a,b)$ with $a>0$, then $E_H(J)\,H\,E_H(J)\geq aE_H(J)$, so the Mourre estimate holds in this case as well.

Summing up, we have established:

Theorem IV.4 (The Mourre estimate for Schrödinger operators)**.** *Let $H=H_0+V$, where V is bounded. Assume* (IV.25) *and* (IV.24)*. Then the Mourre estimate holds for H on any bounded open interval J which does not contain* 0*.*

Remark IV.3 (The free Hamiltonian)**.** The strict Mourre estimate holds for H_0 on any bounded open interval J which does not contain 0.

About the assumptions

The hypotheses (IV.25) and (IV.24) are essentially restrictions on the asymptotic behaviour of V. For instance, sufficient conditions which guarantee the hypotheses are given by (*cf* [4, Prop. 4.1.3])

$$V(x)\xrightarrow[|x|\to\infty]{}0\quad\Longrightarrow\quad\text{(IV.25)}\,,\qquad x\cdot\nabla V(x)\xrightarrow[|x|\to\infty]{}0\quad\Longrightarrow\quad\text{(IV.24)}\,.$$

However, what really (IV.24) (respectively (IV.22)) means is that the form defined for ϕ and ψ in the Schwartz space $\mathcal{S}(\mathbb{R}^d)$ by

$$(\phi,\psi)\mapsto\int_{\mathbb{R}^d}V(x)\;\nabla\cdot\Big\{x\,\overline{[(H_0+1)^{-1}\phi](x)}\,[(H_0+1)^{-1}\psi](x)\Big\}\,dx$$

extends to the form of a compact (respectively bounded) operator. Note that V need not have derivatives in the classical sense for this to hold. For instance, if $\langle\cdot\rangle V$ is relatively compact (respectively bounded) with respect to H_0, then (IV.24) (respectively (IV.22)) holds. Hence, a sufficient condition which guarantees the hypothesis (IV.24) is given by

$$\langle x\rangle V(x)\xrightarrow[|x|\to\infty]{}0\quad\Longrightarrow\quad\text{(IV.24)}\,.$$

IV.3.4 Control of embedded eigenvalues

We now turn to consequences of the validity of a Mourre estimate for H on its spectral properties. We first focus on properties of embedded eigenvalues. The following technical result is useful also in other areas of spectral analysis.

Theorem IV.5 (Virial theorem)**.** *Let H and A be self-adjoint operators such that $H \in C^1(A)$. Then*

$$\psi \text{ is an eigenfunction of } H \qquad \Longrightarrow \qquad \big(\psi, i[H,A]\psi\big) = 0\,.$$

Remark IV.4 (About the mistake in [8])**.** Formally, the statement is obvious, just by expanding the commutator. However, when the operators are unbounded, some care is required. This is probably best demonstrated by the fact that the proof presented in the first edition of the 1987 book [8] contained a mistake. This was discovered by V. Georgescu and C. Gérard in 1999 [12] and corrected in the second (2008) edition of the book [7]. The present proof is overtaken from [4]; its simplicity demonstrates the usefulness of the C^1-regularity framework.

Proof. More generally, we show that ($\lambda \in \mathbb{R}$)

$$\psi_1, \psi_2 \in \mathfrak{D}(H) \quad \text{satisfy} \quad H\psi_k = \lambda\psi_k \qquad \Longrightarrow \qquad \big(\psi_1, i[H,A]\psi_2\big) = 0\,.$$

Note that the eigenvalue equations imply

$$\psi_1 = (\lambda - i)R_i\psi_1\,, \qquad \psi_2 = (\lambda + i)R_{-i}\psi_2\,. \tag{IV.26}$$

Then the formula (IV.17) yields

$$\begin{aligned}\big(\psi_1, i[H,A]\psi_2\big) &= \big(\psi_1, (H+i)\, i[A, R_{-i}]\,(H+i)\psi_2\big) \\ &= (\lambda+i)^2\big(\psi_1, i[A,R_{-i}]\psi_2\big)\,.\end{aligned}$$

Recalling the definition (IV.16),

$$\begin{aligned} i[A, R_z] &\equiv \text{s-}\lim_{t\to 0} \frac{e^{iAt}R_z e^{-iAt} - R_z}{t} \\ &= \text{s-}\lim_{t\to 0} \frac{[e^{iAt}, R_z]\, e^{-iAt}}{t} \\ &= \text{s-}\lim_{t\to 0} \Bigg[\underbrace{\frac{e^{iAt} - I}{t}}_{B_t}, R_z\Bigg]\,. \end{aligned}$$

we therefore have

$$\begin{aligned}\big(\psi_1, [A, R_{-i}]\psi_2\big) &= \text{s-}\lim_{t\to 0} \big(\psi_1, [B_t, R_{-i}]\psi_2\big) \\ &= \text{s-}\lim_{t\to 0} \big\{\big(\psi_1, B_t R_{-i}\psi_2\big) - \big(R_i\psi_1, B_t\psi_2\big)\big\}\,,\end{aligned}$$

where the expression in the curly brackets is zero for all $t \neq 0$ due to (IV.26). This shows that $\big(\psi_1, i[H,A]\psi_2\big) = 0$. □

As a consequence of the virial theorem, we readily see that the point spectrum of H is empty in any open interval J on which the *strict* Mourre estimate holds for H. Indeed, if ψ were an eigenfunction corresponding to an eigenvalue in J, then we would get a contradiction

$$0 = \big(\psi, i[H,A]\psi\big) \geq a > 0\,.$$

It is more interesting that we have a control of eigenvalues also in intervals where the weaker form (IV.14) of the Mourre estimate holds.

Corollary IV.2 (Finiteness of point spectrum). *Let H and A be self-adjoint operators such that $H \in C^1(A)$. If A is conjugate to H on an open interval J, then $J \cap \sigma_{\mathrm{p}}(H)$ is composed of a finite number of eigenvalues, and each of these eigenvalues has finite multiplicity.*

Proof. Assume that the conclusion of the corollary is false. Then there exists an infinite orthonormal sequence $\{\psi_n\}_{n=1}^{\infty} \subset E_H(J)\mathcal{H}$ of eigenfunctions of H. By the virial theorem and the Mourre estimate,

$$0 = \big(\psi_n, i[H,A]\psi_n\big) = \big(\psi_n, E_H(J)\, i[H,A]\, E_H(J)\psi_n\big) \geq a + (\psi_n, K\psi_n)\,.$$

Now, since $\psi_n \to 0$ weakly in $\mathcal{H}$ as $n \to \infty$ and K is compact, one then has $(\psi_n, K\psi_n) \to 0$ as $n \to \infty$. This contradicts the positivity $a > 0$. □

As a consequence of this corollary and Theorem IV.4, we get

Theorem IV.6 (Finiteness of point spectrum for Schrödinger operators). *Let $H = H_0 + V$, where V is bounded. Assume* (IV.25) *and* (IV.24). *Then*

1. $\sigma_{\mathrm{p}}(H) \cup \{0\}$ *is closed and countable,*
2. $\sigma_{\mathrm{p}}(H) \setminus \{0\}$ *is composed of finitely degenerated eigenvalues which can accumulate at* 0 *(and $+\infty$) only.*

IV.3.5 Absence of singularly continuous spectrum

A abstract setting

In the preceding section, as a consequence of the Mourre estimate, we have obtained information about properties of the singular spectrum of H represented by eigenvalues just by requiring $H \in C^1(A)$. It turns out that it is essential to require some additional regularity of H with respect to A in order to deduce the absence of singularly continuous spectrum from the Mourre estimate.

Definition IV.4 (C^2-regularity class). We say that H is of class $C^2(A)$ if the map (IV.15) is of class C^2 for the strong topology of $\mathcal{B}(\mathcal{H})$.

This regularity class is far from being optimal for what we are going to state, but it is easily characterizable in terms of the double commutator $i[i[H,A],A]$, thought as the operator associated to a sesquilinear form initially defined on $\mathfrak{D}(H) \cap \mathfrak{D}(A)$ (note that such a form is well defined if $H \in C^1(A)$).

Theorem IV.7 ([4, Thm. 6.3.4]). *Assume that the unitary one-parameter group $\{e^{iAt}\}_{t\in\mathbb{R}}$ leaves the domain $\mathfrak{D}(H)$ invariant,* i.e., $e^{iAt}\,\mathfrak{D}(H) \subset \mathfrak{D}(H)$. *Then*

$$H \in C^2(A) \quad \Longleftarrow \quad \begin{cases} i[H,A] \in \mathcal{B}\big(\mathfrak{D}(H), \mathcal{Q}(H)^*\big)\,, \\ i[i[H,A],A] \in \mathcal{B}\big(\mathfrak{D}(H), \mathfrak{D}(H)^*\big)\,. \end{cases}$$

Here $\mathcal{Q}(H) := \mathfrak{D}(|H|^{1/2})$ denotes the form domain of H.

Notice that the first condition (about the single commutator) is stronger than that of Theorem IV.3.

We say that a self-adjoint operator *has a spectral gap* if $\sigma(H) \neq \mathbb{R}$.

Theorem IV.8 (Absence of singularly continuous spectrum for operators with a spectral gap)**.** *Let H and A be self-adjoint operators such that $H \in C^2(A)$. Assume that H has a spectral gap. If A is conjugate to H on an open interval J, then*

$$J \cap \sigma_{\mathrm{sc}}(H) = \varnothing \,.$$

In fact, the spectral result follows as a consequence of some sort of LAP in a scale spaces given by $\mathfrak{D}(A)$. Unfortunately the proof of the theorem (adapted from [4, Thm. 7.4.2]) is rather lengthy and we have to omit it. We only mention that the proof centers about the analysis of the operator

$$G_\varepsilon(z) := \big(H - i\varepsilon\, i[H, A] - z\big)^{-1} \,.$$

This operator is not as mysterious as it appears to be at first glance: G_ε is the resolvent of the operator $H - \varepsilon[H, A]$, which is the first term in the formal power series expansion of the complex dilated Hamiltonian $e^{\varepsilon A} H e^{-\varepsilon A}$ (*cf* [4, opening of Sec. 7] or [8, Sec. 4.3] for more details).

An application to Schrödinger operators

Sufficient conditions for the validity of the Mourre estimate for Schrödinger operators $H = H_0 + V$ are established in Theorem IV.4. Since V is assumed to be bounded and $\sigma(H_0) = [0, \infty)$, H is bounded from below, hence it has a spectral gap. To apply Theorem IV.8, we only need to impose additional conditions on the potential V in order to have $H \in C^2(A)$, where A is again the dilation operator (IV.20).

We employ Theorem IV.7, for which we recall that $\mathfrak{D}(H)$ is left invariant by the dilation group (IV.21). Recall also that $\mathfrak{D}(H) = W^{2,2}(\mathbb{R}^d)$ and $\mathcal{Q}(H) = W^{1,2}(\mathbb{R}^d)$. Then it is obvious that the commutator (IV.23) extends to an operator in $\mathcal{B}(\mathfrak{D}(H), \mathcal{Q}(H)^*)$, provided that (IV.22)) is strengthen to

$$(H_0 + 1)^{-1/2}(x \cdot \nabla V)(H_0 + 1)^{-1} \in \mathcal{B}\big(L^2(\mathbb{R}^d)\big) \,. \qquad \text{(IV.27)}$$

Again, a sufficient condition which guarantees this hypothesis is that $\langle\cdot\rangle V$ is relatively bounded with respect to H_0.

At the same time, using (IV.23), it is straightforward to compute the double commutator

$$i\big[i[H, A], A\big] = 4H_0 + x \cdot \nabla V + x \cdot \nabla^2 V \cdot x \,, \qquad \text{(IV.28)}$$

where $\nabla^2 V := \nabla V \nabla^<$ is the Hessian tensor of V. The right hand side represents an operator in $\mathcal{B}(\mathfrak{D}(H), \mathfrak{D}(H)^*)$, provided that

$$(H_0 + 1)^{-1}\big(x \cdot \nabla^2 V \cdot x\big)(H_0 + 1)^{-1} \in \mathcal{B}\big(L^2(\mathbb{R}^d)\big) \,. \qquad \text{(IV.29)}$$

Clearly, the boundedness of $\langle\cdot\rangle^2 V$ is sufficient to guarantee (IV.29).

Summing up, we have established $H \in C^2(A)$, and Theorem IV.8 yields:

Theorem IV.9 (Absence of singularly continuous spectrum for Schrödinger operators)**.** *Let $H = H_0 + V$, where V is bounded. In addition to* (IV.25) *and* (IV.24)*, assume also* (IV.27) *and* (IV.29)*. Then*

$$\sigma_{\mathrm{sc}}(H) = \varnothing \,.$$

Chapter V

Geometric aspects

In the last chapters we studied the influence of the presence of potential V on the spectrum of the Schrödinger operator $H = H_0 + V$ on $L^2(\mathbb{R}^d)$. Here $H_0 = -\Delta$ is the Hamiltonian of the free particle and $V = V(x)$ is a multiplication operator representing an external field (*e.g.*, the Coulomb interaction between electrons and nuclei in atoms).

In this chapter we consider the situation when the Hamiltonian H acts as the "free" Hamiltonian H_0, but its configuration space is *restricted* to a non-trivial subset $\Omega \subset \mathbb{R}$ (*i.e.*, the Hilbert space is $L^2(\Omega)$ now). Of course, we have to specify the boundary conditions on $\partial\Omega$; we shall restrict to *Dirichlet boundary conditions* only. Then the present geometric perturbation can be related to the previous potential perturbation of H_0 by formally putting

$$V(x) := \begin{cases} 0 & \text{if} \quad x \in \Omega\,, \\ +\infty & \text{if} \quad x \in \mathbb{R}^d \setminus \Omega\,. \end{cases}$$

Mathematically, the free Hamiltonian on $L^2(\Omega)$ subject to Dirichlet boundary conditions on $\partial\Omega$ is introduced as the *Dirichlet Laplacian* operator $-\Delta_D^\Omega$.

As well as being simple to treat, Dirichlet boundary conditions are directly relevant to a number of physical problems. In classical physics, these include heat flow in a medium whose boundary is kept at zero temperature and vibrations of an elastic membrane whose boundary is fixed. In the quantum context, this hard-wall boundary conditions are for instance used in semiconductor physics to model a quantum particle which is confined to a region by the barrier associated with a large chemical potential.

This last chapter is devoted to an analysis of the significant features of a domain Ω as regards the spectrum of the associated Dirichlet Laplacian. In the first part we state basic spectral properties of the Dirichlet Laplacian in three classes of Euclidean domains: quasi-conical, quasi-cylindrical and quasi-bounded domains. The last part is devoted to a more detailed analysis of *quantum waveguides*, a special class of quasi-cylindrical domains.

V.1 The Dirichlet Laplacian

We begin with defining the hard-wall Hamiltonian H on $L^2(\Omega)$. Here $\Omega \subset \mathbb{R}^d$ is an *arbitrary* domain (*i.e.* an open connected set), bounded or unbounded, no regularity assumptions are required. The norm and inner product in the Hilbert space $L^2(\Omega)$ will be denoted by $\|\cdot\|$ and $(\cdot,\cdot)$, respectively.

V.1.1 Definition

As in Section I.3, we first introduce the minimal operator

$$\mathfrak{D}(\dot{H}) := C_0^\infty(\Omega)\,, \qquad \dot{H}\psi := -\Delta\psi\,,$$

which is densely defined, symmetric and non-negative. It clearly satisfies the Dirichlet boundary conditions, in fact in a very restrictive sense.

We define H to be the (self-adjoint) Friedrichs extension of $\dot{H}$. That is, H is the operator associated with the closure h of the quadratic form $\dot{h}$ defined by

$$\mathfrak{D}(\dot{h}) := C_0^\infty(\Omega)\,, \qquad \dot{h}[\psi] := (\psi, -\Delta\psi) = \|\nabla\psi\|^2\,.$$

However, from the theory of Sobolev spaces [3], we know the closure explicitly:

$$\mathfrak{D}(h) = W_0^{1,2}(\Omega)\,, \qquad h[\psi] = \|\nabla\psi\|^2\,,$$

where ∇ should be interpreted as the distributional gradient. A difference with respect to the whole-space situation (I.12) is that $W_0^{1,2}(\Omega) \neq W^{1,2}(\Omega)$ in general; in fact, the zero in the subscript gives a meaning to the Dirichlet boundary conditions in a generalized sense.

By the representation theorem, it follows that

$$\mathfrak{D}(H) = \left\{\psi \in W_0^{1,2}(\Omega) \,\middle|\, \exists\eta \in L^2(\Omega),\ \forall\phi \in C_0^\infty(\Omega),\ (\nabla\phi, \nabla\psi) = (\phi, \eta)\right\},$$
$$H\psi = \eta\,.$$

Noticing that the identity $(\nabla\phi, \nabla\psi) = (\phi, \eta)$ with $\phi \in C_0^\infty(\Omega)$ is just the definition of the distributional Laplacian $\eta = -\Delta\psi$, we are allowed to write

$$\mathfrak{D}(H) = \left\{\psi \in W_0^{1,2}(\Omega) \,\middle|\, \Delta\psi \in L^2(\Omega)\right\}, \qquad H\psi = -\Delta\psi\,.$$

H is the *Dirichlet Laplacian.* In order to stress the dependence on Ω and the role of Dirichlet boundary conditions, we shall write

$$H =: -\Delta_D^\Omega\,.$$

Obviously, $-\Delta_D^{\mathbb{R}^d} = H_0$, where H_0 is the free Hamiltonian of Section I.3.

We would like to stress that $-\Delta_D^\Omega$ is well defined in this way for an *arbitrary* domain Ω (no regularity assumptions are needed). But one has to give up the "usual" characterization of $\mathfrak{D}(-\Delta_D^\Omega)$ as a subset of the Sobolev space $W^{2,2}(\Omega)$. If, however, $\partial\Omega$ is sufficiently regular, say of class C^2, then we indeed have

$$\mathfrak{D}(-\Delta_D^\Omega) = W_0^{1,2}(\Omega) \cap W^{2,2}(\Omega) = \left\{\psi \in W^{2,2}(\Omega) \mid \psi \upharpoonright \partial\Omega = 0\right\}, \qquad \text{(V.1)}$$

where $\psi \upharpoonright \partial\Omega$ means the boundary trace of ψ. This can be seen as follows. We clearly have $W_0^{1,2}(\Omega) \cap W^{2,2}(\Omega) \subset \mathfrak{D}(-\Delta_D^\Omega)$ for an arbitrary domain Ω. Under the additional regularity assumption, the opposite inclusion follows by standard elliptic regularity theory. Indeed, by [13, Thm. 8.12], the generalized solution $\psi \in W^{1,2}(\Omega)$ to the problem $-\Delta\psi = \eta \in L^2(\Omega)$ is known to belong to $W^{2,2}(\Omega)$. The second equality in (V.1) then follows by the trivial traces theorem [3, Thm. 5.37].

V.1.2 Glazman's classification of domains

In [14], I. M. Glazman introduced the following useful classification (see also [10, Sec. X.6.1]).

Definition V.1 (Glazman's classification of Euclidean domains)**.** A domain $\Omega \subset \mathbb{R}^d$ is

- *quasi-conical* if it contains arbitrarily large balls;
- *quasi-cylindrical* if it is not quasi-conical but it contains infinitely many (pairwise) disjoint identical (*i.e.* of the same radius, congruent) balls;
- *quasi-bounded* if it is neither quasi-conical nor quasi-cylindrical.

Obviously, each domain $\Omega \subset \mathbb{R}^d$ belongs to one of the classes. Bounded domains represent a subset of quasi-bounded domains, but the latter class is much larger as we shall see below. The whole Euclidean space $\mathbb{R}^d$ or its conical sector are examples of quasi-conical domains. Finally, an infinite (solid) cylinder $\mathbb{R} \times B$, where B is a $(d-1)$-dimensional ball, is a quasi-cylindrical domain.

Now we describe the basic spectral properties of the Dirichlet Laplacian $-\Delta_D^\Omega$ as regards the above classification.

Quasi-conical domains

The spectrum is easiest to locate for quasi-conical domains:

Theorem V.1 (Spectrum of quasi-conical domains)**.** *If* Ω *is quasi-conical, then*

$$\sigma(-\Delta_D^\Omega) = \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = [0,\infty)\,.$$

In particular, $\sigma_{\mathrm{disc}}(-\Delta_D^\Omega) = \varnothing$.

Proof. The proof is very similar to the location of spectrum of the free Hamiltonian (Theorem I.5).

1. $\sigma(-\Delta_D^\Omega) \subset [0,\infty)$ This inclusion follows trivially because the Dirichlet Laplacian is a non-negative operator, *i.e.* $-\Delta_D^\Omega \geq 0$.

2. $\sigma(-\Delta_D^\Omega) \supset [0,\infty)$ To prove the opposite inclusion, for every $n \in \mathbb{N}^*$ we set

$$\tilde{\psi}_n(x) := \psi_n(x - x_n)\,,$$

where $\{\psi_n\}_{n\in\mathbb{N}^*}$ is the singular sequence (I.15) of the free Hamiltonian corresponding to the energy $|k|^2$, with $k \in \mathbb{R}^d$, and x_n is the center of the ball of radius so large that

$$\mathrm{supp}(\tilde{\psi}_n) \subset \Omega$$

(by the hypothesis about Ω, such a sequence of points $\{x_n\}_{n\in\mathbb{N}^*}$ exists). Using the results in the proof Theorem I.5, it is straightforward to show that $\{\tilde{\psi}_n\}_{n\in\mathbb{N}^*}$ is a singular sequence of the Dirichlet Laplacian corresponding to the same energy $|k|^2$. Hence the result follows by the Weyl criterion (Theorem I.2).

3. $\sigma(-\Delta_D^\Omega) = \sigma_{\mathrm{ess}}(-\Delta_D^\Omega)$ Finally, it is clear that the spectrum is purely essential because (non-degenerate) intervals have no isolated points. ∎

It follows that the spectrum of (the Dirichlet Laplacian in) quasi-cylindrical domains $\Omega \subset \mathbb{R}^d$ coincides, as a set, with the spectrum of the free Hamiltonian in $\mathbb{R}^d$. Of course, the result does not say anything about the *nature* of the essential spectrum. We do not follow this direction here. [1]

Having located the spectral threshold, we would rather like to ask the question whether the Dirichlet Laplacian is critical or subcritical.

$\boxed{d \geq 3}$ The answer is trivial in high dimensions, *i.e.* $d \geq 3$, where the classical Hardy inequality (Theorem I.6) holds: $-\Delta_D^\Omega$ is always subcritical if $d \geq 3$. This follows easily from the fact that the classical Hardy inequality valid in $\mathbb{R}^d$ remains true in Ω, just because $W_0^{1,2}(\Omega) \subset W^{1,2}(\mathbb{R}^d)$ (by extending the element of $W_0^{1,2}(\Omega)$ by zero to the whole space $\mathbb{R}^d$). More specifically, for $d \geq 3$ we have (*cf* (II.1))

$$-\Delta_D^\Omega \geq \frac{(d-2)^2}{4} \frac{1}{\delta^2},$$

where $\delta(x) := |x|$ is the distance to the origin of $\mathbb{R}^d$.

$\boxed{d = 1}$ The answer is also trivial for $d = 1$. In that case, Ω is either $\mathbb{R}$ or a semi-axis (without loss of generality, it can be identified with $(0, \infty)$). In the former case we already know that $-\Delta_D^\Omega$ is critical (Theorem II.2), while in the latter case it is subcritical due to the classical one-dimensional Hardy inequality (Lemma I.1)

$$-\Delta_D^{(0,\infty)} \geq \frac{1}{4} \frac{1}{\delta^2}.$$

$\boxed{d = 2}$ The situation is less clear for $d = 2$. As in the one-dimensional case, the case $\Omega = \mathbb{R}^2$ is critical, while the semi-plane $\Omega = \mathbb{R} \times (0, \infty)$ can be shown to be subcritical (as a consequence of Lemma I.1 and the separation of variables). On the other hand, removing just one point $a \in \Omega$, *i.e.*, setting $\Omega = \mathbb{R}^2 \setminus \{a\}$ is not enough to make the operator $-\Delta_D^\Omega$ subcritical, essentially because

$$W_0^{1,2}\big(\Omega \setminus \{a\}\big) = W_0^{1,2}(\Omega).$$

This suggests that a "significant part" of Ω has to be removed in order to make the Dirichlet Laplacian subcritical in $d = 2$. (It should be possible to make this statement precise by using the notion of *capacity*.) Without trying to derive the most general result here, a sufficient condition is given by the following theorem (trivially valid in the other dimensions too).

Theorem V.2 (Generic subriticality of quasi-conical domains)**.** *Let Ω be quasi-conical.*

$$\big(\mathbb{R}^d \setminus \Omega\big)^o \quad \textit{is open} \qquad \Longrightarrow \qquad -\Delta_D^\Omega \quad \textit{is subcritical.}$$

Proof. The proof is very similar to the proof of the classical Hardy inequality (Theorem I.6). Without loss of generality, we may assume that $0 \in (\mathbb{R}^d \setminus \Omega)^o$. By hypothesis, there exists $\varepsilon > 0$ such that the ball $B_\varepsilon(0)$ is contained in the complement $(\mathbb{R}^d \setminus \Omega)^o$. Let $\psi \in C_0^\infty(\Omega)$ and extend it by zero to the whole $\mathbb{R}^d$. Then we can proceed exactly as in the proof of Theorem I.6: passing

[1] A reference to the work where this problem is studied.

to spherical coordinates, neglecting the angular-derivative term and using the one-dimensional Hardy inequality (Lemma I.1), we arrive at the inequality ($\mathbb{R}^d$ can be replaced by Ω)

$$\int_{\mathbb{R}^d} |\nabla\psi(x)|^2 \, dx \geq \frac{(d-2)^2}{4} \int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|^2} \, dx \,.$$

By density, it extends to all $\psi \in W_0^{1,2}(\Omega)$. It looks like the classical Hardy inequality of Theorem I.6, but the difference is that the present inequality holds in *all* dimensions. This is due to the fact that the function

$$r \mapsto \sqrt{r^{d-1}}\, \tilde{\psi}(r,\theta) \,,$$

where $\tilde{\psi}$ is the function ψ expressed in the spherical coordinates, belongs (for every $\theta \in S^{d-1}$) to $W_0^{1,2}(\mathbb{R}_+)$ even if $d = 1, 2$, just because it is identically zero in a neighbourhood of $r = 0$. Summing up, there exists a *global* Hardy inequality for $-\Delta_D^\Omega$, which implies that the operator is subcritical. □

Remark V.1. If the boundary $\partial\Omega$ is sufficiently regular, say continuous, then the complement $(\mathbb{R}^d \setminus \Omega)^o$ is always open whenever $\Omega \neq \mathbb{R}^d$.

Quasi-bounded domains

Theorem V.1 says that the spectrum of quasi-conical domains is purely essential, the discrete spectrum is empty. The other extreme case is represented by quasi-bounded domains, for which (as for bounded domains) the spectrum is purely discrete, at least under some regularity assumptions.

More precisely, a sufficient and necessary condition for $-\Delta_D^\Omega$ to have a purely discrete spectrum is that the embedding

$$W_0^{1,2}(\Omega) \hookrightarrow L^2(\Omega) \qquad \text{is compact.} \tag{V.2}$$

(Indeed, the space $W_0^{1,2}(\Omega)$ is the form domain of $-\Delta_D^\Omega$ and the embedding is the composite of the isometry $(-\Delta_D^\Omega + I)^{1/2} : W_0^{1,2}(\Omega) \to L^2(\Omega)$ and the bounded operator $(-\Delta_D^\Omega + I)^{-1/2} : L^2(\Omega) \to L^2(\Omega)$.) Shortly below we shall see that the quasi-boundedness is *necessary* for (V.2) to hold (*i.e.*, there is always an essential spectrum for quasi-conical and quasi-cylindrical domains). However, it is not sufficient [3, Sec. 6.14]. Schematically,

$$\Omega \text{ is quasi-bounded} \qquad \begin{matrix} \not\Longrightarrow \\ \Longleftarrow \end{matrix} \qquad \text{(V.2) holds.}$$

The validity of (V.2) is well studied in the theory of Sobolev spaces (see, *e.g.*, [3, 10]). Here we provide one example of sufficient condition (*cf* [10, Thm. 5.17]):

Theorem V.3 (Discreteness of spectra for quasi-bounded domains)**.** *One has*

$$\limsup_{|x|\to\infty,\ x\in\Omega} \big|\Omega \cap B_1(x)\big| = 0 \qquad \Longrightarrow \qquad \text{(V.2) } \textit{holds.}$$

Consequently, $\sigma(-\Delta_D^\Omega) = \sigma_{\mathrm{disc}}(-\Delta_D^\Omega)$, $\sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = \varnothing$.

It is interesting to compare the sufficient condition of Theorem V.3 with the following equivalent characterization of quasi-bounded domains (*cf* Definition V.1):

$$\Omega \text{ is quasi-bounded} \qquad \Longleftrightarrow \qquad \limsup_{|x|\to\infty,\ x\in\Omega} \operatorname{dist}(x,\partial\Omega) = 0\,.$$

Roughly speaking, quasi-bounded domains are "narrow at infinity", but the narowness must be "inessential in an integral sense" to have (V.2).

Example V.1 (Spiny urchin)**.** To see that Theorem V.3 represents just a sufficient condition, we recall the nice example of *spiny urchin* [3, Sec. 6.17]:

$$\Omega := \mathbb{R}^2 \setminus \bigcup_{k=1}^{\infty} S_k\,, \tag{V.3}$$

where the sets S_k are specified in polar coordinates $(r,\vartheta) \in \mathbb{R}_+ \times [0,2\pi)$ by

$$S_k := \left\{(r,\vartheta) \mid \quad r \geq k \quad \wedge \quad \vartheta = n\pi/2^k \quad \text{for} \quad n = 1,2,\dots,2^{k+1}\right\}\,.$$

Note that this domain, though quasi-bounded, is simply connected and has empty exterior. Clearly, it does not satisfy the hypothesis of Theorem V.3. However, (V.2) holds for it. In fact, it turns out that the compactness of (V.2) depends in an essential way on the dimension of $\partial\Omega$. Any quasi-bounded domain whose boundary consists of reasonably regular $(d-1)$-dimensional surfaces satisfies (V.2).

On the other hand, if we replace the lines in (V.3) by "dots accumulating at infinity", *i.e.*, we define $\dot\Omega$ as the domain in $\mathbb{R}^2$ obtained by deleting from the plane the union of the sets

$$\dot S_k := \Big\{(r,\vartheta) \mid \quad r = k + \sqrt{m} \quad \text{for} \quad m \in \mathbb{N} \\ \wedge \quad \vartheta = n\pi/2^k \quad \text{for} \quad n = 1,2,\dots,2^{k+1}\Big\}\,,$$

then exactly the same proof as that of Theorem V.1 for quasi-conical domains imply that

$$\sigma(-\Delta_D^{\dot\Omega}) = \sigma_{\mathrm{ess}}(-\Delta_D^{\dot\Omega}) = [0,\infty)\,.$$

This is obvious since a finite number of points in an open planar set (*e.g.*, an arbitrarily large disc) form a polar set. □

More generally, we have

Theorem V.4 ([2])**.** *Let $d \geq 2$. If $\partial\Omega$ consists only of isolated points with no finite accumulation point, then* (V.2) *does not hold.*

Finally, let us remark that in $d = 1$ one knows that quasi-boundedness is necessary and sufficient for an arbitrary (not necessary connected) open subset $\Omega \subset \mathbb{R}$ to satisfy (V.2). In higher dimensions, the necessary and sufficient conditions for the validity of (V.2) can be obtained in terms of capacity.

Recall that an operator having an eigenvalue as the lowest point in its spectrum is always critical (Proposition II.1). Hence, the issue of criticality is trivial for quasi-bounded domains for which (V.2) holds (under this condition, $-\Delta_D^\Omega$ is critical).

Quasi-cylindrical domains

Finally, we consider the class of quasi-cylindrical domains. They are most interesting because they generally contain both the essential and discrete spectra. But this make them also most difficult to study. The following result is probably the only one which can be stated in general.

Theorem V.5 (Spectrum of quasi-cylindrical domains)**.** *Let Ω be quasi-cylindrical. Set*

$$R_{\max} := \sup \big\{ R \mid \Omega \textit{ contains a sequence of disjoint balls of radius } R \big\} .$$

Then

$$\inf \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) \leq \frac{\mu_1}{R_{\max}^2} ,$$

where μ_1 denotes the lowest eigenvalue of the Dirichlet Laplacian in the unit ball in $\mathbb{R}^d$ (μ_1 depends exclusively on the dimension d).
Consequently, $\sigma(-\Delta_D^\Omega) = \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) \cup \sigma_{\mathrm{disc}}(-\Delta_D^\Omega)$ in general.

Proof. The idea is to construct a non-compact sequence supported on the disjoint balls. Let $\{x_n\}_{n\in\mathbb{N}^*} \subset \Omega$ be a set of points such that $\{B_R(x_n)\}_{n\in\mathbb{N}^*} \subset \Omega$ is the set of mutually disjoint balls for all $R \in (0, R_{\max})$. Let ψ be the first eigenfunction of $-\Delta_D^{B_R(0)}$, normalized to 1 in $L^2(B_R(0))$. For all $n \in \mathbb{N}^*$, we set

$$\psi_n(x) := \psi(x - x_n)$$

and extend it by zero to the whole Ω. Then ψ_n's are mutually orthonormal in $L^2(\Omega)$ and satisfy $\|\nabla\psi_n\|_{L^2(\Omega)}^2 = \mu_1/R^2$. Hence, choosing the n-dimensional subspace $\mathcal{L}^n = \mathrm{span}\{\psi_1, \dots, \psi_n\}$ in the minimax principle (Theorem I.3), we get

$$\lambda_n \leq \mu_1/R^2$$

for *all* $n \in \mathbb{N}^*$. Consequently, $\inf \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = \lambda_\infty \equiv \lim_{n\to\infty} \lambda_n \leq \mu_1/R^2$. Since the argument held for all $R \in (0, R_{\max})$, we conclude with the stated inequality. □

Remark V.2. It is not necessary to assume that Ω is quasi-cylindrical in Theorem V.5. The result applies to quasi-conical domains as well (with $R_{\max} = \infty$), in agreement with Theorem V.1.

For quasi-cylindrical domains the precise location of the essential spectrum is difficult. More generally, we can say that the question of criticality constitutes a very challenging problem, and one can hardly study it in the full generality. For this reason, we focus on a special class of quasi-cylindrical domains in the sequel.

V.2 Quantum waveguides

In this last section we are concerned with a special class of quasi-cylindrical domains: *tubes*. Our motivation is twofold. First, the tubular geometry is rich enough to demonstrate the complexity of the class of quasi-cylindrical domains. Second, the Dirichlet Laplacian in tubes is a reasonable model for the Hamiltonian in quantum-waveguide nanostructures. For simplicity, and also because we have the physical motivation in mind, we restrict to three-dimensional tubes.

V.2.1 The geometry of tubes

The tubes we consider are obtained as a suitable deformation of the *straight tube* $\Omega_0 := \mathbb{R} \times \omega$. Here $\omega \subset \mathbb{R}^2$ is a bounded domain, which plays the role of cross-section of the tube. We do not assume any regularity conditions about the boundary $\partial\omega$. The characteristic features of the deformed geometry are as follows:

- unboundedness,
- uniform cross-section,
- local perturbation of Ω_0.

The deformed tube, denoted by Ω, is introduced as follows (the geometric preliminaries follow [18]).

The reference curve

We begin with a smooth (*i.e.* infinitely smooth) curve $\Gamma : \mathbb{R} \to \mathbb{R}^3$, which is assumed to be parameterized by its arc-length. Regarding Γ as a path of a unit-speed traveller in the space, it is convenient to describe its motion in a (non-inertial) reference frame moving along the curve. One usually adopts the so-called *distinguished Frenet frame* $\{e_1, e_2, e_3\}$ which satisfies the Serret-Frenet formulae

$$\begin{pmatrix} e_1 \\ e_2 \\ e_3 \end{pmatrix}^{\cdot} = \begin{pmatrix} 0 & \kappa & 0 \\ -\kappa & 0 & \tau \\ 0 & -\tau & 0 \end{pmatrix} \begin{pmatrix} e_1 \\ e_2 \\ e_3 \end{pmatrix}. \tag{V.4}$$

Here κ and τ is the *curvature* and *torsion* of Γ, respectively (actually defined by (V.4)). The elements of the triad $\{e_1, e_2, e_3\}$ are called the *tangent*, *normal* and *binormal* vectors, respectively, and are obtained from $\{\dot\Gamma, \ddot\Gamma, \dddot\Gamma\}$ by the Gramm-Schmidt orthonormalization process. One has to keep in mind that not every curve in $\mathbb{R}^3$ possesses the distinguished Frenet frame (see Problem V.1), but it always exists if the curvature is never vanishing, *i.e.* $\kappa > 0$. We refer to the books [17, 28] for more details about the geometry of space curves.

Problem V.1. Give an example of smooth curve which does not possess the distinguished Frenet frame.
Solution: [28, Chap. 1, p. 34]. [2]

The general moving frame

A general moving frame along Γ can be introduced by rotating normal components of the distinguished Frenet frame. More specifically, given a smooth function $\theta : \mathbb{R} \to \mathbb{R}$, we define a rotation matrix-valued function $\mathcal{R}^\theta : \mathbb{R} \to \mathrm{SO}(3)$ by

$$\mathcal{R}^\theta := \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}.$$

[2] Elaborate details.

This give rise to a new moving frame $\{e_1^\theta, e_2^\theta, e_3^\theta\}$ by setting

$$e_i^\theta := \sum_{j=1}^{3} \mathcal{R}_{ij}^\theta \, e_j \,, \qquad i \in \{1,2,3\} \,. \tag{V.5}$$

Note that $e_1^\theta(s) = e_1(s)$ for all $s \in \mathbb{R}$, while $e_2^\theta(s)$ (respectively $e_3^\theta(s)$) is rotated with respect to $e_2(s)$ (respectively $e_3(s)$) by the angle $\theta(s)$. Using (V.4), it is easy to check that the new frame evolves along the curve via

$$\begin{pmatrix} e_1^\theta \\ e_2^\theta \\ e_3^\theta \end{pmatrix}^{\cdot} = \begin{pmatrix} 0 & \kappa\cos\theta & \kappa\sin\theta \\ -\kappa\cos\theta & 0 & \tau-\dot\theta \\ -\kappa\sin\theta & -(\tau-\dot\theta) & 0 \end{pmatrix} \begin{pmatrix} e_1^\theta \\ e_2^\theta \\ e_3^\theta \end{pmatrix} . \tag{V.6}$$

The curved tube

The *curved tube* Ω is defined by moving the cross-section ω along the reference curve Γ together with a generally rotated frame (V.5). More precisely, we set

$$\Omega := \mathcal{L}(\Omega_0) \,,$$

where Ω_0 is the straight tube and

$$\mathcal{L} : \mathbb{R}^3 \to \mathbb{R}^3 : \left\{ (s,t) \mapsto \Gamma(s) + \sum_{j=2}^{3} t_j \, e_j^\theta(s) \right\} . \tag{V.7}$$

Since the curve Γ can be reconstructed from the curvature functions κ and τ (*cf* [17, Thm. 1.3.6]), the tube Ω is fully determined by giving the cross-section ω (including its position in $\mathbb{R}^2$) and the triple of functions κ, τ and θ.

The image of Ω_0 by $\mathcal{L}$ can be quite complex, in particular Ω can have self-intersections we would like to avoid. Furthermore, our strategy to deal with the curved geometry of the tube will be to use the identification

$$\Omega \simeq (\Omega_0, G) \,,$$

where the latter is the Riemannian manifold Ω_0 equipped with the metric $G = (G_{ij})$ induced by the mapping $\mathcal{L}$, *i.e.*,

$$G_{ij} := (\partial_i \mathcal{L}) \cdot (\partial_j \mathcal{L}) \,, \qquad i,j \in \{1,2,3\} \,.$$

Here the dot denotes the scalar product in $\mathbb{R}^3$. In other words, we parameterize Ω globally by means of the "coordinates" (s,t) of (V.7). To this aim, we need to impose natural restrictions in order to ensure that $\mathcal{L}$ induces a smooth *diffeomorphism* between Ω_0 and Ω.

Using (V.6), we find

$$G = \begin{pmatrix} f^2 + f_2^2 + f_3^2 & f_2 & f_3 \\ f_2 & 1 & 0 \\ f_3 & 0 & 1 \end{pmatrix}, \quad \begin{aligned} f(s,t) &:= 1 - [t_2\cos\theta(s) + t_3\sin\theta(s)]\,\kappa(s)\,, \\ f_2(s,t) &:= -t_3\,[\tau(s) - \dot\theta(s)]\,, \\ f_3(s,t) &:= t_2\,[\tau(s) - \dot\theta(s)]\,. \end{aligned} \tag{V.8}$$

Consequently,

$$|G| := \det(G) = f^2 \,.$$

By virtue of the inverse function theorem, the mapping $\mathcal{L}$ induces a *local* diffeomorphism provided that the Jacobian f does not vanish on Ω_0. In view of the uniform bounds

$$0 < 1 - a\,\|\kappa\|_{L^\infty(\mathbb{R})} \;\leq\; f \;\leq\; 1 + a\,\|\kappa\|_{L^\infty(\mathbb{R})} < \infty\,, \tag{V.9}$$

where the cross-section quantity

$$a := \sup_{t\in\omega} |t|$$

measures the distance of the farthest point of $\overline{\omega}$ to the origin of $\mathbb{R}^2$, the positivity of f is guaranteed by the hypothesis

$$\kappa \in L^\infty(\mathbb{R}) \qquad \text{and} \qquad a\,\|\kappa\|_{L^\infty(\mathbb{R})} < 1\,. \tag{V.10}$$

The mapping then becomes a *global* diffeomorphism if, in addition to (V.10), we assume that

$$\mathcal{L} \quad \text{is injective}\,. \tag{V.11}$$

Summing up, we have:

Proposition V.1. *Assume* (V.10) *and* (V.11)*. Then* $\mathcal{L} : \Omega_0 \to \Omega$ *is a smooth diffeomorphism. Consequently,* Ω *can be identified with the Riemannian manifold* (Ω_0, G)*. In particular,* Ω *is not self-intersecting.*

The natural hypotheses

For the convenience of the reader, we summarize here characteristic conditions needed for the construction of the tube Ω:

1. *the reference curve* Γ *is smooth and possesses the distinguished Frenet frame;*
2. *the cross-section* ω *is bounded;*
3. *the angle function* θ *is smooth;*
4. (V.10) *and* (V.11) *hold.*

These hypotheses will be assumed henceforth, without any further repetitions.

Relaxing the geometrical interpretation of Ω being a non-self-intersecting tube in $\mathbb{R}^3$, it is possible to consider (Ω_0, G) as an abstract Riemannian manifold where only the reference curve Γ is embedded in $\mathbb{R}^3$. Then one does not need to assume (V.11), and the spectral results below hold in this more general situation, too.

V.2.2 The Hamiltonian

Now we associate to Ω the Dirichlet Laplacian $-\Delta_D^\Omega$.

The initial Laplacian

Let us recall that, under the hypotheses (V.10) and (V.11), the tube Ω is an open subset of $\mathbb{R}^3$. Hence, the corresponding Dirichlet Laplacian can be introduced in the way as described in Section V.1.1:

$$\mathfrak{D}(-\Delta_D^\Omega) := \left\{\psi \in W_0^{1,2}(\Omega) \;\middle|\; \Delta\psi \in L^2(\Omega)\right\}, \qquad -\Delta_D^\Omega\psi := -\Delta\psi\,.$$

The Laplacian in curvilinear coordinates

Our strategy to investigate $-\Delta_D^\Omega$ is to express it in the coordinates determined by (V.7). More specifically, recalling the diffeomorphism between Ω_0 and Ω given by $\mathcal{L}$ (*cf* Proposition V.1), we can identify the Hilbert space $L^2(\Omega)$ with

$$\mathcal{H} := L^2\big(\Omega_0, f(s,t)\, ds\, dt\big)$$

and the Dirichlet Laplacian can be identified with the Laplace-Beltrami operator

$$\mathfrak{D}(H) := \Big\{\psi \in W_0^{1,2}(\Omega_0, G) \,\Big|\, \Delta_G \psi \in \mathcal{H}\Big\}, \qquad H\psi := -\Delta_G \psi\,.$$

Here

$$-\Delta_G := -|G|^{-1/2}\partial_i |G|^{1/2} G^{ij}\partial_j \tag{V.12}$$

is a general expression for the Laplacian expressed in curvilinear coordinates (the Einstein summation convention is adopted, with the range of indices being $1,2,3$) and $W_0^{1,2}(\Omega_0, G)$ denotes the completion of $C_0^\infty(\Omega_0)$ with respect to the norm

$$\|\psi\|_{\mathcal{H}_1} := \sqrt{(\partial_i\psi, G^{ij}\,\partial_j\psi)_{\mathcal{H}} + \|\psi\|_{\mathcal{H}}^2}\,.$$

In our case, when the metric is given by (V.8), we have $|G|^{1/2} = f$ and

$$G^{-1} = \frac{1}{f^2}\begin{pmatrix} 1 & -f_2 & -f_3 \\ -f_2 & f^2 + f_2^2 & f_2 f_3 \\ -f_3 & f_3 f_2 & f^2 + f_3^2 \end{pmatrix}.$$

The quadratic form associated with H is given by, $\mathfrak{D}(h) = W_0^{1,2}(\Omega_0)$,

$$\begin{aligned} h[\psi] &= \big(\partial_i\psi, G^{ij}\,\partial_j\psi\big)_{\mathcal{H}} \\ &= \big\|f^{-1}\big[\partial_1\psi - (\tau - \dot\theta)\partial_u\psi\big]\big\|_{\mathcal{H}}^2 + \|\nabla'\psi\|_{\mathcal{H}}^2\,, \end{aligned}$$

where $\nabla' := (\partial_2, \partial_3)$ is the transverse gradient and $\partial_u := t_3\partial_2 - t_2\partial_3$ is the transverse angular derivative.

If the functions κ and $\tau - \dot\theta$ are bounded, then the $\mathcal{H}_1$-norm is equivalent to the usual norm in $W^{1,2}(\Omega_0)$ and $W_0^{1,2}(\Omega_0, G) = W_0^{1,2}(\Omega_0)$.

Problem V.2. Calculate the eigenvalues of G.
Solution:

$$1\,,$$
$$\tfrac{1}{2}\left(1 + f^2 + f_2^2 + f_3^2 - \sqrt{-4f^2 + \big(1 + f^2 + f_2^2 + f_3^2\big)^2}\right),$$
$$\tfrac{1}{2}\left(1 + f^2 + f_2^2 + f_3^2 + \sqrt{-4f^2 + \big(1 + f^2 + f_2^2 + f_3^2\big)^2}\right).$$

The passage from $L^2(\Omega)$ to $\mathcal{H}$ is explicitly given by the unitary transform

$$U : L^2(\Omega) \to \mathcal{H} : \{\Psi \mapsto \Psi \circ \mathcal{L} =: \psi\}\,.$$

Then $H = U(-\Delta_D^\Omega)U^{-1}$. In particular, $\mathfrak{D}(H) = U\mathfrak{D}(-\Delta_D^\Omega)$ and

$$W_0^{1,2}(\Omega_0, G) = \mathfrak{D}(H^{1/2}) = U\mathfrak{D}\big((-\Delta_D^\Omega)^{1/2}\big) = UW_0^{1,2}(\Omega_0)\,.$$

As usual, the idea of expressing the Laplacian in curvilinear coordinates is that a simple operator $(-\Delta)$ acting on a complicated space (Ω) is transformed to a more complicated operator $(-\Delta_G)$ acting on a simple space (Ω_0).

A unitarily equivalent operator

Finally, we transform H on $\mathcal{H}$ into a unitarily equivalent operator on a fully straighten Hilbert space $L^2(\Omega_0)$. This is enabled by the unitary transform

$$\hat{U} : \mathcal{H} \to L^2(\Omega_0) : \Big\{ \psi \mapsto f^{1/2}\psi \Big\} \,,$$

which leads to $\hat{H} := \hat{U} H \hat{U}^{-1}$. To find an explicit form of $\hat{H}$, we note that the differential expression (V.12) is transformed to

$$\begin{aligned} |G|^{1/4}(-\Delta_G)|G|^{-1/4} &= -|G|^{-1/4}\partial_i |G|^{1/2} G^{ij} \partial_j |G|^{-1/4} \\ &= -\partial_i G^{ij}\partial_j + V \,, \end{aligned}$$

where

$$V := \partial_i (G^{ij} F_j) + F_i G^{ij} F_j \qquad \text{with} \qquad F_i := \partial_i (\log |G|^{1/4}) \,.$$

(This is a general formula valid for any smooth metric G.) Hence,

$$\begin{aligned} \mathfrak{D}(\hat{H}) &= \Big\{ \psi \in \mathfrak{D}(\hat{h}) \;\Big|\; -\partial_i G^{ij}\partial_j \psi + V\psi \in L^2(\Omega_0) \Big\} \,, \\ \hat{H}\psi &= -\partial_i G^{ij}\partial_j\psi + V\psi \,, \end{aligned}$$

in the distributional sense, where

$$\begin{aligned} \mathfrak{D}(\hat{h}) &:= \overline{C_0^\infty(\Omega_0)}^{\sqrt{\hat{h}[\cdot] + \|\cdot\|^2}} \,, \\ \hat{h}[\psi] &:= \big(\partial_i \psi, G^{ij}\partial_j\psi\big) - 2\,\Re\big(\partial_i\psi, G^{ij} F_j \psi\big) + \big(\psi, F_i G^{ij} F_j \psi\big) \,. \end{aligned}$$

Here we denote by $\|\cdot\|$ and $(\cdot,\cdot)$ the norm and inner product in $L^2(\Omega_0)$, respectively.

Again, if κ, $\dot{\kappa}$, τ and $\dot{\theta}$ are bounded functions, then the topology of $\mathfrak{D}(\hat{h})$ is equivalent to that of $W^{1,2}(\Omega_0)$ and we have $\mathfrak{D}(\hat{h}) = W_0^{1,2}(\Omega_0)$. Moreover, if in addition $\ddot{\kappa}$, $\dot{\tau}$ and $\ddot{\theta}$ are bounded, then V is a bounded function and

$$\hat{h}[\psi] = \big\| f^{-1}\big[\partial_1\psi - (\tau - \dot{\theta})\partial_u \psi\big]\big\|^2 + \|\nabla'\psi\|^2 + (\psi, V\psi) \,.$$

Then the study of $-\Delta_D^\Omega$ is reduced to the study of a Schrödinger-type operator $\hat{H}$.

V.2.3 Shrinking cross-section limit

Now, let us rescale the transverse variables

$$t \mapsto \varepsilon t \,,$$

where $\varepsilon > 0$, which corresponds to initially considering the Dirichlet Laplacian $-\Delta_D^{\Omega_\varepsilon}$ in a tube $\Omega_\varepsilon := \mathcal{L}(\mathbb{R} \times \varepsilon\omega)$ with shrinking cross-section $\varepsilon\omega := \{\varepsilon t \,|\, t \in \omega\}$. Inspecting the dependence of the metric G_ε on ε, where $G_\varepsilon(s,t) := G(s, \varepsilon t)$, it turns out that $\hat{H}_\varepsilon$ (the operator obtained from $\hat{H}$ by replacing G by G_ε) satisfies

$$\hat{H}_\varepsilon \;\sim\; L_\varepsilon := -\big(\partial_1 - (\tau - \dot{\theta})\partial_u\big)^2 - \frac{1}{\varepsilon^2}\,\Delta' - \frac{\kappa^2}{4} \qquad \text{as} \qquad \varepsilon \to 0 \,. \qquad \text{(V.13)}$$

Here $-\Delta' := -\partial_2^2 - \partial_3^2$ is the transverse Laplacian and the curvature-induced potential $-\kappa^2/4$ is the only term which survives from V after taking the limit $\varepsilon \to 0$.

(V.13) can be easily checked if it is understood as the corresponding quadratic-forms limit

$$\forall \phi, \psi \in W_0^{1,2}(\Omega_0), \qquad \hat{h}_\varepsilon(\phi,\psi) - l_\varepsilon(\phi,\psi) \xrightarrow[\varepsilon\to 0]{} 0$$

(assuming the boundedness of κ, $\dot{\kappa}$, $\ddot{\kappa}$, τ, $\dot{\tau}$, $\dot{\theta}$, $\ddot{\theta}$, the (form) domains of $\hat{H}_\varepsilon$ and L_ε coincide). This can be in turn used to prove the norm-resolvent convergence

$$\|(\hat{H}_\varepsilon + i)^{-1} - (L_\varepsilon + i)^{-1}\| \xrightarrow[\varepsilon\to 0]{} 0 .$$

Obviously, one cannot expect the operator $\hat{H}_\varepsilon$ or L_ε to have a limit as $\varepsilon \to 0$, because their spectra explode (*i.e.*, tend to infinity) in the limit. However, (V.13) suggests that the spectrum of $\hat{H}_\varepsilon$ can be approximated by the spectrum of the simpler operator L_ε, in the limit when the cross-section of the tube shrinks to zero.

Moreover, the diverging term in (V.13) is less diverging when projected on the lowest transverse mode $\mathcal{J}_1$, *i.e.*, the eigenfunction of $-\Delta_D^\omega$ corresponding to its lowest eigenvalue E_1, normalized to 1 in $L^2(\omega)$. This suggests that

$$L_\varepsilon \;\sim\; M_\varepsilon := P_1 L_\varepsilon P_1 \qquad \text{as} \qquad \varepsilon \to 0\,, \tag{V.14}$$

where P_1 is the lowest-transverse-mode projection

$$(P_1\psi)(s,t) := \mathcal{J}_1(t)\,\big(\mathcal{J}_1, \psi(s,\cdot)\big)_{L^2(\omega)} .$$

M_ε is essentially a one-dimensional operator. A simple calculation shows

$$M_\varepsilon = \left(-\partial_1^2 + C(\omega)(\tau - \dot{\theta})^2 - \frac{\kappa^2}{4} + \frac{E_1}{\varepsilon^2}\right) P_1 \qquad \text{with} \qquad C(\omega) := \|\partial_u \mathcal{J}_1\|^2_{L^2(\omega)} .$$

Summing up, the spectrum of $\hat{H}_\varepsilon$ (and therefore of $-\Delta_D^{\Omega_\varepsilon}$) in tubes of shrinking cross-section is asymptotically determined by the exploding lowest transverse eigenvalue E_1/ε^2 plus the spectrum of the one-dimensional operator

$$-\Delta + C(\omega)(\tau - \dot{\theta})^2 - \frac{\kappa^2}{4} \qquad \text{on} \qquad L^2(\mathbb{R}) .$$

From the effective potential we identify the different role of curvature κ on one side and torsion τ, rotations $\dot{\theta}$ of cross-section ω and asymmetry of the cross-section (given by $C(\omega)$) on the other side.

Definition V.2 (bending)**.** The tube Ω is said to be *bent* if the reference curve Γ is not a straight line, *i.e.*, $\kappa \neq 0$.

Definition V.3 (twisting)**.** The tube Ω is said to be *twisted* if the cross-section ω is not rotationally invariant with respect to the origin and $\tau - \dot{\theta} \neq 0$.

We can conclude that (at least in the asymptotic regime of $\varepsilon \to 0$)

- bending acts as an attractive interaction,
- twisting acts as a repulsive interaction.

It turns out that these effect hold for *all* positive ε (admissible with (V.10) and (V.11)). In particular, bending leads to the existence of geometrically induced bound states below the essential spectrum, while twisting induces geometrically induced Hardy inequalities. See [18, 19] for more details.

Appendix A

Elements of spectral theory

Here we recall the fundamental notions of spectral theory of unbounded operators in Hilbert spaces. More account on the theory can be found in the books [16, 29, 6, 9].

A.1 Unbounded linear operators

Let H be a linear operator in a separable complex Hilbert space $\mathcal{H}$, *i.e.*, a linear mapping of a subspace $\mathfrak{D}(H) \subset \mathcal{H}$ into $\mathcal{H}$; $\mathfrak{D}(H)$ is called the *domain* of H. H is said to be *densely defined* if $\mathfrak{D}(H)$ is dense in $\mathcal{H}$. $\tilde{H}$ is called an *extension* of H (or H is a *restriction* of $\tilde{H}$) if we have

$$\mathfrak{D}(H) \subset \mathfrak{D}(\tilde{H}) \qquad \text{and} \qquad \forall \psi \in \mathfrak{D}(H), \quad \tilde{H}\psi = H\psi \, .$$

Any bounded operator on $\mathcal{H}$ can be extended to a bounded operator with domain $\mathcal{H}$ (extension principle). Moreover, the *boundedness* of an operator H is equivalent to its *continuity* (*i.e.*, for any sequence ψ_n with limit ψ, it follows that $H\psi_n$ converges to $H\psi$). The set of bounded operators on $\mathcal{H}$ will be denoted by $\mathcal{B}(\mathcal{H})$.

The continuity of bounded operators is so useful that we need to have a replacement for it in the general situation. This is provided by the notion of closedness: H is said to be *closed* if for any sequence $\psi_n \in \mathfrak{D}(H)$ we have

$$\left.\begin{aligned} \psi_n &\xrightarrow[n\to\infty]{} \psi \in \mathcal{H} \\ H\psi_n &\xrightarrow[n\to\infty]{} \phi \in \mathcal{H} \end{aligned}\right\} \quad \Longrightarrow \quad \psi \in \mathfrak{D}(H) \quad \text{and} \quad H\psi = \phi \, .$$

An operator H on $\mathcal{H}$ is said to be *closable* if H has a closed extension. H is closable if, and only if, for any sequence $\psi_n \in \mathfrak{D}(H)$ we have

$$\left.\begin{aligned} \psi_n &\xrightarrow[n\to\infty]{} 0 \\ H\psi_n &\xrightarrow[n\to\infty]{} \phi \in \mathcal{H} \end{aligned}\right\} \quad \Longrightarrow \quad \phi = 0 \, .$$

When H is closable, there exists a closed extension $\overline{H}$, called the *closure* of H, whose domain is smallest among all closed extensions. If H is closed, a subset $D \subset \mathfrak{D}(H)$ is called a *core* for H if $\overline{H \restriction D} = H$. The subset D is a core for H if, and only if, for all ψ in $\mathfrak{D}(H)$ there exists a sequence ψ_n in D such that $\psi_n \to \psi$ and $H\psi_n \to H\psi$ as $n \to \infty$.

A.2 Unbounded sesquilinear forms

A mapping $h : \mathfrak{D}(h) \times \mathfrak{D}(h) \to \mathbb{C}$, with $\mathfrak{D}(h) \subset \mathcal{H}$, such that $\psi \mapsto h(\phi, \psi)$ is linear for each fixed $\phi \in \mathfrak{D}(h)$ and $\phi \mapsto h(\phi, \psi)$ is semilinear for each fixed $\psi \in \mathfrak{D}(h)$ is called a *sesquilinear form* on $\mathcal{H}$; $\mathfrak{D}(h)$ is called the domain of h. h is said to be *densely defined* if $\mathfrak{D}(h)$ is dense in $\mathcal{H}$. *Extensions* and *restrictions* of forms are defined in an obvious way as in the case of operators.

The mapping from $\mathfrak{D}(h)$ to $\mathbb{C}$ defined by $\psi \mapsto h[\psi] := h(\psi, \psi)$ is called the *quadratic form* associated with h. $h[\psi]$ determines $h(\phi, \psi)$ uniquely according to the polarization identity

$$h(\phi, \psi) = \frac{1}{4}\Big(h[\phi + \psi] - h[\phi - \psi] + ih[\phi - i\psi] - ih[\phi + i\psi]\Big). \tag{A.1}$$

With each sesquilinear form h is associated an *adjoint* form h^* defined as follows:

$$\mathfrak{D}(h^*) := \mathfrak{D}(h)\,, \qquad h^*(\phi, \psi) := \overline{h(\psi, \phi)}\,. \tag{A.2}$$

A sesquilinear form h is said to be *symmetric* if $h^* = h$. As is seen from the polarization identity (A.1), h is symmetric if, and only if, $h[\psi]$ is real-valued.

A symmetric form h is said to be *bounded from below* if there exists a real constant c such that

$$\forall \psi \in \mathfrak{D}(h), \qquad h[\psi] \geq c\, \|\psi\|^2\,.$$

In this case we simply write $h \geq c$. The symmetric form h is said to be *non-negative* if $h \geq 0$.

A symmetric sesquilinear form h bounded from below is said to be *closed* if for any sequence $\psi_n \in \mathfrak{D}(h)$ we have

$$\left.\begin{array}{r} \psi_n \xrightarrow[n\to\infty]{} \psi \in \mathcal{H} \\ h[\psi_n - \psi_m] \xrightarrow[n,m\to\infty]{} 0 \end{array}\right\} \quad \Longrightarrow \quad \psi \in \mathfrak{D}(h) \quad \text{and} \quad h[\psi_n - \psi] \xrightarrow[n\to\infty]{} 0\,.$$

Let h be a symmetric sesquilinear form bounded from below. h is said to be *closable* if it has a closed extension. h is closable if, and only if, for any sequence $\psi_n \in \mathfrak{D}(h)$ we have

$$\left.\begin{array}{r} \psi_n \xrightarrow[n\to\infty]{} 0 \\ h[\psi_n - \psi_m] \xrightarrow[n,m\to\infty]{} 0 \end{array}\right\} \quad \Longrightarrow \quad h[\psi_n] \xrightarrow[n\to\infty]{} 0\,.$$

When this condition is satisfied, h has the *closure* (*i.e.* the smallest closed extension) $\overline{h}$ defined in the following way:

$$\begin{aligned} \mathfrak{D}(\overline{h}) &:= \left\{ \psi \in \mathcal{H} \;\middle|\; \exists \{\psi_n\} \subset \mathfrak{D}(h),\ \psi_n \xrightarrow[n\to\infty]{} \psi,\ h[\psi_n - \psi_m] \xrightarrow[n,m\to\infty]{} 0 \right\}, \\ h(\phi, \psi) &:= \lim_{n\to\infty} h(\phi_n, \psi_n)\,; \end{aligned}$$

any closed extension of h is also and extension of $\overline{h}$. If h is closed, a subset $D \subset \mathfrak{D}(h)$ is called a *core* for h if $\overline{h \restriction D} = h$. The subset D is a core for h if, and only if, for all ψ in $\mathfrak{D}(h)$ there exists a sequence ψ_n in D such that $\psi_n \to \psi$ and $h[\psi_n - \psi] \to 0$ as $n \to \infty$.

A.3 Self-adjointness

If H is a densely defined operator on $\mathcal{H}$, its *adjoint* H^* is (uniquely) defined as follows:

$$\begin{aligned} \mathfrak{D}(H^*) &:= \left\{ \phi \in \mathcal{H} \mid \exists \phi^* \in \mathcal{H},\ \forall \psi \in \mathfrak{D}(H), \quad (\phi, H\psi) = (\phi^*, \psi) \right\}, \\ H^*\phi &:= \phi^* . \end{aligned}$$

H^* is always a closed operator (regardless whether H is closed or closable).

An operator H on $\mathcal{H}$ is said to be *symmetric* if it is densely defined and its adjoint H^* is an extension of H, *i.e.*,

$$H^* \supset H .$$

H is symmetric if, and only if, it is densely defined and (I.7) holds.

An operator H on $\mathcal{H}$ is said to be *self-adjoint* if it is densely defined and coincides with its adjoint H^*, *i.e.*,

$$H^* = H .$$

Hence, H is self-adjoint if, and only if, it is symmetric and $\mathfrak{D}(H) = \mathfrak{D}(H^*)$.

A symmetric operator H is called *essentially self-adjoint* if its closure $\overline{H}$ is self-adjoint.

A symmetric operator H is said to be *bounded from below* if (I.8) holds.

A.4 Spectrum

The spectrum of an unbounded operator H on $\mathcal{H}$ is conventionally introduced by means of the *resolvent* operator

$$R(z) := (H - z)^{-1} ,$$

well defined for all z which are not eigenvalues of H (*i.e.* $H - z$ is injective). The set

$$\rho(H) := \left\{ z \in \mathbb{C} \,\middle|\, \quad H - z \quad \text{is injective} \quad \wedge \quad R(z) \in \mathcal{B}(\mathcal{H}) \right\}$$

is called the *resolvent set* of H and its complement

$$\sigma(H) := \mathbb{C} \setminus \rho(H)$$

is called the *spectrum* of H.

For a closed operator H on $\mathcal{H}$ we have by the closed graph theorem [16, Sec. III.5.4] that

$$\rho(H) = \{ z \in \mathbb{C} \mid \quad H - z \quad \text{is bijective} \} .$$

Consequently, $\sigma(H)$ coincides with the set of points $\lambda \in \mathbb{C}$ such that either $H - \lambda$ is not invertible or it is invertible but has range smaller than $\mathcal{H}$. Since H is closed, $\rho(H)$ is open, consequently $\sigma(H)$ is closed.

If H is not closed, then $H - \lambda$ is not closed, consequently $\sigma(H) = \mathbb{C}$. In other words $\rho(H) = \varnothing$ and the (resolvent) operator-valued function $z \mapsto R(z)$ is nowhere defined. This is why the closedness of H is so important in spectral theory.

The set $\sigma_{\mathrm{p}}(H)$ of all eigenvalues of H, *i.e.*,

$$\sigma_{\mathrm{p}}(H) := \big\{\lambda \in \mathbb{C} \mid \quad \exists\psi \subset \mathfrak{D}(H), \quad \|\psi\| = 1, \quad H\psi = \lambda\psi\big\}$$

is called the *point spectrum* of H. It is obviously contained in $\sigma(H)$, but does not exhaust the spectrum for a general unbounded operator H. If λ is an eigenvalue of H then the dimension of the kernel of $H-\lambda$ is called the (geometric) *multiplicity* of λ.

The remaining part of the spectrum of a closed operator H is divided as follows:

$$\sigma_{\mathrm{c}}(H) := \big\{\lambda \in \sigma(H) \mid \quad H-\lambda \quad \text{is injective} \quad \wedge \quad \mathfrak{R}(H-\lambda) \quad \text{is dense in } \mathcal{H}\big\},$$
$$\sigma_{\mathrm{r}}(H) := \big\{\lambda \in \sigma(H) \mid \quad H-\lambda \quad \text{is injective} \quad \wedge \quad \overline{\mathfrak{R}(H-\lambda)} \neq \mathcal{H}\big\}.$$

Here $\sigma_{\mathrm{c}}(H)$ is called the *continuous spectrum* of H and $\sigma_{\mathrm{r}}(H)$ is called the *residual spectrum* of H. In this way, the spectrum decomposes into three disjoint sets:

$$\sigma(H) = \sigma_{\mathrm{p}}(H) \cup \sigma_{\mathrm{c}}(H) \cup \sigma_{\mathrm{r}}(H).$$

For self-adjoint operators H, $\sigma(H) \subset \mathbb{R}$ and $\sigma_{\mathrm{r}}(H) = \varnothing$. We rather use the following, alternative disjoint partition of the spectrum of a self-adjoint operator H:

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

Here the *discrete spectrum* $\sigma_{\mathrm{disc}}(H) \subset \sigma_{\mathrm{p}}(H)$ consists of those eigenvalues of H which are isolated points of $\sigma(H)$ and have finite multiplicity. The complement

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

is called the *essential spectrum* of H and, by definition, it contains either accumulation points of $\sigma(H)$ or isolated eigenvalues of infinite multiplicity.

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Notation

Here we point out some special notation used in the lectures.

- $\mathbb{N}^* := \mathbb{N} \setminus \{0\}$ where $\mathbb{N} = \{0, 1, 2, \dots\}$.
- $\mathbb{R}_+ := (0, +\infty)$, $\mathbb{R}_- := (-\infty, 0)$.