Introduction to Spectral Theory of Schrödinger Operators

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Preface

Here are lecture notes of the course delivered at the Giessen University during my visit as DFG guest professor (1999-2000 teaching year). The audience consisted of graduate and PhD students, as well as young researchers in the field of nonlinear analysis, and the aim was to provide them with a starting point to read monographs on spectral theory and mathematical physics. According to introductory level of the course, it was required a standard knowledge of real and complex analysis, as well as basic facts from linear functional analysis (like the closed graph theorem). It is desired, but not necessary, some familiarity with differential equations and distributions. The notes contain simple examples and exercises. Sometimes we omit proofs, or only sketch them. One can consider corresponding statements as problems (not always simple). Remark also that the second part of Section 9 is not elementary. Here I tried to describe (frequently, even without rigorous statements) certain points of further development. The bibliography is very restricted. It contains few books and survey papers of general interest (with only one exception: [11]). We also add references [1] and [4] to show how spectral theory can be used in applications of critical point theory.

It is a pleasant duty for me to thank Thomas Bartsch who initiated my visit and the subject of course, as well as all the members of the Mathematical Institute of Giessen University, for many interesting and fruitful discussions. Also, I am grateful to Petra Kuhl who converted my handwritten draft into a high quality type-setting.

1 A bit of quantum mechanics

1.1 Axioms

Quantum mechanics deals with microscopic objects like atoms, molecules, etc. Here, as in any physical theory, we have to consider only those quantities which may be measured (at least in principle). Otherwise, we go immediately to a kind of scholastic. Physical quantities, values of which may be found by means of an experiment (or measured) are called observables. It turns out to be that in quantum mechanics it is impossible, in general, to predict exactly the result of measurement. This result is a (real) random variable and, in fact, quantum mechanics studies lows of distribution of such random variables.

Now we discuss a system of axioms of quantum mechanics suggested by J. von Neumann.

Axiom 1.1. *States of a quantum system are nonzero vectors of a complex separable Hilbert space $\mathcal{H}$, considered up to a nonzero complex factor. There is a one-to-one correspondence between observable and linear self-adjoint operators in $\mathcal{H}$. In what follows we consider states as unit vectors in $\mathcal{H}$.*

If a is an observable, we denote by $\hat{a}$ the corresponding operator. We say that observables $a_1, \dots, a_n$ are *simultaneously measurable* if their values may be measured up to an arbitrarily given accuracy in the same experiment. This means that for an arbitrary state $\psi \in \mathcal{H}$ the random variables $a_1, \dots, a_n$ have a simultaneous distribution function $\mathcal{P}_\psi(\lambda_1, \dots, \lambda_n)$, i.e. $\mathcal{P}_\psi(\lambda_1, \dots, \lambda_n)$ is a probability that the values of observables $a_1, \dots, a_n$ measured in the state ψ are less or equal to $\lambda_1, \dots, \lambda_n$, respectively.

Axiom 1.2. *Observables $a_1, \dots, a_n$ are simultaneously measurable if and only if the self-adjoint operators $\hat{a}_1, \dots, \hat{a}_n$ mutually commutes. In this case*

$$\mathcal{P}_\psi(\lambda_1, \dots, \lambda_n) = \|E^{(1)}_{\lambda_1} E^{(2)}_{\lambda_2} \dots E^{(n)}_{\lambda_n} \psi\|^2, \tag{1.1}$$

where $E^{(k)}_\lambda$ is the spectral decomposition of unit corresponding to the operator $\hat{a}_k$.

It is clear that the right-hand side of (1.1) depends on the state itself, not on representing unit vector ψ (ψ is defined up to a complex factor ζ, $|\zeta = 1$). Also this expression does not depend on the order of observables, since the spectral projectors $E^{(k)}_\lambda$ commute.

Among all observables there is one of particular importance: the energy. Denote by H the corresponding operator. This operator is called frequently the (quantum) *Hamiltonian*, or the *Schrödinger operator.* It is always assumed that $\mathcal{H}$ does not depend explicitly on time.

Axiom 1.3. *There exists a one parameter group U_t of unitary operators (evolution operator) that map an initial state ψ_0 at the time $t = 0$ to the state $\psi(t) = U_t\psi_0$ at the time t. The operator U_t is of the form*

$$U_t = e^{-\frac{i}{h}tH}, \tag{1.2}$$

where h is the Plank constant. If $\psi_0 \in D(H)$, the domain of H, then the $\mathcal{H}-$valued function $\psi(t)$ is differentiable and

$$ih\frac{d\psi(t)}{dt} = H\psi(t). \tag{1.3}$$

Thus, the evolution of quantum systems is completely determined by its Hamiltonian H. Equation (1.3) is called the *Schrödinger equation.*

Axiom 1.4. *To each non-zero vector of $\mathcal{H}$ it corresponds a state of quantum system and every self-adjoint operator in $\mathcal{H}$ corresponds to an observable.*

The last axiom is, in fact, too strong and sometimes one needs to weaken it. However, for our restricted purpose this axiom is sufficient.

Now let us discuss some general consequences of the axioms. Let a be an observable and $\hat{a}$ the corresponding self-adjoint operator with the domain $D(\hat{a})$. We denote by $\overline{a}_\psi$ the mean value, or mathematical expectation, of the observable a at the state ψ.

If $\psi \in D(\hat{a})$, then the mean value $\overline{a}_\psi$ exists and

$$\overline{a}_\psi = (\hat{a}\psi, \psi). \tag{1.4}$$

Indeed, due to the spectral theorem

$$(\hat{a}\psi, \psi) = \int_{-\infty}^{\infty} \lambda d(E_\lambda\psi, \psi)$$

However,

$$(E_\lambda\psi, \psi) = (E_\lambda^2, \psi, \psi) = (E_\lambda\psi, E_\lambda\psi) = \|E_\lambda\psi\|^2.$$

Using (1.1), we see that

$$(\hat{a}\psi, \psi) = \int_{-\infty}^{\infty} \lambda d\|E_\lambda\psi\|^2 = \int_{-\infty}^{\infty} \lambda d\mathcal{P}_\psi(\lambda) = \overline{a}_\psi.$$

Denote by $\delta_\psi a$ the dispersion of a at the state ψ, i.e. the mean value of $(a - \overline{a}_\psi)^2$.

The dispersion $\delta_\psi a$ exists if $\psi \in D(\hat{a})$. In this case

$$\delta_\psi a = \|\hat{a}\psi - \overline{a}_\psi \psi\|^2. \tag{1.5}$$

The first statement is a consequence of the spectral theorem (consider it as an exercise). Now consider a self-adjoint operator $(\hat{a} - \overline{a}_\psi I)^2$, where I is the identity operator. Applying (1.4) to this operator, we have

$$\delta_\psi a = ((\hat{a} - \overline{a}_\psi I)^2\psi, \psi) = ((\hat{a} - \overline{a}_\psi I)\psi, (\hat{a} - \overline{a}_\psi I)\psi) = \|\hat{a}\psi - \overline{a}\psi\|^2.$$

Now we have the following important

Claim 1.5. *An observable a takes at a state ψ a definite value λ with probability* 1 *if and only if ψ is an eigenvector of $\hat{a}$ with the eigenvalue λ.*

Indeed, if a takes at ψ the value λ with probability 1, then $\overline{a}_\psi = \lambda$ and $\delta_\psi a = 0$. Hence, by (1.5), $\|\hat{a}\psi - \lambda\psi\| = 0$, i. e. $\hat{a}\psi = \lambda\psi$. Conversely, if $\hat{a}\psi = \lambda\psi$, then (1.4) implies that $\overline{a}_\psi = (\hat{a}\psi, \psi) = \lambda(\psi, \psi) = \lambda$. Hence, $\delta_\psi = \|\hat{a}\psi - \overline{a}_\psi\psi\|^2 = \|\hat{a}\psi - \lambda\psi\|^2 = 0$.

Consider a particular case $\hat{a} = H$. Assume that at the time $t = 0$ the state of our system is an eigenvector ψ_0 of H with the eigenvalue λ_0. Then

$$\psi(t) = e^{-i\lambda_0 t/h}\psi_0$$

solves the Schrödinger equation. However, $\psi(t)$, differs from ψ_0 by a scalar factor and, hence, define the same state as ψ_0. Assume now that $U_t\psi_0 = c(t)\psi_0$. The function $c(t) = (U_t\psi_0, \psi_0)$ is continuous, while the group low $U_{t+s} = U_tU_s$ implies that $c(t+s) = c(t)c(s)$. Hence, $c(t)$ is an exponential function. Therefore, it is differentiable and

$$H\psi_0 = ih\frac{d}{dt}U_t\psi_0|_{t=0} = \lambda_0\psi_0,$$

with $\lambda_0 = ih\frac{dc(t)}{dt}|_{t=0}$.

Thus, the state of quantum system is a stationary state, i. e. it does not depend on time, if and only if it is represented by an eigenvector of the Hamiltonian. The equation

$$H\psi = \lambda\psi$$

for stationary states is called *stationary Schrödinger equation.*

1.2 Quantization

Let us consider a classical dynamical systems, states of which are defined by means of (generalized) coordinates $q_1, \dots, q_n$ and (generalized) impulses $p_1, \dots, p_n$. Assume that the (classical) energy of our system is defined by

$$H_{cl} = \sum_{k=1}^{n} \frac{p_k^2}{2m_k} + v(q_1, \dots, q_n), \tag{1.6}$$

where m_k are real constants, $q_k \in \mathbb{R}, p_k \in \mathbb{R}$. A typical example is the system of l particles with a potential interaction. Here $n = 3l$, the number of degrees of freedom, $q_{3r-2}, q_{3r-1}, q_{3r}$ are Cartesian coordinates of rth particle, $p_{3r-2}, p_{3r-1}, p_{3r}$ are the components of corresponding momentum, $m_{3r-2} = m_{3r-1} = m_{3r}$ is the mass of rth particle, and $v(q_1, q_2, \dots, q_n)$ is the potential energy.

There is a heuristic rule of construction of corresponding quantum system such that the classical system is, in a sense, a limit of the quantum one. As the space of states we choose the space $L^2(\mathbb{R}^n)$ of complex valued functions of variables $q_1, \dots, q_n$. To each coordinate q_k we associate the operator $\hat{q}_k$ of multiplication by q_k

$$(\hat{q}_k \psi)(q_1, \dots, q_n) = q_k \psi(q_1, \dots, q_n).$$

Exercise 1.6. Let $h(q_1, \dots, q_n)$ be a real valued measurable function. The operator $\hat{h}$ defined by

$$(\hat{h}\psi)(q_1, \dots, q_n) = h(q_1, \dots, q_n)\psi(q_1, \dots, q_n),$$
$$D(\hat{h}) = \{\psi \in L^2(\mathbb{R}^n) : h(q)\psi(q) \in L^2(\mathbb{R}^n)\},$$

is self-adjoint.

Thus, $\hat{q}_k$ is a self-adjoint operator. We set also

$$\hat{p}_k = \frac{h}{i} \frac{\partial}{\partial q_k},$$

with

$$D(\hat{p}_k) = \{\psi(q) \in L^2(\mathbb{R}^n) : \frac{\partial \psi}{\partial q_k} \in L^2(\mathbb{R}^n)\},$$

where $\partial\psi/\partial q_k$ is considered in the sense of distributions.

Exercise 1.7. Show that $\hat{p}_k$ is a self-adjoint operator.

Now we should define the quantum Hamiltonian as a self-adjoint operator generated by the expression

$$H = -\frac{h^2}{2}\sum_{k=1}^{n}\frac{1}{m_k}\frac{\partial^2}{\partial q_k^2} + v(q_1, \ldots, q_n). \tag{1.7}$$

However, at this point some problems of mathematical nature arise. Roughly speaking, what does it mean operator (1.7)? It is easy to see that operator (1.7) is well-defined on the space $C_0^\infty(\mathbb{R}^n)$ of smooth finitely supported functions and is symmetric. So, the first question is the following. Does there exist a self-adjoint extension of operator (1.7) with $C_0^\infty(\mathbb{R}^n)$ as the domain? If no, there is no quantum analogue of our classical system. If yes, then how many of self-adjoint extensions do exist? In the case when there are different self-adjoint extensions we have different quantum versions of our classical system. In good cases we may except that there exists one and only one self-adjoint operator generated by (1.7). It is so if the closure of H defined first on $C_0^\infty(\mathbb{R}^n)$ is self-adjoint. In this case we say that H is *essentially self-adjoint* on $C_0^\infty(\mathbb{R}^n)$.

By means of direct calculation one can verify that the operators of impulses and coordinates satisfy the following Heisenberg commutation relations

$$[\hat{p}_k, \hat{q}_k] = \frac{h}{i}I, [\hat{p}_k, \hat{q}_j] = 0, k \neq j. \tag{1.8}$$

In fact, these relations are easy on $C_0^\infty(\mathbb{R}^n)$, but there are some difficulties connected with the rigorous sense of commutators in the case of unbounded operators. We do not go into details here. Remark that there is essentially one set of operators satisfying relations (1.8). In the classical mechanics coordinates and impulses are connected by relations similar to (1.8), but with respect to the Poisson brackets. In our (coordinate) representation of quantum system with Hamiltonian (1.7) a state is given by a function $\psi(q_1, \ldots, q_n, z)$ with belongs to $L^2(\mathbb{R}^n)$ for every fixed time t. Moreover,

$$\psi(q_1, \ldots, q_n, t) = e^{-\frac{i}{h}tH}\psi(q_1, \ldots, q_n, 0)$$

The Schrödinger equation is now of the form

$$ih\frac{\partial\psi}{\partial t} = -\frac{h^2}{2}\sum_{k=1}^{n}\frac{1}{m_k}\frac{\partial^2\psi}{\partial q_k^2} + v(q_1, \ldots, q_n)\psi.$$

The function $\psi(q_1, \ldots, q_n, t)$ is called a *wave function* of the quantum system. (The same term is used frequently for functions $\psi(q_1, \ldots, q_n) \in L^2(\mathbb{R}^n)$ representing states of the system).

Let $E_\lambda^{(k)}$ be a decomposition of identity for $\hat{q}_k$,

$$\hat{q}_k = \int_{-\infty}^{\infty} \lambda dE_\lambda^{(k)}.$$

Then $E_\lambda^{(k)}$ is just the operator of multiplication by the characteristic function of the set

$$\{q = (q_1, \dots, q_n) \in \mathbb{R}^n : q_k \leq \lambda\}$$

Hence the simultaneous distribution of $q_1, \dots, q_n$ is given by

$$\mathcal{P}_\psi(\lambda_1, \dots, \lambda_n) = \int_{-\infty}^{\lambda_1} \dots \int_{-\infty}^{\lambda_n} |\psi(q_1, \dots, q_n)|^2 dq_1 \dots dq_n.$$

Therefore, the square of modulus of a wave function is exactly the density of simultaneous distribution of $q_1, \dots, q_n$. Thus, the probability that a measurement detects values of coordinates $q_1, \dots, q_n$ in the intervals $(a_1, b_1), \dots, (a_n, b_n)$ respectively is equal to

$$\int_{a_1}^{b_1} \dots \int_{a_n}^{b_n} |\psi(q_1, \dots, q_n)|^2 dq_1, \dots, dq_n.$$

We have just described the so-called coordinate representation which is, of course, not unique. There are other representations, e. g. so-called impulse representation (see [2] for details).

We have considered quantization of classical systems of the form (1.6). For more general classical systems quantization rules are more complicated. In addition, let us point out that there exist quantum systems which cannot be obtained from classical ones by means of quantization, e.g. particles with spin.

1.3 Heisenberg uncertainty principle

Let us consider two observables a and b, with corresponding operators $\hat{a}$ and $\hat{b}$. Let ψ be a vector such that $(\hat{a}\hat{b} - \hat{b}\hat{a})\psi$ makes sense. The uncertainties of the results of measurement of a and b in the state ψ are just

$$\Delta a = \Delta_\psi a = \sqrt{\delta_\psi a} = \|\hat{a}\psi - \overline{a}_\psi \psi\|$$
$$\Delta b = \Delta_\psi b = \sqrt{\delta_\psi b} = \|\hat{b}\psi - \overline{b}_\psi \psi\|.$$

We have

$$\Delta a \Delta b \geq \frac{1}{2} |((\hat{a}\hat{b} - \hat{b}\hat{a})\psi, \psi)| \tag{1.9}$$

Indeed, let $\hat{a}_1 = \hat{a} - \overline{a}_\psi I, \hat{b}_1 = \hat{b} - \overline{b}_\psi I$. Then $\hat{a}_1\hat{b}_1 - \hat{b}_1\hat{a}_1 = \hat{a}\hat{b} - \hat{b}\hat{a}$. Hence,

$$\begin{aligned}
|((\hat{a}\hat{b} - \hat{b}\hat{a})\psi, \psi)| &= |((\hat{a_1}\hat{b_1} - \hat{b_1}\hat{a_1})\psi, \psi)| \\
&= |(\hat{a_1}\hat{b_1}\psi, \psi) - (\hat{b_1}\hat{a_1}\psi, \psi)| = |(\hat{b_1}\psi, \hat{a_1}\psi) - (\hat{a_1}\psi, \hat{b_1}\psi)| \\
&= 2|\mathrm{Im}(\hat{a_1}\psi, \hat{b_1}\psi)| \leq 2|(\hat{a_1}\psi, \hat{b_1}\psi)| \leq 2\|\hat{a_1}\psi\|\|\hat{b_1}\psi\| \\
&= 2\|\hat{a}\psi - \overline{a_\psi}\psi\|\|\hat{b}\psi\| - \overline{b_\psi}\psi = 2\Delta a\Delta b.
\end{aligned}$$

We say that the observables a and b are canonically conjugate if

$$\hat{a}\hat{b} - \hat{b}\hat{a} = \frac{h}{i}I$$

In this case the right hand part of (1.8) is independent of ψ and

$$\Delta a\Delta b \geq h/2 \tag{1.10}$$

It is so for the components q_k and p_k of coordinates and momenta, and, as consequence, we get the famous Heisenberg uncertainly relations

$$\Delta p_k\Delta q_k \geq h/2. \tag{1.11}$$

Due to Axiom 1.2, two observables are simultaneously measurable if the corresponding operators commute. Relation (1.11) gives us a quantitative version of this principle. If an experiment permits us to measure the coordinate q_k with a high precision, then at the same experiment we can measure the corresponding impulse p_k only very roughly: the accuracies of these two measurements are connected by (1.11).

1.4 Quantum oscillator

The classical (1-dimensional) oscillator is a particle with one degree of freedom which moves in the potential field of the form

$$v(x) = \frac{\omega^2}{2}x^2, \quad x \in \mathbb{R}.$$

The classical energy is of the form

$$M_{cl} = \frac{m}{2}(\dot{x})^2 + \frac{m\omega^2}{2}x^2 = \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2,$$

where m is the mass of the particle, and $p = m\dot{x}$ is its momentum.

The space of states of the quantum analogue is $\mathcal{H} = L^2(\mathbb{R})$, the operators of coordinate and momentum were defined above, and the quantum Hamiltonian H is a self-adjoint operator generated by the expression

$$-\frac{h}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2}{2}x^2.$$

For the sake of simplicity we set $h = m = \omega = 1$. Then

$$H = \frac{1}{2}(-\frac{d^2}{dx^2} + x^2).$$

Let $\tilde{\mathcal{H}}$ be a linear subspace of $L^2(\mathbb{R})$ (not closed!) that consists of all functions of the form

$$P(x)e^{-\frac{x^2}{2}},$$

where $P(x)$ is a polynomial.

Exercise 1.8. $\tilde{\mathcal{H}}$ is dense in $L^2(\mathbb{R})$.

Now let us introduce the so-called operators of annihilation and birth.

$$A = \frac{1}{\sqrt{2}}(\hat{x} + i\hat{p}) \ , \ A^* = \frac{1}{\sqrt{2}}(\hat{x} - 1\hat{p})$$

In fact, one can show that A^* is the adjoint operator to A, defined on $\tilde{H}$. However, we do not use this fact. So, one can consider A^* as a single symbol. These operators, as well as $\hat{p}$, $\hat{x}$ and H, are well-defined on the space $\tilde{\mathcal{H}}$ and map $\tilde{\mathcal{H}}$ into itself (verify this). As consequence, on the space $\tilde{\mathcal{H}}$ products and commutators of all these operators are also well-defined. Verify the following identities (on $\tilde{\mathcal{H}}$):

$$[A, A^*] \ = \ I, \tag{1.12}$$

$$H \ = \ A^*A \ = \ \frac{1}{2}I \ = \ AA^* - \frac{1}{2}I, \tag{1.13}$$

$$[H, A] - A \ , \ [H, A^*] \ = \ A^* \tag{1.14}$$

Exercise 1.9. Let $\psi \in \tilde{\mathcal{H}}$ be an eigenvector of H with the eigenvalue λ and $A^*\psi \neq 0$. Then $A^*\psi$ is an eigenvector of H with the eigenvalues $\lambda + 1$.

Now let

$$\psi_0(x) = e^{-\frac{x^2}{2}}$$

Then

$$H\psi_0 = \frac{1}{2}\psi_0,$$

and $\psi_0 \in \tilde{\mathcal{H}}$ is an eigenvector of H with the eigenvalue $\frac{1}{2}$ (verify!). Let us define vectors $\psi_k \in \tilde{\mathcal{H}}$ by

$$\psi_{k+1} = \sqrt{2}A^*\psi_k,$$

or

$$\psi_k = (\sqrt{2}A^*)^k\psi_0.$$

Exercise 1.10. $H\psi_k = (k + \frac{1}{2})\psi_k$.

Hence, ψ_k is an eigenvector of H with the eigenvalue $(k + \frac{1}{2})$. Since $\psi_k \in \tilde{\mathcal{H}}$, we have

$$\psi_k(x) = H_k(x)e^{-\frac{x^2}{2}},$$

where $H_k(x)$ are polynomials (the so-called *Hermite polynomials*). The functions ψ_k are said to be *Hermite functions.*

Exercise 1.11. Calculate $(H\psi_k, \psi_l)$ and verify that $\{\psi_k\}$ is an orthogonal systems in $L^2(\mathbb{R})$ (not normalized).

Exercise 1.12. Show that the system $\{\psi_k\}$ may be obtained by means of orthogonalization of the system

$$x^n e^{-\frac{x^2}{2}}.$$

Exercise 1.13. Verify the following identities

$$\begin{aligned} H_n(x) &= (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2} \ , \\ \frac{d^n H_n}{dx^n} &= 2^n \cdot n! \ , \\ H_{n+1}(x) &= 2xH_n(x) - 2nH_{n-1}(x) \ . \end{aligned}$$

Calculate $H_0(x), H_1(x), H_2(x), H_3(x)$ and $H_n(x)$.

Exercise 1.14. Show that $\{\psi_k\}$ is an orthogonal basis in $L^2(\mathbb{R})$. Moreover,

$$\|\psi_k\|^2 = 2^k \cdot k!\sqrt{\pi}.$$

As consequence, the functions

$$\tilde{\psi}_k(x) = \frac{\psi_k(x)}{\sqrt{2^k k! \sqrt{\pi}}} = \frac{1}{\sqrt{2^k \cdot k! \sqrt{\pi}}} H_k(x) e^{-\frac{x^2}{2}}$$

form an orthonormal basis. In addition,

$$\tilde{\psi}_k = \frac{1}{\sqrt{k!}} (A^*)^k \tilde{\psi}_0.$$

Since, with respect to the basis $\{\psi_k\}$, the operator H has a diagonal form, we can consider this operator as self-adjoint, with the domain

$$D(H) = \{\psi \in L^2(\mathbb{R}) : \sum_{k=0}^{\infty} |(\psi, \tilde{\psi}_k)(k + \frac{1}{2})|^2 < \infty\}.$$

Therefore, the spectrum of H consists of simple eigenvalues (energy levels) $k + \frac{1}{2}$, $k = 0, 1, \ldots$, with corresponding eigenvectors (stationary states of the oscillator) $\tilde{\psi}_k$. In general case, the energy levels are

$$h_k = h\omega(k = +\frac{1}{2}), k = 0, 1, \ldots, \tag{1.15}$$

with corresponding stationary states

$$P_h(x) = \sqrt[4]{\frac{m\omega}{\pi h}} \sqrt{\frac{1}{2^k \cdot k!}} H_k(\xi) e^{-\frac{\xi}{2}},$$

where

$$\xi = x\sqrt{\frac{m\omega}{h}}$$

The last change of variable reduces general problem to the case $h = m = \omega = 1$. Moreover, in general case we also have corresponding operators of annihilation and birth, A and A^*. Formula (1.15) means that the oscillator may gain or loss energy by portions (quanta) multiple of $h\omega$. The minimal possible energy level is equal to

$$h_0 = h\omega/_2 \neq 0,$$

i.e. the quantum oscillator cannot be at absolute rest. Operators A and A^*, acting on wave functions of stationary states decrease and increase, respectively, the number of quanta, i.e. A^* generates new quanta while A annihilates them. This explains the names "birth" and "annihilation". Finally, let point out that the picture we see in the case of quantum oscillator is not so typical. In general, the spectrum of a quantum Hamiltonian may contain points of continuous spectrum, not only eigenvalues.

2 Operators in Hilbert spaces

2.1 Preliminaries

To fix notation, we recall that a Hilbert space $\mathcal{H}$ is a complex linear space equipped with an inner product $(f, g) \in \mathbb{C}$ such that

$$\begin{aligned}(f, g,) &= (g, f),\\ (\lambda, f_1 + \lambda_2 f_2, g) &= \lambda_1(f_1, g) + \lambda_2(f_2, g),\\ (f, \lambda, g_1 + \lambda_2 g_2) &= \overline{\lambda}_1(f, g_1) + \overline{\lambda}_2(f, g_2),\end{aligned}$$

where $\lambda_1, \lambda_2 \in \mathbb{C}$ and $^-$stands for complex conjugation,

$$(f, f) \geq 0, f \in \mathcal{H},$$

$(f, f) = 0$ iff $f = 0$. Such inner product defines a norm

$$\|f\| = (f, f)^{1/2}$$

and, by definition, $\mathcal{H}$ is complete with respect to this norm.

Exercise 2.1. Prove the following polarization identity

$$\begin{aligned}(f, g) = \frac{1}{4}[(f + g, f + g) - (f - g, f - g)\\ + i(f + ig, f + ig) - i(f - ig, f - ig)]\end{aligned}$$

for every $f, g \in \mathcal{H}$.

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two Hilbert spaces. By definition, a *linear operator* $A : \mathcal{H}_1 \to \mathcal{H}_2$ is a couple of two objects:

- a linear (not necessary dense, or closed) subspace $D(A) \subset \mathcal{H}_1$ which is called the domain of A;
- a linear map $A : D(A) \to \mathcal{H}_2$.

We use the following notations

$$\begin{aligned}\ker A &= \{f \in D(A) : Af = 0\},\\ \operatorname{im} A &= \{g \in \mathcal{H}_2 : g = Af, f \in D(A)\}\end{aligned}$$

for kernel and image of A respectively. (Distinguish $\operatorname{im} A$ and $Im\lambda$, the imaginary part of a complex number.)

The operator A is said to be *bounded* (or *continuous*), if there exists a constant $C > 0$ such that

$$\|Af\| \le C\|f\|, \quad f \in D(A). \tag{2.1}$$

The norm $\|A\|$ of A is defined as the minimal possible C in (2.1), or

$$\|A\| = \sup_{f\in D(A), f\neq 0} \frac{\|Af\|}{\|f\|}. \tag{2.2}$$

In this case A can be extended by continuity to the closure $\overline{D(A)}$ of $D(A)$. Usually, we deal with operators defined on dense domains, i.e. $\overline{D(A)} = \mathcal{H}_1$. If such an operator is bounded, we consider it to be defined on the whole space $\mathcal{H}_1$.

If $\ker A = \{0\}$, we define the *inverse* operator $A^{-1} : \mathcal{H}_2 \to \mathcal{H}_1$ in the following way: $D(A^{-1}) = \operatorname{im} A$ and for every $g \in \operatorname{im} A$ we set $A^{-1}g = f$, where $f \in D(A)$ is a (uniquely defined) vector such that $g = Af$.

Let $A : \mathcal{H}_1 \to \mathcal{H}_2$ and $B : \mathcal{H}_2 \to \mathcal{H}_3$ be linear operators. Their *product* (or *composition*) $BA : \mathcal{H}_1 \to \mathcal{H}_3$ is defined by

$$D(BA) = \{f \in D(A) : Af \in D(B)\}, (BA)f = B(Af), f \in D(BA).$$

Certainly, it is possible that $\operatorname{im} A \cap D(B) = \{0\}$. In this case $D(BA) = \{0\}$.

The *sum* of $A : \mathcal{H}_1 \to \mathcal{H}_2$ and $A_2 : \mathcal{H}_1 \to \mathcal{H}_2$ is an operator $A_1 + A_2 : \mathcal{H}_1 \to H_2$ defined by

$$\begin{aligned} D(A_1 + A_2) &= D(A_1) \cap D(A_2), \\ (A_1 + A_2)f &= A_1 f + A_2 f. \end{aligned}$$

Again, the case $D(A_1 + A_2) = \{0\}$ is possible.

Let $A : \mathcal{H}_1 \to \mathcal{H}_2$ be a linear operator. By definition the *graph* $G(A)$ of A is a linear subspace of $\mathcal{H}_1 \oplus \mathcal{H}_2$ consisting of all vectors of the form $\{f, Af\}$, $f \in D(A)$.

Exercise 2.2. A linear subspace of $\mathcal{H}_1 \oplus \mathcal{H}_2$ is the graph of a linear operator if it does not contain vectors of the form $\{0, g\}$ with $g \neq 0$.

A linear operator $A : \mathcal{H}_1 \to \mathcal{H}_2$ is said to be *closed* if its graph $G(A)$ is a closed subspace of $\mathcal{H}_1 \times \mathcal{H}_2$. A is called *closable* if $\overline{G(A)}$ is the graph of some operator $\overline{A}$. In this case $\overline{A}$ is called the *closure* of A. Equivalently, $A : \mathcal{H}_1 \to \mathcal{H}_2$ is closed if $f_n \in D(A)$, $f_n \to f$ in $\mathcal{H}_1$ and $Af_n \to g$ in $\mathcal{H}$ imply $f \in D(A)$ and $Af = g$. A is closable if $f_n \in D(A)$, $f_n \to 0$ in $\mathcal{H}_1$ and $Af_n \to g$ in $\mathcal{H}_2$ imply $g = 0$.

Now let us list some simple properties of such operators.

- *Every bounded operator A is closable. Such an operator is closed provided $D(A)$ is closed.*

- *If A is closed, then* $\ker A$ *is a closed subspace of* $\mathcal{H}_1$.

- *If A is closed and* $\ker A = 0$, *then A^{-1} is a closed operator.*

Let $A_1, A_2 : \mathcal{H}_1 \to \mathcal{H}_2$ be two linear operators. We say that A_2 is an *extension* of A_1 (in symbols $A_1 \subset A_2$) if $D(A_1) \subset D(A_2)$ and $A_2 f = A_1 f$, $f \in D(A_1)$. Obviously, the closure $\overline{A}$ of A (if it exists) is an extension of A.

2.2 Symmetric and self-adjoint operators

First, let us recall the notion of adjoint operator. Let $A : \mathcal{H}_1 \to \mathcal{H}_2$ be a linear operator such that $\overline{D(A)} = \mathcal{H}_1$ (important assumption!). The *adjoint* operator $A^* : \mathcal{H}_2 \to \mathcal{H}_1$ is defined as follows. The domain $D(A^*)$ of A^* consists of all vectors $g \in \mathcal{H}_2$ with the following property:

there exists $g^* \in \mathcal{H}_1^*$ such that $(Af, g) = (f, g^*)$ $\forall f \in D(A)$.

Since $D(A)$ is dense in $\mathcal{H}_1$, the vector g^* is uniquely defined, and we set

$$A^* g = g^*$$

In particular, we have

$$(Af, g) = (f, A^* g), f \in D(A), g \in D(A^*).$$

Evidently, $g \in D(A^*)$ iff the linear functional $l(f) = (Af, g)$ defined on $D(A)$ is continuous. Indeed, in this case on can extend l to $\overline{D(A)} = \mathcal{H}_1$ by continuity. Then, by the Riesz theorem, we have $l(f) = (Af, g) = (f, g^*)$ for some $g^* \in \mathcal{H}_1$.

Let us point out that the operation * of passage to the adjoint operator reverses arrows: *if $A : \mathcal{H}_1 \to \mathcal{H}_2$, then $A^* : \mathcal{H}_2 \to \mathcal{H}_1$*. In the language of the theory of categories this means that * is a contravariant functor.

Now we list a few simple properties of adjoint operators.

- *If $A_1 \subset A_2$, then $A_2^* \subset A_1^*$.*

- *If A is bounded and $D(A) = \mathcal{H}_1$, then $D(A_2) = \mathcal{H}_2$ and A^* is bounded. Moreover, $\|A^*\| = \|A\|$.*

- *For every linear operator A, with $\overline{D(A)} = \mathcal{H}_1$, A^* is a closed operator.*

If E is a linear subspace of $\mathcal{H}$, we denote by $E^\perp$ the orthogonal complement of E, i.e.

$$E^\perp = \{g \in \mathcal{H} : (f, g) = 0 \ \forall f \in E\}.$$

Evidently,$E^\perp$ is a closed subspace of $\mathcal{H}$, and $E^\perp = (\overline{E})^\perp$.

Exercise 2.3. (i) $\ker A^* = (\operatorname{im} A)^\perp$.

(ii) Operators $(A^*)^{-1}$ and $(A^{-1})^*$ exist iff $\ker A = \{0\}$ and $\operatorname{im} A$ is dense in $\mathcal{H}_2$.

(iii) In the last case, $(A^*)^{-1} = (A^{-1})^*$.

Proposition 2.4. *$D(A^*)$ is dense in $\mathcal{H}_2$ iff A is closable. In this case $\overline{A} = A^{**} = (A^*)^*$.*

Proof. By definition of $\mathcal{H}_1 \oplus \mathcal{H}_2$,

$$(\{f_1, g_1\}, \{f_2, g_2\}) = (f_1, f_2) + (g_1, g_2).$$

Now we have easily that $\{g, g^*\} \in G(A^*)$ iff $\{g^*, -g\} \perp G(A)$ (prove!). This means that the vectors $\{A^*g, -g\}$ form the orthogonal complement of $G(A)$. Hence, $\overline{G(A)}$ is the orthogonal complement to the space of all vectors of the form $\{A^*g, -g\}$.

The space $D(A^*)$ is not dense in $\mathcal{H}_2$ if and only if there exists a vector $h \in \mathcal{H}_2$ such that $h \neq 0$ and $h \perp D(A^*)$, or, which is the same, $\{0, h\} \perp \{A^*_g, -g\}$ for all $g \in D(A^*)$. The last means that $\{0, h\} \in G(A)$, i.e. $G(A)$ cannot be a graph of an operator and, hence, A is not closable.

The last statement of the proposition is an exercise. (*Hint*: $G(A^{**}) = \overline{G(A)}$). □

Now we will consider operators acting in the same Hilbert space $\mathcal{H}(\mathcal{H} = \mathcal{H}_1 = \mathcal{H}_2)$. Let $A : \mathcal{H} \to \mathcal{H}$ be an operator with dense domain, $\overline{D(A)} = \mathcal{H}$. We say that A is *symmetric* if $A \subset A^*$, i.e.

$$(Af, g) = (f, Ag) \quad \forall f, g \in D(A).$$

First, we remark that every symmetric operator is closable. Indeed, we have $\underline{G(A)} \subset G(A^*)$. Since A^* is closed, (i.e. $\overline{G(A^*)} = G(A^*)$), we see that $\overline{G(A)} \subset G(A^*) = \overline{G(A^*)}$. Hence, $\overline{G(A)}$ does not contain any vector of the form $\{0, h\}, h \neq 0$. Therefore, $\overline{G(A)}$ is the graph of an operator. It is easy to see that the closure $\overline{A}$ of symmetric operator A is a symmetric operator.

An operator $A : \mathcal{H} \to \mathcal{H}$ is said to be *self-adjoint* if $A = A^*$. If $\overline{A}$ is self-adjoint, we say that A is *essentially self-adjoint*. Each self-adjoint operator is obviously closed. If A is self-adjoint and there exists A^{-1}, then A^{-1} is self-adjoint. Indeed, $(A^{-1})^* = (A^*)^{-1} = A^{-1}$.

Proposition 2.5. *A closed symmetric operator A is self-adjoint if and only if A^* is symmetric.*

Proof. We prove the first statement only. If A is closed, then, due to Proposition 2.4, $A^{**} = A$. Since A^* is symmetric, we have $A^* \subset A^* * = A$. However, A itself is symmetric: $A \subset A^*$. Hence, $A \subset A^* \subset A$ and we conclude. $\square$

Exercise 2.6. An operator A with the dense domain is essentially self-adjoint if and only if A^* and A^{**} are well-defined, and $A^* = A^{**}$.

Theorem 2.7. *An operator A such that $\overline{D(A)} = \mathcal{H}$ is essentially self-adjoint iff there is one and only one self-adjoint extension of A.*

The proof is not trivial and based on the theory of extension of symmetric operators. It can be found, e.g., in [10].

2.3 Examples

We consider now a few examples.

Example 2.8. Let J be an interval of real line, not necessary finite and $a(x)$ a real valued measurable function which is finite almost everywhere. Let A be the operator of multiplication by $a(x)$ defined by

$$\begin{aligned} D(A) &= \{f \in L^2(J) : af \in L^2(J)\}, \\ (Af)(x) &= a(x)f(x). \end{aligned}$$

Then A is a self-adjoint operator. To verify this let us first prove that $\overline{D(A)} = L^2(J)$. Let $g \in L^2(J)$ be a function such that

$$\int_J f\overline{g}dx = 0 \quad \forall f \in D(A).$$

We show that $g = 0$. With this aim, given $N > 0$ we consider the set

$$J_N = \{x \in J : |a(x)| < N\}.$$

Since $a(x)$ is finite almost everywhere, we have

$$\text{meas}(J \setminus \cup_{N=1}^{\infty} J_N) = 0.$$

Hence, it suffices to prove that $g|_{J_N} = 0$ for all integer N. Let χ_N be the characteristic function of J_N, i.e. $\chi_N = 1$ on J_N and $\chi_N = 0$ on $J \setminus J_N$. For every $f \in L^2(J)$ we set $f_N = \chi_N f$.

Then, obviously, $f_N \in L^2(J)$ and $af_N \in L^2(J)$. Therefore, for all $f \in L^2(J)$ we have

$$\int_{J_N} f\overline{g}dx = \int_J f_N\overline{g}dx = 0.$$

If we take here $f = g$, we get

$$\int_{J_N} g\overline{g}dx = \int_{J_N} |g|^2 dx = 0,$$

and, hence, $g = 0$ on J_N.

Now, let $g \in D(A^*)$, i.e. there exists $g^* \in L^2(J)$ such that

$$\int_J af\overline{g}dx = \int_J f\overline{g^*}dx \quad \forall f \in D(A).$$

If we take as f an arbitrary function in $L^2(J)$ vanishing outside J_N, we see as above that $ag = g^*$ almost everywhere, i.e. $g \in D(A)$. Hence, $D(A^*) = D(A)$ and $A^*g = Ag$, i.e. $A = A^*$.

To consider next examples we need some information on weak derivatives (see, e.g., [8], [10]). Let $f \in L^2(J)$. Recall that a function $g \in L^2(J)$ is said to be the weak derivative of f if

$$\int_J g\overline{\varphi}dx = -\int_J f\overline{\varphi}'dx \quad \forall \varphi \in C_0^\infty(J). \tag{2.3}$$

In this case we write $g = f'$. For any integer m we set $H^m(J) = \{f \in L^2(J) : f^{(k)} \in L^2(J), k = 1, \ldots, m\}$. Endowed with the norm

$$\|f\|_{H^m} = (\sum_{k=0}^{m} \|f^{(k)}\|_{L^2}^2)^{1/2}$$

this is a Hilbert space. One can prove that the expression

$$(\|f\|_{L^2}^2 + \|f^{(m)}\|_{L^2}^2)^{1/2}$$

defines an equivalent norm in H^m. We have also to point out the following properties:

(i) *$f \in H^m(J)$ iff $f \in L^2(J) \cap C(\overline{J})$, is continuously differentiable up to order $m-1$, $f^{(m)}$ exists almost everywhere, and $f^{(m)} \in L^2(J)$. Moreover, in this case all the functions $f, f', \ldots, f^{(m-1)}$ are absolutely continuous.*

(ii) *For* $f, g, \in H^1(J)$ *the following formula (integration by parts) holds true*:

$$\text{(2.4)} \quad \int_{t_2}^{t_2} fg'dx = f(t_2)g(t_2) - f(t_1)g(t_1) - \int_{t_2}^{t_2} f'gdx, t_1, t_2 \in J, t_1 < t_2$$

(iii) *In the case of unbounded* J, *if* $f \in H^1(J)$, *then* $\lim_{x\to\infty} f(x) = 0$.

Let us recall that a function $f(x)$ is said to be absolutely continuous if, for every $\epsilon > 0$ there exists $\delta > 0$ such that

$$\sum |f(\beta_j) - f(\alpha_j)| < \epsilon,$$

whenever $(\alpha_1, \beta_1), \ldots, (\alpha_k, \beta_k)$ is a finite family of intervals with $\sum(\beta_j - \alpha_j) < \delta$.

Example 2.9. Operator id/dx on real line. Define an operator B_0 in the following way:

$$D(B_0) = C_0^\infty(\mathbb{R}),$$
$$(B_0 f)(x) = i\frac{df}{dx}.$$

This operator is symmetric. Directly from definition of weak derivative we see that $D(B_0^*) = H^1(\mathbb{R})$ and

$$(B_0^* g)(x) = i\frac{dg}{dx}, g \in D(B_0^*).$$

Moreover, properties (ii) and (iii) above imply that B_0^* is self-adjoint. Now we prove that the closure $B = \overline{B_0}$ of B_0 coincides with B_0^*. To end this it suffices to show that for any $f \in D(B_0^*) = H^1(\mathbb{R})$ there exists a sequence $f_n \in C_0^\infty(\mathbb{R})$ such that $f_n \to f$ in $L^2(\mathbb{R})$ and $f_n' \to f'$ in $L^2(\mathbb{R})$, i.e. $f_n \to f$ in $H^1(\mathbb{R})$. This is well-known, but let us to explain briefly the proof. Choose a function $\chi_n \in C_0^\infty(\mathbb{R})$ such that $\chi_n = 1$ if $|x| \le N$, $\chi_N = 0$ if $|x| \ge N+1$, and $|\chi_N'(x)| \le C$ (independently of N). Then cut off f: set $f_N = \chi_n f$. We have $f_N \to f$ in $H^1(\mathbb{R})$. So, we can assume that $f = 0$ outside a compact set. Now choose an even function $\varphi \in C_0^\infty(\mathbb{R})$ such that $\varphi(x) \ge 0$, $\varphi(x) = 0$, if $|x| \ge 1$,

$$\int_{\mathbb{R}} \varphi(x)dx = 1$$

and set $\varphi_\epsilon(x) = \epsilon^{-1}\varphi(x/\epsilon)$. Let

$$f_\epsilon(x) = \int_{\mathbb{R}} \varphi_\epsilon(x-y)f(y)dy.$$

One can easily verify that $f_\epsilon \in C_0^\infty(\mathbb{R})$ and $(f')_\epsilon = (f_\epsilon)'$. From this one can deduce that $f_\epsilon \to f$ in $H^1(\mathbb{R})$, i.e. $f_\epsilon \to f$ in $L^2(\mathbb{R})$ and $f'_\epsilon \to f'$ in $L^2(\mathbb{R})$. Thus, $B = B_0^*$ is a self-adjoint operator.

Remark 2.10. Let F be the Fourier transform

$$(Ff)(\xi) = \frac{1}{(2\pi)^{1/2}} \int_{\mathbb{R}} f(x) e^{-ix\xi} dx.$$

It is well-known that F is a bounded operator in $L^2(\mathbb{R})$. Moreover, F is a unitary operator, i.e. F has a bounded inverse operator F^{-1} defined on $L^2(\mathbb{R})$ and

$$(Ff, Fg) = (f, g), \quad \forall f, g \in L^2(\mathbb{R}).$$

In fact,

$$(F^{-1}h)(x) = \frac{1}{(2\pi)^{1/2}} \int_{\mathbb{R}} h(\xi) e^{i\xi x} d\xi.$$

One can verify, that

$$B = F^{-1}AF. \tag{2.5}$$

In particular, $FD(B) = D(A)$. Equation (2.5) means that the operators A and B are unitary equivalent.

Example 2.11. Operator id/dx on a half-line. Let B_0 be the operator id/ix in $L^2(\mathbb{R}^+)$, where $\mathbb{R}^+ = \{x \in \mathbb{R} : x > 0\}$, with $D(B_0) = C_0^\infty(\mathbb{R}^+)$. As in Example 2.9, B_0^* is id/dx, with $D(B_0^*) = H^1(\mathbb{R}^+)$. On the other hand, $\overline{B}_0$ is id/dx, with

$$D(\overline{B}_0) = \{f \in H^1(\mathbb{R}^+) : f(0) = 0\} = H_0^1(\mathbb{R}^+).$$

Indeed, it is easy that $D(\overline{B}_0) \subset H_0^1(\mathbb{R}^+)$. Now, a function $f \in H_0^1(\mathbb{R}^+)$ can be considered as a member of $H^1(\mathbb{R})$: extend f to the whole $\mathbb{R}$ by 0. If we set $f_\epsilon(x) = f(x - \epsilon)$, we see that $f_\epsilon \to f$ in $H^1(\mathbb{R}^+)$. Therefore, to show that each $f \in H_0^1(\mathbb{R}^+)$ belongs to $D(\overline{B}_0)$, we can assume without loss of generality that f vanishes in a neighborhood of 0. Now we may repeat the same cut-off and averaging arguments as in Example 2.9. We also see that B_0 and $\overline{B}_0$ are symmetric operators. Since $\overline{B}_0 = B_0^{**} \neq B_0^* = (\overline{B}_0)^*$, $\overline{B}_0$ is not self-adjoint and B_0 is not essentially self-adjoint. Moreover, B_0 has no self-adjoint extension at all. Indeed, if C is an extension of $\overline{B}_0$, then

$$D(\overline{B}_0) = H_0^1(\mathbb{R}^+) \subset D(C) \subset D(B_0^*) = H^1(\mathbb{R}^+).$$

However,

$$\dim H^1(\mathbb{R}^+)/H_0^1(\mathbb{R}^+) = 1$$

(prove!) and, hence, $D(C) = H_0^1(\mathbb{R}^+)$ or $H^1(\mathbb{R}^+)$. i.e. $C = \overline{B}_0$ or $C = B_0^*$. Both these operators are not self-adjoint.

Example 2.12. Operator $-d^2/dx^2$ on real line. Consider an operator H_0 in $L^2(\mathbb{R})$ defined as $-d^2/dx^2$, with $D(H_0) = C_0^\infty(\mathbb{R})$. Then H_0^* is $-d^2/dx^2$, with $D(H_0^*) = H^2(\mathbb{R})$. Moreover, $H = \overline{H}_0 = H_0^*$ is a self-adjoint operator, and H_0 is essentially self-adjoint. This can be shown, basically, along the same lines as in Example 2.9.

Example 2.13. Operator $-d^2/dx^2$ on a half-line. Let $H_{0,\min}$ be $-d^2/dx^2$, with $D(H_{0,\min}) = C_0^\infty(\mathbb{R}^+)$. This operator is symmetric. $(H_{0,\min})^* = H_{\max}$ is just $-d^2/dx^2$, with the domain $H^2(\mathbb{R}^+)$, while $H_{\min} = \overline{H_{0,\min}}$ is the operator $-d^2/dx^2$, with the domain

$$D(H_{\min}) = H_0^2(\mathbb{R}^+) = \{f \in H^2(\mathbb{R}^+) : f(0) = f'(0) = 0\}.$$

[We use such notation, since $H_{\min}$ is the minimal closed operator generated by $-d^2/dx^2$, while $H_{\max}$ is the maximal one]. $H_{\min}$ is a symmetric operator. Now we define H_0 as $-d^2/dx^2$, with the domain $D(H_0)$ consisting of all functions $f \in C^2(\overline{\mathbb{R}}^+)$ such that $f(0) = 0$ and $f(x) = 0$ for x sufficiently large. Prove that

$$\begin{aligned} D(H_0^*) &= \{f \in H^2(\mathbb{R}^+) : f(0) = 0\} \\ H^* f &= \frac{d^2 f}{dx^2}, f \in D(H_0^*). \end{aligned}$$

Moreover, H_0^* is self-adjoint and $H = \overline{H}_0 = H_0^*$. Therefore, H is a self-adjoint operator and H_0 essentially self-adjoint.

Certainly, $H_{\min} \subset H \subset H_{\max}$, and the next problem is to find all self-adjoint extensions of $H_{\min}$. It turns out to be (this is an exercise) that every self-adjoint extension of $H_{\min}$ is of the form $H_{(\zeta)}$, $\zeta = e^{i\varphi} \in \mathbb{C}$, where

$$\begin{aligned} D(H_{(\zeta)}) &= \{f \in H^2(\mathbb{R}^+) : \cos\varphi \cdot f(0) + \sin\varphi \cdot f'(0) = 0\}, \\ H(\zeta) f &= -\frac{d^2 f}{dx}, f \in D(H_{(\zeta)}). \end{aligned}$$

Hint: the domain of any such extension lies between $H_0^2(\mathbb{R}^+)$ and $H^1(\mathbb{R}^+)$. On the other hand, the rule $f \mapsto \{f(0), f'(0)\}$ defines an isomorphism of $H^2(\mathbb{R}^+)/H_0^2(\mathbb{R}^+)$ onto $\mathbb{C}^2$. This means that all such extensions form, or are parametrized by, the unit circle in $\mathbb{C}$.

Example 2.14. Let us define an operator B_0 in $L^2(0,1)$ as id/dx, with

$$D(B_0) = H_0^1(0,1) = \{f \in H^1(0,1) : f(0) = f(1) = 0\}.$$

Then B_0 is symmetric and B_0^* is again id/dx with $D(B_0^*) = H^1(0,1)$. Every self-adjoint extension of B_0 is of the form $B_{(\zeta)}$, $\zeta \in \mathbb{C}$, $|\zeta| = 1$, where

$$D(B_{(\zeta)}) = \{f \in H^1(0,1) : f(1) = e^{i\varphi} f(0)\},$$

and $B_{(\zeta)} = id/dx$ on this domain. All such extensions again form the unit circle in $\mathbb{C}$.

Example 2.15. Let H be the operator $-d^2/dx^2$ in $L^2(0,1)$, with

$$D(H) = H^2(0,1) \cap H_0^1(0,1) = \{f \in H^2(0,1) : f(0) = f(1) = 0\}.$$

This operator is self-adjoint (prove!)

2.4 Resolvent

Let $A : \mathcal{H} \to \mathcal{H}$ be a linear operator. We say that $z \in \mathbb{C}$ belongs to the *resolvent set* of A if there exists the operator $R_z = (A - zI)^{-1}$ which is bounded and $\overline{D(R_z)} = \mathcal{H}$. The operator function R_z is called the *resolvent* of A. The complement of the resolvent set is called the *spectrum*, $\sigma(A)$, of A.

If A is a closed operator, and $z \notin \sigma(A)$, then $D(R_z) = \mathcal{H}$, since R_z is closed. One can verify that the resolvent set is open. Hence, $\sigma(A)$ is closed. Moreover, R_z is an analytic operator function of z on the resolvent set.

Remark 2.16. There are various equivalent definitions of analytic operator functions. The simplest one is the following. An operator valued function $B(z)$ defined on an open subset of $\mathbb{C}$ is said to be *analytic* if each its value is a bounded operator and for every $f, g \in \mathcal{H}$ a scalar valued function $(B(z)f, g)$ is analytic.

For $z, z' \in \mathbb{C} \setminus \sigma(A)$, the following Hilbert identity

$$R_z - R_{z'} = (z - z')R_z R_{z'} \tag{2.6}$$

holds true.

Proof.

$$\begin{aligned}
R_z - R_{z'} &= R_z(A - z'I)R_{z'} - R_{z'} \\
&= R_z[(A - zI) + (z - z')I]R_{z'} - R_{z'} \\
&= [I + (z - z')R_z]R_{z'} - R_{z'} \\
&= (z - z')R_z R_{z'}.
\end{aligned}$$

□

Let us introduce the following notations:

$$\begin{aligned}
\mathbb{C}^+ &= \{z \in \mathbb{C} : \ Imz > 0\} \\
\mathbb{C}^- &= \{z \in \mathbb{C} : \ Imz < 0\}.
\end{aligned}$$

We have $\mathbb{C} = \mathbb{C}^+ \cup \mathbb{R} \cup \mathbb{C}^-$, where $\mathbb{R}$ is considered as the real axis.

Proposition 2.17. *Suppose A to be a self-adjoint operator. The $\sigma(A) \subset \mathbb{R}$ and the resolvent set contains both C^+ and $\mathbb{C}^-$. If $z \in \mathbb{C}^+ \cup \mathbb{C}^-$, then $R_z^* = R_{\overline{z}}$. Moreover,*

$$\|R_z\| \leq |Imz|^{-1}. \tag{2.7}$$

Proof. Let us calculate $\|(A - zI)f\|^2$, where $f \in D(A)$, $z = x + iy$, $y \neq 0$. We have

$$\begin{aligned} \|(A - zI)f\|^2 &= ((A - zI)f, (A - zI)f) \\ &= ((A - xI)f - iyf, (A - xI)f - iyf) \\ &= \|(A - xI)f\|^2 + y^2\|f\|^2. \end{aligned}$$

This implies that

$$\|(A - zI)f\|^2 \geq y^2\|f\|^2.$$

From the last inequality it follows that $(A - zI)$ has a bounded inverse operator and

$$\|(A - zI)^{-1}\| \leq 1/|y|.$$

Now let us prove that $(A - Iz)^{-1}$ is everywhere defined. Indeed,

$$(A - zI)^* = A^* - \overline{z}I = A - \overline{z}I. \tag{2.8}$$

Next,

$$[\mathrm{im}(A - zI)l]^\perp = \ker(A - \overline{z}I) = \{0\}.$$

Hence, $\mathrm{im}(A - zI) = D((A - zI)^{-1})$ is dense in $\mathcal{H}$. However, the operator $(A - zI)^{-1}$ is bounded and closed. Therefore, $D((A - zI)^{-1}) = \mathcal{H}$.

The identity $R_z^* = R_{\overline{z}}$ follows from (2.6) and the identity $(B^{-1})^* = (B^*)^{-1}$. □

A self-adjoint operator A is said to be *positive* (resp. *non-negative*) if there is a constant $\alpha > 0$ such that

$$(Af, f) \geq \alpha\|f\|^2, \quad \forall f \in D(A)$$

(resp., if $(Af, f) \geq 0 \quad \forall f \in D(A)$). In symbols $A > 0$ and $A \geq 0$, respectively.

Exercise 2.18. If $A > 0$ (resp., $A \geq 0$), then $\sigma(A) \subset (0, +\infty)$ (resp., $\sigma(A) \subset [0, +\infty)$).

Exercise 2.19. (i) For the operator H defined in Example 2.4 (or in Example 2.5), prove that $H \geq 0$.

(ii) Let H be the operator of Example 2.15. Prove that $H > 0$.

For more details we refer to [10] and [14].

3 Spectral theorem of self-adjoint operators

3.1 Diagonalization of self-adjoint operators

In Example 2.1 we have shown that operators of multiplication by a measurable (almost everywhere finite) functions are self-adjoint. It was also pointed out (Remark 2.1) that the self-adjoint operator in $L^2(\mathbb{R})$ generated by id/dx is unitary equivalent to the operator of multiplication by the independent variable x, i.e. it is essentially of the same form as in Example 2.1.

Let us now look at an extremely simple situation, the case when $\mathcal{H}$ is finite dimensional, $\dim \mathcal{H} = n < \infty$. We recall that in this case each linear operator is bounded and everywhere defined, provided it is densely defined. If A is a self-adjoint operator in $\mathcal{H}$, then, as it is well-known, there exists a complete orthogonal system $\{e_1, \dots, e_n\}$ of normalized eigenvectors, with corresponding eigenvalues $\lambda_1, \dots, \lambda_n \in \mathbb{R}$. Denote be $\mathcal{E}$ a linear space of all functions $f : \{1, \dots, n\} \to \mathbb{C}$. Endowed with the natural inner product, $\mathcal{E}$ is a Hilbert space. Denote by $b(k)$ the function $b(k) = \lambda_k, k = 1, \dots, n$, and by B the corresponding multiplication operator:

$$(Bf)(k) = b(k)f(k), k = 1, \dots, n.$$

It is easy that B is a self-adjoint operator in $\mathcal{E}$. Let us also define an operator $U : \mathcal{H} \to \mathcal{E}$, letting

$$(Ue_j)(k) = \delta_{jk}, j, k = 1, \dots, n,$$

where δ_{jk} is the Kronecker symbol. It is a simple exercise that U is a unitary operator and

$$A = U^{-1}BU.$$

Therefore, each self-adjoint operator in an finite dimensional Hilbert space is unitary equivalent to an operator of multiplication.

In fact, there is something similar for general self-adjoint operators. To formulate corresponding result rigorously, let us recall some basic notions from measure theory. A *measure space* is a triple $(M, \mathcal{F}, \mu)$, where M is a set, $\mathcal{F}$ is a σ-algebra of subsets of M, and $\mu : \mathcal{F} \to \mathbb{R} \cup \{\infty\}$ is a measure on M. Further, one says that a collection $\mathcal{F}$ of subsets is a σ-algebra if it is closed with respect to complements and countable unions (hence, countable intersections), and, in addition, $\emptyset \in \mathcal{F}$ (hence, $M \in \mathcal{F}$). A *measure* on M is a nonnegative function on $\mathcal{F}$, with values in $\mathbb{R} \cup \{\infty\}$, which is σ-additive, i.e.

$$\mu(\cup X_\alpha) = \sum \mu(X_\alpha),$$

where $\{X_\alpha\}$ is at most countable family of mutually disjoint members of $\mathcal{F}$. Moreover, $\mu(\emptyset) = 0$. A real-valued function f on M is said to be *measurable* if it is finite almost everywhere, i.e. outside a set of measure 0, and every sublevel set

$$\{m \in M : f(m) \leq \lambda\}, \lambda \in \mathbb{R}_0$$

is measurable, i.e. belongs to F. A complex valued function is measurable if both its real and imaginary parts are measurable. On a measurable space one develops integration theory, like Lebesgue's theory. Particularly, the space $L^2(M, d\mu)$ is well-defined. This space consists of all complex valued functions with square integrable modulus. Any two such functions are considered to be equal if they may differ only on a set of measure 0. Endowed with the natural inner product

$$(f, g) = \int_M f(m)\overline{g}(m)d\mu(m),$$

$L^2(M, \mu)$ becomes a Hilbert space.

Proposition 3.1. *Let $a(m)$ be a real-valued measurable function on M, A an operator of multiplication by $a(m)$ with*

$$D(A) = \{f \in L^2(M, d\mu) : a(m)f(m) \in L^2(M, d\mu)\}.$$

Then A is a self-adjoint operator.

Proof. Repeat the arguments of Example 2.1 □

Now we formulate, without proof, the following

Theorem 3.2. *Let A be a self-adjoint operator in a Hilbert space. Then there exist a measure space M, with measure σ, a real-valued measurable function $a(m)$ on M, and a unitary operator U from $\mathcal{H}$ onto $L^2(M, \sigma)$ such that*

(i) $f \in D(A)$ iff $f \in \mathcal{H}$ and $a(m)(Uf)(m) \in L^2(M, \sigma)$;

(ii) for every $f \in D(A)$ we have

$$(UAf)(m) = a(m)(Uf)(m).$$

This means that

$$A = U^{-1}aU.$$

See, e.g., [2], [10] and [14] for proofs.

In the case of separable $\mathcal{H}$, one can choose M, σ, and $a(m)$ in the following manner. The space M is a union of finite, or countable, number of straight lines l_j of the form

$$l_j = \{(x, y) \in \mathbb{R}^2 : y = j\}.$$

On each such line it is given a monotone decreasing function σ_j having finite limits at $+\infty$ and $-\infty$. The function σ_j defines the Lebesgue-Stieltjes measure $d\sigma_j$ on l_j. We always assume that σ_j is right-continuous, i.e. $\sigma_j(k+0, j) = \sigma_j(x, j)$. [For every interval $\Delta = \{(x, j) : \alpha < x \leq \beta\} \subset l_j$ we have $d\sigma_j(\Delta) = \sigma_j(\beta) - \sigma_j(\alpha)$]. By definition, a set $B \subset M$ is measurable iff each $B \cap l_j$ is measurable, and in this case

$$d\sigma(B) = \sum d\sigma_j(B \cap l_j).$$

The function $a(m)$ is now

$$a(m) = x, m = (x, j).$$

We also have the following orthogonal direct decomposition

$$L^2(M, \sigma) = \oplus L^2(l_j, d\sigma_j).$$

It must be pointed out that the measurable space $(M, d\sigma)$ is not uniquely determined and, therefore, is not an invariant of a self-adjoint operator.

Example 3.3. Consider again the operator of multiplication by x in $L^2(\mathbb{R})$. It is not exactly of the form described after Theorem 3.1. To obtain that one, we consider $M = \cup l_j$ and define σ_j by

$$\sigma_j(j, x) = \begin{cases} 0 & \text{if } x \leq j \\ x - j & \text{if } x \in [j, j+1] \\ 1 & \text{if } x \geq j+1. \end{cases}$$

With respect to $d\sigma_j$, the sets $(-\infty, j]$ and $[j+1, +\infty]$ in l_j have measure 0. Therefore, $L^2(l_j, d\sigma_j) \simeq L^2(j, j+1)$. Now we see that

$$L^2(\mathbb{R}) \simeq \oplus L^2(l_j, d\sigma_j) \simeq \oplus L^2(j, j+1),$$

where the isomorphism is defined by $f \mapsto \{f|_{[j,j+1]}\}_{j \in \mathbb{Z}}$. In both these spaces our operator acts as multiplication by x.

3.2 Spectral decomposition

Now we describe the so-called spectral decomposition of a self-adjoint operator A. We start with a construction of corresponding decomposition of identity. By Theorem 2.1, $A = U^{-1}aU$, where $U : \mathcal{H} \to L^2(M\sigma)$ is a unitary operator and $a(m)$ is a real valued measurable function on M. Let us denote by $\chi_\lambda = \chi_\lambda(m)$ the characteristic function of the set

$$M_\lambda = \{m \in M : a(m) \leq \lambda\},$$

i.e. $\chi_\lambda = 1$ on M_λ and $\chi_\lambda = 0$ on $M \setminus M_\lambda$. Define operators E_λ, $\lambda \in \mathbb{R}$, acting in $\mathcal{H}$ by

$$E_\lambda = U^{-1}\chi_\lambda U. \tag{3.1}$$

Here and subsequently, we do not make notational distinction between function and corresponding operators of multiplication. All the operators E_λ are bounded and $\|E_\lambda\| \leq 1$. We collect certain properties of the family E_λ which is called decomposition of identity. All these properties are unitary invariant, and we can (and will) assume that $A = a$. Certainly, every time such unitary invariance should be verified, but this is a simple thing.

Proposition 3.4. *The operator E_λ is an orthogonal (=self-adjoint) projector*

Proof. Since χ_λ is real valued, E_λ is self-adjoint. Since $\chi_\lambda^2 = \chi_\lambda$, we have $E_\lambda^2 = E_\lambda$. Hence, E_λ is a projector. Being realized in $L^2(M)$, E_λ projects $L^2(M)$ onto a subspace of functions vanishing on $M \setminus M_\lambda$ along a subspace of functions vanishing on M_λ. Each of these two subspaces is an orthogonal complement to another one. $\square$

The next property is a kind of monotonicity of E_λ.

Proposition 3.5.

(i) $E_\lambda E_\mu = E_\mu E_\lambda = E_\lambda$ *if* $\lambda \leq \mu$.

(ii) *For every $f \in \mathcal{H}$ the function $(E_\lambda f, f) = \|E_\lambda f\|^2$ is monotone increasing.*

Proof. It is easily seen that $\chi_\lambda\chi_\mu = \chi_\mu\chi_\lambda = \chi_\lambda$, $\lambda \leq \mu$. This proves (i).

Since $E_\lambda = E_\lambda^2$ and E_λ is self-adjoint, $(E_\lambda f, f) = (E_\lambda^2 f, f) = (E_\lambda f, E_\lambda f) = \|E_\lambda f\|^2$. Next,

$$\|\chi_\lambda f\|^2 = \int_{M_\lambda} f(m)d\sigma(m),$$

and this formula trivially implies (ii). $\square$

Proposition 3.6. *E_λ is right-continuous ($E_{\lambda+0} = E_\lambda$) in the strong operator topology, i.e.*

$$\lim_{\epsilon\to 0, \epsilon>0} \|E_{\lambda+\epsilon} f - E_{\lambda f}\| = 0. \tag{3.2}$$

Proof. Let us first prove (3.2) for $f \in \mathcal{L}$, the space of bounded measurable functions vanishing outside a set of finite measure. For such a function f let $S = \{m : f(m) > 0\}$ (this set has a finite measure). Now

$$\begin{aligned}\|E_{\lambda+\epsilon} f - E_\lambda f\|^2 &= \int_S (\chi_{\lambda+\epsilon} - \chi_\lambda)^2 |f|^2 d\sigma(m) \\ &= \int_{S\cap(M_{\lambda+\epsilon}\setminus M_\lambda)} |f|^2 d\sigma(m) \\ &\le C\sigma((S\cap M_{\lambda+\epsilon}) \setminus (S \cap M_\lambda)).\end{aligned}$$

Since

$$\bigcap_{\substack{\epsilon_k>0\\ \epsilon_k\to 0}} (S\cap M_{\lambda+\epsilon_k}) = S \cap M_\lambda,$$

we have

$$\lim \sigma((S\cap M_{\lambda+\epsilon}) \setminus (S\cap M_\lambda)) = 0.$$

Thus, for $f \in \mathcal{L}$, (3.2) is proved. For $f \in \mathcal{H}$, let us take $f_k \in \mathcal{L}$ such that $\delta_k = \|f - f_k\| \to 0$. Then we have (recall that $\|E_\lambda\| \le 1$)

$$\begin{aligned}\|E_{\lambda+\epsilon} f - E_\lambda f\| &\le \|(E_{\lambda+\epsilon} - E_\lambda) f_k\| + \|(E_{\lambda+\epsilon} - E_\lambda)(f - f_k)\| \\ &\le \|(E_{\lambda+\epsilon} - E_\lambda) f_k\| + \|E_{\lambda+\epsilon}(f - f_k)\| + \|E_\lambda(f - f_k)\| \\ &\le \|(E_{\lambda+\epsilon} - E_\lambda) f_k\| f_k + 2\|f - f_k\| = \|(E_{\lambda+\epsilon} - E_\lambda) f_k\| + 2\delta_k.\end{aligned}$$

This is enough (let first $\epsilon \to 0$ and then $k \to \infty$). □

Proposition 3.7. $\lim_{\lambda\to-\infty} E_\lambda = 0$, $\lim_{\lambda\to+\infty} E_\lambda = I$ *in the strong operator topology.*

Proof. Similar to that of Proposition 3.3. □

Proposition 3.8. *Let $\Delta = (\lambda_1, \lambda_2)(\lambda_1 < \lambda_2)$ and $E(\Delta) = E_{\lambda_2} - E_{\lambda_1}$. Then $E(\Delta)\mathcal{H} \subset D(A)$, $A[E(\Delta)\mathcal{H}] \subset E(\Delta)\mathcal{H}$ and*

$$\lambda_1(f, f) \le (Af, f) \le \lambda_2(f, f), \quad f \in E(\Delta)\mathcal{H}. \tag{3.3}$$

Moreover, for $f \in E(\Delta)\mathcal{H}$

$$\|(A - \lambda I)f\| \le |\lambda_2 - \lambda_1| \cdot |f|, \quad \lambda \in \Delta. \tag{3.4}$$

Remark 3.9. The last inequality means that , for Δ small, elements from $E(\Delta)\mathcal{H}$ are almost eigenvectors of A, with an eigenvalue $\lambda \in \Delta$. Certainly, it is not trivial only in the case $E(\Delta) \neq 0$.

Proof. $\chi_{\lambda_2} - \chi_{\lambda_1}$ vanishes outside $M_{\lambda_2} \setminus M_{\lambda_1}$. On the last set $a(m)$ is bounded (pinched between λ_1 and λ_2). Hence $(\chi_{\lambda_2} - \chi_{\lambda_1})f \in D(A)$ for every $f \in L^2(M)$. Next, $f \in E(\Delta)\mathcal{H}$ iff $f = 0$ outside $M_{\lambda_2} \setminus M_{\lambda_1}$, and we have easily

$$\lambda_1 \int_{M_{\lambda_2} \setminus M_{\lambda_1}} |f|^2 d\sigma(m) \leq \int_{M_{\lambda_2} \setminus M_{\lambda_1}} a(m)|f|^2 d\sigma(m)$$
$$\leq \lambda_2 \int_{M_{\lambda_2} \setminus M_{\lambda_1}} |f|^2 d\sigma(m),$$

which implies (3.3). In a similar way one can prove (3.4). $\square$

Proposition 3.10. *$f \in D(A)$ if and only if*

$$\int_{-\infty}^{\infty} \lambda^2 d(E_\lambda f, f) = \int_{-\infty}^{\infty} \lambda^2 d\|E_\lambda f\|^2 < \infty$$

Moreover, for $f \in D(A)$ the last integral coincides with $\|Af\|^2$ and

$$Af = \int_{-\infty}^{\infty} \lambda d(E_\lambda f), \tag{3.5}$$

where the last integral is the limit in $\mathcal{H}$

$$\lim_{\substack{\alpha \to -\infty \\ \beta \to +\infty}} \int_{\alpha}^{\beta} \lambda d(E_\lambda f),$$

while the integral over a finite interval is the limit of its integral sums (in the norm of $\mathcal{H}$).

Proof. First, let us recall what does it mean

$$\int_{\alpha}^{\beta} \varphi(\lambda) d\theta(\lambda),$$

where φ is continuous, θ is monotone increasing and right-continuous. Given a partition γ of $(\alpha, b]$ by points $\lambda_1 < \lambda_2 < \ldots < \lambda_{n+1} = \beta$ $(\lambda_0 = \alpha)$, we choose $\xi_i \in (\lambda_i, \lambda_{i+1})$ and set

$$\|\gamma\| = \max_i (\lambda_{i+1} - \lambda_i).$$

Then
$$\int_\alpha^\beta \varphi(\lambda)d\theta(\lambda) = \lim_{|\gamma|\to 0}\sum_{i=0}^{n}\varphi(\xi_i)[\theta(\lambda_{i+1}) - \theta(\lambda_i)].$$
We have
$$\begin{aligned}\int_\alpha^\beta \lambda^2 d(E_\lambda f, f) &= \int_\alpha^\beta \lambda^2 d\int_M x_\lambda(m)f(m)\overline{f}(m)d\sigma(m)\\ &= \int_\alpha^\beta \lambda^2 d\int_{M_\lambda}|f(m)|^2 d\sigma(m)\\ &= \lim_{|\gamma|\to 0}\sum \xi_i^2 \int_{M_{\lambda_{i+1}}\setminus M_{\lambda_1}}|f(m)|^2 d\sigma(m)\\ &= \lim_{|\gamma|\to 0}\int_{M_\beta\setminus M_\alpha} h_\gamma^2(m)|f(m)|^2 d\sigma(m),\end{aligned}$$
where $h_\gamma(m) = \xi_i$ on $M_{\lambda_{i+1}}\setminus M_{\lambda_i}$. Since
$$0 \le h_\gamma^2(m) \le \max(\alpha^2, \beta^2) = C,$$
then $h_\gamma^2(m)|f(m)|^2$ is bounded above by an integrable function $C|f(m)^2|$ on $M_\beta \setminus M_\alpha$. Obviously, $h_\gamma(m) \to a(m)$ almost everywhere on $M_\beta\setminus M_\alpha$. By the dominated convergence theorem, we have
$$\int_\alpha^\beta \lambda^2 d(E_\lambda f, f) = \int_{M_\beta\setminus M_\alpha} a(m)^2|f(m)|^2 d\sigma(m).$$
Passing to the limit as $\alpha\to-\infty$ and $\beta\to+\infty$, we get
$$\int_{-\infty}^{\infty}\lambda^2 d(E_\lambda f, f) = \int_M a(m)^2|f(m)|^2 d\sigma(m) = \|Af\|^2.$$
Now an integral sum for the right-hand part of (3.5) is
$$\sum \xi_i[\chi_{\lambda_{i+1}}(m) - \chi_{\lambda_i}(m)]f(m) = h_\gamma(m)f(m), m\in M_\beta\setminus M_\alpha,$$
and vanishes outside $M_\beta\setminus M_\alpha$. Hence,
$$\begin{aligned}&\int_M |(\chi_\beta - \chi_\alpha)a(m)f(m) - (\chi_\beta-\chi_\alpha)h_\gamma(m)f(m)|^2 d\sigma(m)\\ &\qquad\qquad = \int_{M_\beta\setminus M_\alpha}|a(m) - h_\gamma(m)|^2|f(m)|^2 d\sigma(m).\end{aligned}$$

As above, we see that the last integral tends to 0. Therefore

$$(\chi_\beta - \chi_\alpha)af = \int_\alpha^\beta \lambda d(E_\lambda f).$$

Letting $\alpha \to -\infty$, $\beta \to +\infty$, we conclude. □

A family E_λ satisfying the properties listed in Propositions 3.1 - 3.6 is called a *decomposition of identity* corresponding to a given self-adjoint operator A. We proved its existence. Remark without proof that given a self-adjoint operator there is only one decomposition of identity.

3.3 Functional calculus

Let $\varphi(\lambda), \lambda \in \mathbb{R}$, be a function which is measurable (and almost everywhere finite) with respect to the measure $d(E_\lambda f, f)$ for each $f \in \mathcal{H}$. Let $M, d\sigma, a(m)$ and U diagonalize A. Then $\varphi(a(m))$ is measurable. By definition,

$$\varphi(A) = U^{-1}\varphi(a(m))U$$

Proposition 3.11.

$$D(\varphi(A)) = \{f \in \mathcal{H} : \int_{-\infty}^{\infty} |\varphi(\lambda)|^2 d(E_\lambda f, f) < \infty).$$

Moreover, for every $f \in D(\varphi(A))$ and $g \in \mathcal{H}$

$$(\varphi(A)f, g) = \int_{-\infty}^{\infty} \varphi(\lambda) d(E_\lambda f, g).$$

Since the proof makes use the same kind of arguments as in section 3.2, we omit it. Due to this proposition, the operator $\varphi(A)$ is well-defined: it does not depend on a choice of $M, d\sigma, a(m)$ and U. The following statement is easy to prove by means of diagonalization.

Proposition 3.12.

(i) *If $\varphi(\lambda)$ is bounded, then $\varphi(A)$ is a bounded operator.*

(ii) *If $\varphi(\lambda)$ is real valued, then $\varphi(A)$ is a self-adjoint operator.*

(iii) *If $|\varphi(\lambda)| = 1$, then $\varphi(A)$ is a unitary operator.*

(iv) $\varphi_1(A)\varphi_2(A) = (\varphi_1\varphi_2)(A)$.

Remark 3.13. If A is bounded, then $(\varphi_1 + \varphi_2)(A) = \varphi_1(A) + \varphi_2(A)$. For unbounded A the situation is more complicated. Take $\varphi_1(\lambda) = \lambda, \varphi_2(\lambda) = -\lambda$. Then $(\varphi_1 + \varphi_2)(A) = 0$, with the domain $\mathcal{H}$, while $\varphi_1(A) + \varphi_2(A)$ is the same operator, but considered only on $D(A) \neq \mathcal{H}$.

Proposition 3.14. $\lambda_0 \in \mathbb{R} \setminus \sigma(A)$ *if and only if* E_λ *does not depend on* λ *in a neighborhood of* λ_0. *In other words,* $\sigma(A)$ *is exactly the set of increasing of* E_λ.

Proof. Let $\lambda_0 \in \mathbb{R} \setminus \sigma(A)$. We know that the resolvent set is open and R_λ depends continuously on λ. Therefore, there exists $\epsilon > 0$ such that $(\lambda_0 - \epsilon, \lambda_0 + \epsilon) \cap \sigma(A) = \emptyset$ and $\|R_\lambda\| \leq C$ for $|\lambda - \lambda_0| < \epsilon$. (Pass to the diagonalization $M, a(m), \ldots$). Evidently, R_λ, if exists, must coincide with multiplication by $1/(a(m) - \lambda)$. Recall now that the operator of multiplication by, say, $b(m)$ is bounded if $b(m)$ is essentially bounded, and the norm of this operator is exactly ess sup$|b(m)|$. Hence,

$$\text{ess sup} \frac{1}{|a(m) - \lambda|} \leq C, \lambda \in (\lambda_0 - \epsilon, \lambda_0 + \epsilon).$$

This implies directly that the set $a^{-1}(\lambda_0 - \epsilon, \lambda_0 + \epsilon)$ is of measure 0. Therefore, due to construction of E_λ, $E_\lambda = \text{const}$ for $\lambda \in (\lambda_0 - \epsilon, \lambda_0 + \epsilon)$. The converse statement is almost trivial. If $E_\lambda = \text{const}$ on $(\lambda_0 - \epsilon, \lambda_0 + \epsilon]$, then $\chi_{\lambda_0 + \epsilon} - \chi_{\lambda_0 - \epsilon} = 0$ almost everywhere, i.e. $a^{-1}((\lambda_0 - \epsilon, \lambda_0 + \epsilon])$ is of measure 0. Therefore, $1/[a(m) - \lambda_0]$ is essentially bounded. ☐

Exercise 3.15. Let $E_{\lambda_0 - 0} \neq E_{\lambda_0}$. Then there exists an eigenvector of A with the eigenvalue λ_0. If, in addition, $E_\lambda = E_{\lambda_0 - 0}$ for $\lambda_0 - \lambda > 0$ small enough, and $E_\lambda = E_{\lambda_0}$ for $\lambda - \lambda_0 > 0$ small, then $P_{\lambda_0} = E_{\lambda_0} - E_{\lambda_0 - 0}$ is the orthogonal projector onto the subspace of all eigenvectors with eigenvalue λ_0.

Now let $\varphi(\lambda) = \varphi_t(\lambda) = \exp(it\lambda)$. Then, due to Proposition 3.12 $U_t = \exp(itA)$ is a unitary operator. Moreover,

$$\begin{aligned} U_{t+s} &= U_t U_s, \quad t, s \in \mathbb{R}, \\ U_0 &= I \end{aligned}$$

Exercise 3.16. Prove that U_t is a strongly continuous family of operators, i.e. for every $f \in \mathcal{H}$ the function $U_t f$ of t is continuous.

In other words, operators U_t form a *strongly continuous group* of unitary operators.

Exercise 3.17. The derivative

$$\frac{d}{dt}(U_t f)|_{t=0} = \lim_{t\to 0} \frac{1}{t}(U_t f - f)$$

exists if and only if $f \in D(A)$. In this case the derivative is equal to iAf.

Exercise 3.18. Prove that for all $t \in \mathbb{R}$

$$\frac{d}{dt} U_t f = iAU_t f, \quad f \in D(A).$$

The last means that U_t is the so-called evolution operator for the Schrödinger equation

$$\frac{du}{dt} = iAu,$$

since, for $f \in D(A)$, the function $u(t) = U_t f$ is a solution of the last equation with the Cauchy data $u(0) = f$.

Remarkably, that the famous Stone theorem states: if U_t is a strongly continuous group of unitary operators, then there exists a self-adjoint operator A such that $U_t = \exp(itA)$. The operator A is called the *generator* of U_t.

Exercise 3.19. In $L^2(\mathbb{R})$ consider a family of operators U_t defined by

$$(U_t f)(x) = f(x - t), \quad f \in L^2(\mathbb{R}).$$

Prove that U_t is a strongly continuous group of unitary operators and find its generator.

3.4 Classification of spectrum

Let $d\sigma$ be a finite Lebesgue-Stieltjes measure generated by a bounded monotone increasing function σ. Then [13] it may be decomposed as

$$d\sigma = d\sigma_{ac} + d\sigma_{sc} + d\sigma_p, \tag{3.6}$$

where $d\sigma_{ac}$ is absolutely continuous with respect to the Lebesgue measure, $d\sigma_{sc}$ is purely singular, i.e. its support has Lebesgue measure 0 and at the same time $d\sigma_{sc}$ has no points of positive measure, and $d\sigma_p$ is a purely point measure. The last means that there are countably many atoms (points of positive measure with respect to $d\sigma_p$) and the measure of any set is equal to the sum of measures of atoms contained in this set. On the level of distribution function σ, we have

$$\sigma = \sigma_{ac} + \sigma_{sc} + \sigma_p.$$

Here σ_{ac} is a monotone absolutely continuous function, σ_{sc} is a monotone continuous function, whose derivative vanishes almost everywhere with respect to the Lebesgue measure, and σ_p is a function of jumps:

$$\sigma_p(x) = \sum_{x_j < x} \alpha_j,$$

where $\{x_j\}$ a countable set of points, $\alpha_j > 0$ and $\sum \alpha_j < \infty$.

Now we introduce the following subspaces:

$$\begin{aligned} \mathcal{H}_p &= \{f \in \mathcal{H} : d(E_\lambda f, f) \text{ is a purely point measure}\}\,, \\ \mathcal{H}_{ac} &= \{f \in \mathcal{H} : d(E_\lambda f, f) \text{ is absolutely continuous}\}\,, \\ \mathcal{H}_{sc} &= \{f \in \mathcal{H} : d(E_\lambda f, f) \text{ is purely singular}\}\,. \end{aligned}$$

It turns out that these subspaces are orthogonal, invariant with respect to A and

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

The spectra of the parts of A in the spaces $\mathcal{H}_p$, $\mathcal{H}_{ac}$ and $\mathcal{H}_{sc}$ are called *pure point spectrum* $\sigma_p(A)$, *absolutely continuous spectrum* $\sigma_{ac}(A)$ and *singular spectrum* $\sigma_{sc}(A)$, respectively. If, for example, $\mathcal{H}_{sc} = \{0\}$, we say that A has no singular spectrum and write $\sigma_{sc}(A) = \emptyset$, etc. See [10], [2] for details.

4 Compact operators and the Hilbert-Schmidt theorem

4.1 Preliminaries

First, let us recall several properties of bounded operators. The set $L(\mathcal{H})$ of all bounded operators is a Banach space with respect to the operator norm $\|A\|$. In $L(\mathcal{H})$ there is an additional operation, the multiplication of operators, such that

$$\|AB\| \leq \|A\|\|B\|.$$

Another way to express this is to say that $L(\mathcal{H})$ is a *Banach algebra* (not commutative!). Moreover, passage to the adjoint operator, $A \mapsto A^*$, is an anti-linear involution ($A^{**} = A$) and

$$\|A^*\| = \|A\|$$

(prove this). In other words, $L(\mathcal{H})$ is a Banach algebra with involution. Even more, we have

$$\|AA^*\| = \|A\|^2$$

(prove this) and this means that $L(\mathcal{H})$ is a C^*-algebra. We summarize these facts here, since later on we will deal with particular subsets of $L(\mathcal{H})$ which are (two-side) ideals.

Proposition 4.1. *Let $A \in L(\mathcal{H})$ be a self-adjoint operator. Then*

$$\|A\| = \sup_{\|f\|=1} |(Af, f)|.$$

Proof. Let $m = \sup_{\|f\|=1} |(Af, f)|$. Clearly,

$$|(Af, f)| \leq \|Af\|\|f\| \leq \|A\|\|f\|^2$$

and, hence, $m \leq \|A\|$. To prove the opposite inequality, note that

$$(A(f+g), f+g) - (A(f-g), f-g) = 4Re(Af, g).$$

Therefore,

$$Re(Af, g) \leq \frac{1}{4}m(\|f+g\|^2 + \|f-g\|^2) = \frac{1}{2}m(\|f\|^2 + \|g\|^2).$$

Assuming that $\|f\| = 1$, take here $g = Af/\|Af\|$. We get $\|Af\| = Re(Af, g) \leq m$. Hence $\|A\| \leq m$.

$\square$

4.2 Compact operators

An operator $A \in L(\mathcal{H})$ is said to be *compact* if for any bounded sequence $\{f_k\} \subset \mathcal{H}$ the sequence $\{Af_k\}$ contains a convergent subsequence. The set of all such operators is denoted by $S(\mathcal{H})$ (more natural would be $S_\infty(\mathcal{H})$, as we will see later on). Obviously, the sum of two compact operators is a compact operator. Moreover, if $A \in L(\mathcal{H})$ and $B \in S(\mathcal{H})$, then $AB \in S(\mathcal{H})$ and $BA \in S(\mathcal{H})$. Thus, $S(\mathcal{H})$ is a two-side ideal in $L(\mathcal{H})$. If $\dim \mathcal{H} < \infty$, all linear operators in $\mathcal{H}$ are compact. It is not so if $\dim H = \infty$. For example, the identity operator I is not compact. As consequence, we see that a compact operator cannot have a bounded inverse operator.

Theorem 4.2. *If $A \in S(\mathcal{H})$, then $A^* \in S(\mathcal{H})$.*

Proof. Let B be the unit ball in $\mathcal{H}$. Then its image $M = A(B)$ is compact. Consider the set of functions $F = \{\varphi : \varphi(x) = (x, y), y \in B\}$ defined on M, i.e. here $x \in M$. F is a subset in $C(M)$, the spaces of continuous functions on M. The set F is bounded, since

$$|\varphi(x)| \leq \|x\| \cdot \|y\| \leq \|x\|, \quad x \in M,$$

and M is bounded. Moreover, F is equicontinuous, since $\|\varphi(x) - \varphi(x')\| \leq \|x - x'\|$. By the Arzela theorem, F is a compact subset of $C(M)$.

Now, for any $\epsilon > 0$ there exists a finite number of functions $\varphi_1(x) = (x, y_1), \dots, \varphi_N(x) = (x, y_N)$ with the following property. For any $\varphi \in F$, we have $|\varphi(x) - \varphi_j(x)| \leq \epsilon$ for some j and all $x \in M$. This means that for any $y \in B$ there exists an element y_j such that

$$|(Ax, y - y_j)| \leq \epsilon \quad \forall x \in B,$$

or

$$|(x, A^*y - A^*y_j)| \leq \epsilon \quad \forall x \in B.$$

The last means that

$$\|A^*y - A^*y_j\| \leq \epsilon.$$

Since ϵ is arbitrary, the closure of $A^*(B)$ is compact ($A^*(B)$ is precompact) and the proof is complete. □

Theorem 4.2 means that the ideal $S(\mathcal{H})$ is invariant with respect to the involution, or *-ideal.

Now let us point out that any finite dimensional operator A, i.e. a bounded operator whose image $\operatorname{im} A$ is a finite dimensional subspace of $\mathcal{H}$, is obviously a compact operator. The set $S_0(\mathcal{H})$ of all finite dimensional operators is a two-side *-ideal (not closed!).

Exercise 4.3. Prove the last statement.

Theorem 4.4. *$S(\mathcal{H})$ is closed. Moreover, $S(\mathcal{H})$ is the closure of $S_0(\mathcal{H})$.*

Proof. Assume that $A_k \in S(\mathcal{H})$ and $A_k \to A$. Let $\{f_j\}$ be a bounded sequence in $\mathcal{H}$. Then $\{A_1 f_j\}$ contains a convergent subsequence $\{A_1 f_j^{(1)}\}$, the sequence $\{A_2 f_j^{(1)}\}$ contains a convergent subsequence $\{A_2 f_j^{(2)}\}$, etc. Let $y_j = f_j^{(j)}$ be the diagonal sequence. Certainly, $\{A_k f_j\}$ is convergent for each k. One can prove that $\{Ay_j\}$ is convergent.

Now let $A \in S(H)$. For arbitrarily chosen orthogonal basis $\{e_k\}$, denote by P_k the orthogonal projector onto the subspace spanned on $\{e_1, \dots, e_k\}$. Then $P_k A$ is a finite dimensional operator and $P_k A \to A$ in $L(\mathcal{H})$. □

Exercise 4.5. Complete the proof of Theorem 4.4.

4.3 The Hilbert-Schmidt theorem

Now we will clarify spectral properties of compact self-adjoint operators.

Proposition 4.6. *A compact self-adjoint operator has at least one eigenvalue.*

Proof. Assume $A \neq 0$ (otherwise the assertion is trivial). Then

$$m = \sup_{\|f\|=1} |(Af, f)| \neq 0.$$

For definiteness, assume that

$$m = \sup_{\|f\|=1} (Af, f).$$

There exists a sequence $\{f_k\}$ such that $\|f_k\| = 1$ and

$$(Af_k, f_k) \to m.$$

Since A is compact, we can assume that $Af_k \to g$. By Proposition 4.1, $m = \|A\|$ and

$$\begin{aligned}\|Af_k - f_k\| &= \|Af_k\|^2 - 2m(Af_k, f_k) + m^2 \\ &\leq \|A\|^2 - 2m(Af_k, f_k) + m^2 = 2(m^2 - m(Af_k, f_k))\end{aligned}$$

The right-hand side here tends to 0, hence, $\|Af_k - mf_k\| \to 0$. Therefore, $f_k \to g/m = f_0$ and $\|f_0\| = 1$. Evidently, $Af_0 = mf_0$. □

Proposition 4.7. *Let A be a compact self-adjoint operator. For any $r > 0$ there is at most a finite number of linearly independent eigenvectors, with eigenvalues outside of $[-r, r]$. In particular, each eigenspace with nonzero eigenvalue is finite dimensional.*

Proof. Assume there is an infinite sequence of mutually orthogonal eigenvectors f_k, $\|f_k\| = 1$, with eigenvalues λ_k, $|\lambda_k| > r$. The sequence $g_k = f_k/\lambda_k$ is bounded and therefore the sequence Ag_k contains a convergent subsequence. However, the last is impossible, since $Ag_k = f_k$ and $\|f_k - f_j\| = \sqrt{2}$, $j \neq k$. □

The next result is known as the Hilbert-Schmidt theorem.

Theorem 4.8. *Let A be a compact self-adjoint operator. Then there exists an orthogonal system $\{e_k\}$ of eigenvectors, with nonzero eigenvalues $\{\lambda_k\}$, such that each vector $f \in \mathcal{H}$ has a unique representation of the form*

$$f = \sum_{k=1}^{\infty} c_k e_k + f_0,$$

where $f_0 \in \ker A$. Moreover,

$$Af = \sum_k c_k \lambda_k e_k$$

and $\lambda_k \to 0$, provided the system $\{e_k\}$ is infinite.

Proof. By proposition 4.6, there exists an eigenvector e_1 with the eigenvalue $\lambda = \pm m_1 = \pm m$ (in terms of Proposition 4.6). Let $\mathcal{X}_1$ be the 1-dimensional subspace generated by e_1 and $\mathcal{H} = \mathcal{X}_1^{\perp}$. It is not difficult to see that $A\mathcal{H}_1 \subset \mathcal{H}_1$. If $A|\mathcal{H}_1 = 0$, the proof is complete. Otherwise, there exists $e_2 \in \mathcal{H}_2$ such that $\|e_2\| = 1$, $Ae_2 = \pm m_2 e_2$, where

$$m_2 = \sup_{\|f\|=1, f \in \mathcal{H}_1} |(Af, f)|.$$

And so on. □

Thus, for a self-adjoint compact operator A any non-zero point $\lambda \in \sigma(A)$ is an eigenvalue. Certainly, $0 \in \sigma(A)$ and may be not an eigenvalue. Let P_{λ_j} be an orthogonal projector onto the eigenspace with eigenvalue λ_j. Then for the corresponding decomposition of identity, we have

$$E_\lambda = \sum_{\lambda_j < \lambda} P_{\lambda_j}.$$

Let us remark that a non self-adjoint compact operator in an infinite dimensional Hilbert space may have no eigenvalues. In the case of finite dimensions any operator has an eigenvalue.

Exercise 4.9. Let ℓ^2 be the Hilbert space of all sequences $x = \{x_k\}$ such that

$$\|x\| = (\sum_{k=1}^{\infty} |x_k|^2)^{1/2}.$$

The operator A is defined by $Ax = y$, where $y_1 = 0$, $y_k = 2^{-k}x_{k-1}$, $k = 2, 3, \ldots$. Then A is compact, but has no eigenvalues. In fact, $\sigma(A) = \{0\}$.

Example 4.10. In $L^2(0,1)$ let us consider an operator A defined by

$$(Af)(x) = \int_0^x f(t)dt.$$

This operator is compact, $\sigma(A) = \{0\}$ and there are no eigenvalues.

Compact operators with $\sigma(A) = \{0\}$ are commonly known as *Volterra operators.*

4.4 Hilbert-Schmidt operators

An operator $K \in L(\mathcal{H})$ is called a Hilbert-Schmidt operator if for some orthonormal basis $\{e_k\}$ the following norm

$$\|K\|_2 = (\sum \|Ke_k\|^2)^{1/2} \tag{4.1}$$

is finite. The set of all Hilbert-Schmidt operators is denoted by $S_2(\mathcal{H})$. Certainly, one has to prove that this notion is well-defined.

Proposition 4.11. *If the quantity (4.1) is finite for some orthonormal basis, than same is for every orthonormal basis and $\|K\|_2$ is independent on the choice of basis. If $K \in S_2(\mathcal{H})$, then $K^* \in S_2(\mathcal{H})$ and*

$$\|K^*\|_2 = \|K\|. \tag{4.2}$$

Moreover,

$$\|K\| \le \|K\|_2 \tag{4.3}$$

Proof. Inequality (4.3) follows immediately: if

$$f = \sum f_k e_k,$$

then

$$\|Kf\|^2 = \|\sum f_k Ke_k\|^2 \le (\sum |f_k| \|Ke_k\|)^2$$
$$\le \sum |f_k|^2 \sum \|Ke_k\|^2 = \|K\|_2^2 \|f\|^2.$$

Now let $\{e'_k\}$ be an orthonormal basis (perhaps, the same as $\{e_k\}$). We have

$$\|Ke_k\|^2 = \sum |(Ke_k, e'_j)|^2$$

Hence,

$$\sum_k \|Ke_k\|^2 = \sum_{k,j} |(e_k, K^* e'_j)| = \sum_j \|K^* e'_j\|^2 \tag{4.4}$$

This implies (4.2) and independence of $\|K\|_2$ on the basis. ☐

Proposition 4.12. *Every Hilbert-Schmidt operator is a compact operator, i. e. $S_2(\mathcal{H}) \subset S(\mathcal{H})$.*

Proof. We have

$$Kf = \sum (f, e_k) Ke_k.$$

Set

$$K_N f = \sum_{k=1}^{N} (f, e_k) Ke_k.$$

Then

$$\|K - K_N\|^2 \le \|K - K_N\|_2^2 \le \sum_{k=N+1}^{\infty} \|Ke_n\|^2 \to 0.$$

☐

Proposition 4.13. *Let K be a compact self-adjoint operator. $K \in S_2(\mathcal{H})$ iff*

$$\sum \lambda_k^2 < \infty,$$

where $\{\lambda_k\}$ are all nonzero eigenvalues of K, counting multiplicity.

Proof. Obvious. ☐

Now we want to study Hilbert-Schmidt operators in the space $L^2(M, d\sigma)$ (for simplicity, one can think that M is an open subset of $\mathbb{R}^n$, and $d\sigma$ is the Lebesgue measure, or a Lebesgue-Stieltjes measure).

Proposition 4.14. *Let K be a bounded linear operator in $L^2(M, d\sigma)$. K is a Hilbert-Schmidt operator iff there exists a function*

$$\mathcal{K}(m_2, m_1) \in L^2(M \times M, d\sigma \times d\sigma)$$

(the kernel function of K) such that

$$(Kf)(m_2) = \int_{M_1} \mathcal{K}(m_2, m_1) f(m_1) d\sigma(m_1). \tag{4.5}$$

The function $\mathcal{K}$ is uniquely defined, up to a set of $d\sigma \times d\sigma$-measure 0 and

$$\|K\|_2^2 = \int\int |\mathcal{K}(m_2, m_1)|^2 d\sigma(m_2) d\sigma(m_1). \tag{4.6}$$

Proof. Let $\{e_k\}$ be an orthonormal basis in $L^2(M, d\sigma)$ (for simplicity we assume that $L^2(M, d\sigma)$ is separable) and $K \in S_2(L^2(M, d\sigma))$. We have

$$Kf = K\sum_k (f, e_k)e_k = \sum_k (f, e_k)Ke_k = \sum_{k,j} (Ke_k, e_j)(f, e_k)e_j. \tag{4.7}$$

By (4.4),

$$\|K\|_2^2 = \sum_{k,j} |(Ke_k, e_j)|^2.$$

The functions $\{e_k(m_2)\overline{e_j(m_1)}\}$ form an orthonormal basis in $L^2(M \times M, d\sigma \times d\sigma)$ (check this). Now we set

$$\mathcal{K}(m_2, m_1) = \sum (Ke_k, e_j)e_j(m_2)\overline{e_k(m_1)}. \tag{4.8}$$

Then $\mathcal{K} \in L^2(M \times M, d\sigma \times d\sigma)$ and

$$\|\mathcal{K}\|^2_{L^2(M\times M)} = \sum |(Ke_k, f_j)|^2 = \|K\|_2^2.$$

Equation (4.5) follows directly from (4.7).

Now let K is defined by (4.5), with $\mathcal{K} \in L^2(M \times M)$ Then

$$\mathcal{K}(m_2, m_1) = \sum_{k,j} c_{kj} f_j(m_2)\overline{e_k(m_1)}, \tag{4.9}$$

where $\sum |e_{kj}|^2 < \infty$. By (4.4),

$$\|K\|_2^2 = \sum |c_{kj}|^2,$$

since $Ke_k = \sum_j c_{kj}e_j$. ☐

Exercise 4.15. Prove uniqueness of $\mathcal{K}$.

Exercise 4.16. Prove that $S_2(\mathcal{H})$ is a two-side ideal in $L(\mathcal{H})$ (not closed!).

4.5 Nuclear operators

First, we introduce an inner product on $S_2(\mathcal{H})$, so that $S_2(\mathcal{H})$ becomes a Hilbert space. Set

$$(K, L)_2 = \sum (Ke_k, Le_k), \quad K, L \in S_2(\mathcal{H}), \tag{4.10}$$

where $\{e_k\}$ is an orthonormal basis. Certainly, this inner product induces the norm in $S_2(\mathcal{H})$ defined above.

An operator $A \in L(\mathcal{H})$ is said to be nuclear if it can be written in the form

$$A = \sum_{i=1}^{N} B_j C_j, \quad B_j, C_j \in S_2(\mathcal{H}), \tag{4.11}$$

where N depends on A. We denote the set of all such operators by $S_1(\mathcal{H})$. One can verify that $S_1(\mathcal{H})$ is a two-side ideal in $L(\mathcal{H})$ (not closed), and $S_1(\mathcal{H}) \subset S_2(\mathcal{H})$. In algebraic terms, $S_1(\mathcal{H})$ is the square of the ideal $S_2(\mathcal{H})$: $S_1(\mathcal{H}) = S_2(\mathcal{H})^2$.

Proposition 4.17. *Let $A \in S_1(\mathcal{H})$ and $\{e_k\}$ an orthonormal basis. Then*

$$\sum |(Ae_k, e_k)| < \infty \tag{4.12}$$

and

$$\operatorname{tr} A = \sum (Ae_k, e_k), \tag{4.13}$$

the trace of A, is independent on the choice of $\{e_k\}$. The trace of A is a linear functional on $S_1(\mathcal{H})$ such that $\operatorname{tr} A \geq 0$ for $A \geq 0$ and

$$\operatorname{tr} A^* = \overline{\operatorname{tr} A}. \tag{4.14}$$

Moreover,

$$(K, L)_2 = \operatorname{tr}(L^* K), K, L \in S_2(\mathcal{H}). \tag{4.15}$$

Proof. Using (4.11), we have

$$(Ae_k, e_k) = \sum_{j=1}^{N} (B_j C_j e_k, e_k) = \sum_{j=1}^{N} (Cje_k, Bj^* e_k),$$

which implies (4.12) and the following equation

$$\sum_k (Ae_k, e_k) = \sum_{j=1}^{N} (C_j, B_j^*)_2.$$

Hence $\operatorname{tr} A$ does not depend on the choice of basis. Nonnegativity of $\operatorname{tr} A$ and (4.14), (4.15) are evident. $\square$

Proposition 4.18. *Let A be a self-adjoint compact operator and $\lambda_1, \lambda_2, \ldots$ all its nonzero eigenvalues (counting multiplicity). $A \in S_1(\mathcal{H})$ iff*

$$\sum |\lambda_j| < \infty. \tag{4.16}$$

Moreover,

$$\operatorname{tr} A = \sum \lambda_j \tag{4.17}$$

Proof. Let $A \in S_1(\mathcal{H})$. Choosing as $\{e_k\}$ the eigenbasis (it exists!), we get (4.16) and (4.17). Conversely, assume (4.16). Let $\{e_k\}$ be the eigenbasis of A, i.e. $Ae_k = \lambda_k e_k$. Define the operators B and C by

$$Be_k = |\lambda_k|^{1/2} e_k,$$
$$Ce_k = \lambda_k |\lambda_k|^{-1/2} e_k.$$

We have $B, C \in S_2(\mathcal{H})$ and $A = BC$. Hence $A \in S_1(\mathcal{H})$. □

The next statement is, perhaps, the most important property of trace.

Proposition 4.19. *If $A \in S_1(\mathcal{H})$ and $B \in L(\mathcal{H})$, then*

$$\operatorname{tr}(AB) = \operatorname{tr}(BA). \tag{4.18}$$

Lemma 4.20. *Every operator $B \in L(\mathcal{H})$ is a linear combination of four unitary operators.*

Proof. We have

$$B = B_1 + iB_2,$$

where

$$B_1 = B_1^* = (B + B^*)/2, \quad B_2 = B_2^* = (B - B^*)/2i.$$

Hence, we need to prove that each self-adjoint operator B is a linear combination of two unitary operators. In addition, we may assume that $\|B\| \leq 1$. Now

$$B = \frac{1}{2}(B + i\sqrt{I - B^2}) + \frac{1}{2}(B - i\sqrt{I - B^2}).$$

To verify that $B \pm i\sqrt{I - B^2}$ is a unitary operator one can use the functional calculus. □

Proof of Proposition 4.19. Due to the Lemma, we can assume that B is a unitary operator. In this case the operators AB and BA are unitary equivalent:

$$AB = B^{-1}(BA)B$$

However, unitary equivalent nuclear operators have the same trace, since trace does not depend on the choice of basis. □

4.6 A step apart: polar decomposition

An operator $U \in L(\mathcal{H})$ is said to be partially isometric if it maps isometrically $(\ker U)^\perp$ onto $\operatorname{im} U$, i. e. $\|Uf\| = \|f\|$ for $f \in (\ker U)^\perp$. Remark that in this case $\operatorname{im} U$ is a closed subspace of $\mathcal{H}$. As consequence,

$$U^*U = E, \quad UU^* = F, \tag{4.19}$$

where E is the orthogonal projector onto $(\ker U)^\perp$ and F the orthogonal projector onto $\operatorname{im} U$. Certainly, if $\ker U = \{0\}$ and $\operatorname{im} U = \mathcal{H}$, then U is a unitary operator.

Exercise 4.21. Prove (4.19).

Let $A \in L(\mathcal{H})$. If

$$A = US, \tag{4.20}$$

where $S \in L(\mathcal{H})$, $S^* = S$, $S \geq 0$, and U is a partially isometric operator with

$$\ker U = \ker S = (\operatorname{im} S)^\perp, \tag{4.21}$$

we say that (4.20) is a *polar decomposition* of A. In the case $\mathcal{H} = \mathbb{C}$, we have $L(\mathcal{H}) = \mathbb{C}$ and polar decomposition is exactly the representation of a complex number in the form $r\exp(i\theta)$.

Proposition 4.22. *For each bounded linear operator there exists a unique polar decomposition.*

Proof. Assume that (4.20) is a polar decomposition. Then $A^* = SU^*$. Hence

$$A^*A = SU^*US = SES.$$

Due to (4.21), $ES = S$. Therefore,

$$A^*A = S^2 \tag{4.22}$$

which implies

$$S = \sqrt{A^*A}. \tag{4.23}$$

Due to (4.20), the operator U is uniquely determined on $\operatorname{im} S$, hence, on $\overline{\operatorname{im} S}$. Since, by (4.21),

$$\ker U = (\operatorname{im} S)^\perp = (\overline{\operatorname{im} S})^\perp,$$

the operator U is unique.

To prove existence, we first define S by (4.23). Here A^*A is a nonnegative self-adjoint operator and the square root exists due to functional calculus. Now we define U letting

$$\begin{aligned} Uf &= 0\,, \qquad & f &\in (\operatorname{im} S)^\perp = (\overline{\operatorname{im} S})^\perp \\ Uf &= Ag\,, \qquad & f &= Sg \in \operatorname{im} S. \end{aligned}$$

Equation (4.22) implies immediately that if $Sg = 0$, then $Ag = 0$. Therefore, U is well-defined on $\operatorname{im} S \oplus (\operatorname{im} S)^\perp$ which is, in general, only a dense subspace of $\mathcal{H}$ ($\overline{\operatorname{im} S} \oplus (\operatorname{im} S)^\perp = \mathcal{H}$!). However, (4.22) implies

$$\|Sg\|^2 = (Sg, Sg) = (S^2 g, g) = (A^*Ag, g) = (Ag, Ag) = \|Ag\|^2,$$

i.e. $\|Uf\| = \|f\|$ for $f \in \operatorname{im} S$. Hence, S is bounded and, by continuity, can be extended to a (unique) partially isometric operator on whole $\mathcal{H}$. ☐

For $A \in L(\mathcal{H})$ we denote by $|A|$ the operator S from the polar decomposition of A ($|A| = \sqrt{A^*A}$).

Proposition 4.23. *Let J be a left ideal of $L(\mathcal{H})$. Then $A \in J$ if $|A| \in J$.*

Proof. Obvious, due to formulas $A = U|A|, U^*A = |A|$. ☐

As consequence, $A \in S(\mathcal{H})$ (resp. $S_1(\mathcal{H}), S_2(\mathcal{H})$) if and only if $|A| \in S(\mathcal{H})$ (resp., $S_1(\mathcal{H}), S_2(\mathcal{H})$.

4.7 Nuclear operators II

Proposition 4.24. *If $A, B \in S_2(\mathcal{H})$, then*

$$\operatorname{tr}(AB) = \operatorname{tr}(BA).$$

Proof. We have the following identities:

$$\begin{aligned} 4AB^* &= (AB) + (AB)^* - (A-B)(A-B)^* \\ &\qquad + i(A+iB)(A+iB)^* - i(A-iB)(A-iB)^*, \\ 4B^*A &= (AB)^* + (AB) - (A-B)^*(A-B) \\ &\qquad + i(A+iB)^*(A+iB) - i(A-iB)^*(A-iB). \end{aligned}$$

This implies that we need only to prove that

$$\operatorname{tr}(AA^*) = \operatorname{tr}(A^*A), \quad A \in S_2(\mathcal{H}).$$

From the polar decomposition $A = US$ we get $S = U^*A$. Since $A \in S_2(\mathcal{H})$, this implies that $S \in S_2(\mathcal{H})$. However, $A^* = S^2$ and, by Proposition 4.9,

$$\operatorname{tr}(AA^*) = \operatorname{tr}(US^2U^*) = \operatorname{tr}(U^*US^2) = \operatorname{tr}(S^2) = \operatorname{tr}(A^*A).$$

(Here we have used $U^*U = E$ and $ES = S$). ☐

Now we introduce the so-called nuclear norm. Let $A \in S_2(\mathcal{H})$ and $A = U|A|$ its polar decomposition. Set

$$\|A\|_1 = \operatorname{tr}|A|$$

We collect main properties of nuclear norm.

Proposition 4.25. *We have*

$$\|A\|_2 \le \|A\|_1, \qquad A \in S_1(\mathcal{H}); \tag{4.24}$$
$$\|BA\|_1 \le \|B\| \cdot A_1, \qquad A \in S_1(\mathcal{H}), B \in L(\mathcal{H}); \tag{4.25}$$
$$\|AB\|_1 \le \|A\|_1\|B\|, \qquad A \in S_1(\mathcal{H}), B \in L(\mathcal{H}); \tag{4.26}$$
$$\|BA\|_1 \le \|B\|_2\|A\|_2, \qquad A, B \in S_2(\mathcal{H}); \tag{4.27}$$
$$|\operatorname{tr} A| \le \|A\|_1, \qquad A \in S_1(\mathcal{H}); \tag{4.28}$$
$$\|A^*\|_1 = \|A\|_1, \qquad A \in S_1(\mathcal{H}); \tag{4.29}$$
$$\|A\|_1 = \sup_{\substack{B\in L(\mathcal{H})\\ \|B\|\le 1}} |\operatorname{tr}(BA)|, \qquad A \in S_1(\mathcal{H}). \tag{4.30}$$

(In (4.30) one can replace $B \in L(\mathcal{H})$ by $B \in S_0(\mathcal{H})$, the set of finite dimensional operators).

Proof.

1) Prove (4.24). Let $S = |A|$. Then

$$\|A\|_1 = \|S\|_1 = \operatorname{tr} S,$$
$$\|A\|_2^2 = \operatorname{tr} A^*A = \operatorname{tr} S^2,$$

and (4.24) reduces to the inequality

$$\operatorname{tr} S^2 \le (\operatorname{tr} S)^2.$$

The last inequality becomes easy if we write down $\operatorname{tr} S^2$ and $\operatorname{tr} S$ by means of the eigenbasis of S.

2) To prove (4.29), remark that $A^* = SU^*, AA^* = US^2U^*$ and $|A^*| = USU^*$. Hence

$$\operatorname{tr}|A^*| = \operatorname{tr}(USU^*) = \operatorname{tr}(U^*US) = \operatorname{tr} S = \operatorname{tr}|A|.$$

3) Let us prove (4.28). Let $\{e_k\}$ be an orthonormal eigenbasis of S, $\{s_k\}$ the set of corresponding eigenvalues:

$$Se_k = s_k e_k.$$

Then

$$\operatorname{tr} A = \sum_k (USe_k, e_k) = \sum_k S_k(Ue_k, e_k).$$

However, $|(Ue_k, e_k)| \leq 1$ and, therefore,

$$|\operatorname{tr} A| \leq \sum s_k = \operatorname{tr} s = \|A\|_1.$$

4) To prove (4.25), consider the polar decomposition $BA = VT$ of BA. We have

$$\|BA\|_1 = \operatorname{tr} T = \operatorname{tr}(V^*BA) = \operatorname{tr}(V^*BUS).$$

However, $\|V^*BU\| \leq \|B\|$ and we can use the argument of step 3.

5) Proof of (4.27). As on step 4, we have

$$\begin{aligned}\|BA\|_1 &= \operatorname{tr}(V^*BA) = \operatorname{tr}((B^*V)^*A) = (A, B^*V)_2 \\ &\leq \|A\|_2\|B^*V\|_2 \leq \|A\|_2\|B^*\|_2\|V\| \leq \|A\|_2\|B\|_2.\end{aligned}$$

6) Due to (4.29), estimate (4.26) follows from (4.25).

7) We have

$$|\operatorname{tr}(BA)| \leq \|BA\|_1 \leq \|B\|\|A\|_1.$$

In fact, here we have equality if $B = U^*$ and this implies (4.30). Now let $B = B_n = P_nU^*$, where

$$P_n = E((1/n, +\infty))$$

is the spectral projector of S. We have

$$\lim\|B_nA\|_1 = \lim \operatorname{tr}(P_nS) = \operatorname{tr} A = \|A\|_1.$$

$\square$

Proposition 4.26. *$S_1(\mathcal{H})$ is a Banach space with respect to the nuclear norm.*

Proof.

1) Let us verify the standard properties norm

$$\begin{aligned}\|A'+A''\|_1 &\le \|A'\|_1+\|A''\|_1,\\ \|\lambda A\|_1 &= |\lambda|\|A'\|_1,\\ \|A\|_1 &= 0 \text{ iff } A=0.\end{aligned}$$

Only the first one is nontrivial an we consider it now. Using (4.30), we get

$$\begin{aligned}\|A'+A''\|_1 &\le \sup_{\|B\|\le 1}|\mathrm{tr}(B(A'+A''))|\\ &= \sup_{\|B\|\le 1}|\mathrm{tr}(BA')+\mathrm{tr}(BA'')|\\ &\le \sup_{\|B\|\le 1}(|\mathrm{tr}\, BA'|+|\mathrm{tr}\, BA''|)\\ &\le \sup_{\|B\|\le 1}|\mathrm{tr}(BA')|+\sup_{\|B\|\le 1}|\mathrm{tr}(BA'')|\\ &= \|A'\|_2+\|A''\|_2.\end{aligned}$$

2) Now we want to prove the completeness. Let $A_n \in S_1(\mathcal{H})$ and

$$\|A_n - A_m\|_1 \to 0$$

as $m,n\to\infty$. By (4.24), $\|A_n - A_m\|_2 \to 0$. Hence, there exists $A\in S_2(\mathcal{H})$ such that

$$\lim\|A_n - A\|_2 = 0 \tag{4.31}$$

We prove that $A\in S_1(\mathcal{H})$. Let $A=US$ be the polar decomposition of A and $S_n = U^*A_n$. It is clear that

$$\lim\|S_n - S\|_2 = 0, \tag{4.32}$$

$$\lim\|S_n - S_m\|_1 = 0. \tag{4.33}$$

Let $\{e_k\}$ be an orthonormal eigenbasis of S, with corresponding eigenvalues s_k. Equation (4.31) implies that

$$s_k = (Se_k,e_k) = \lim(S_ne_k,e_k). \tag{4.34}$$

To verify that $A \in S_1(\mathcal{H})$, is suffices to show that

$$\sum s_k < \infty.$$

However, (4.30) implies easily that

$$\sum_k |(Se_k, e_k)| \leq \|S\|_1,\ S \in S_1(\mathcal{H}).$$

Hence,

$$\sup_n \sum_k |(S_n e_k, e_k)| < \infty$$

and this implies the required due to (4.34).

Now it remains to show that

$$\lim \|A_n - A\|_1 = 0.$$

Let $\epsilon > 0$. Choose $N > 0$ such that

$$\|A_m - A_n\|_1 \leq \epsilon, \quad m, n \geq N$$

and prove that

$$\|A_n - A\|_1 \leq \epsilon, n \geq N.$$

Indeed, (4.27) and (4.31) imply that for each finite dimensional $B \in L(\mathcal{H})$

$$\lim \operatorname{tr}(BA_m) = \operatorname{tr}(BA)$$

Therefore,

$$|\operatorname{tr}[B(A_n - A)]| = \lim_m |\operatorname{tr}[B(A_n - A_m)]| \leq \epsilon, n \geq N,$$

provided $\|B\| \leq 1$. We conclude using the last remark of Proposition 4.13.

□

4.8 Trace and kernel function

Now let K be a nuclear operator in $L^2(X)$. We know that K is a Hilbert-Schmidt operator and, therefore, has a kernel $\mathcal{K}(x, y)$:

$$Ku(x) = \int \mathcal{K}(x, y) u(y) dy.$$

Two questions arise: how to express $\operatorname{tr} K$ in terms of its kernel function $\mathcal{K}$. And which kernel functions generate nuclear operators? The first question is answered by the formula

$$\operatorname{tr} K = \int \mathcal{K}(x, x) dx. \tag{4.35}$$

Certainly, since $\mathcal{K}$ is only measurable, the meaning of the right-hand side here is not so clear. It may be clarified, but we will not do this here. Instead, let us explain why formula (4.35) is natural.

First we have

$$K = K_1 + iK_2,$$

where

$$K_1 = \frac{1}{2}(K + K^*), K_2 = \frac{1}{2i}(K - K^*)$$

are self-adjoint nuclear operators. Hence, we can assume that K is self-adjoint. Let $\{e_k\}$ be an eigenbasis of K and $\{\lambda_k\}$ the set of eigenvalues. Then $\{e_k(x)\overline{e_\ell(y)}\}$ is a basis in $L^2(X \times X)$. Therefore, we have an expansion

$$\mathcal{K}(x, y) = \sum_k \lambda_k e_k(x)\overline{e_k(y)}$$

(verify it). Letting $x = y$ and integrating, we get formally (4.35). Certainly, this is not a rigorous argument!

Now let us formulate the following

Proposition 4.27. *Let K be an integral operator in $L^2(X)$, where X is a domain in $\mathbb{R}^n$, and $\mathcal{K}$ its kernel function. Assume that $\mathcal{K}(x, y)$ is continuous and $K \geq 0$. Then K is nuclear if an only if the right-hand side of (4.35) is finite. Moreover,* $\operatorname{tr} K$ *is expressed by (4.35).*

Certainly, there are various situations in which (4.35) can be justified.

5 Perturbation of discrete spectrum

5.1 Introductory examples

Here we discuss formally how to find eigenvalues of perturbation of a given self-adjoint operator. We start with generic situation, the case of simple eigenvalues.

Example 5.1. Let A_0 and B be two self-adjoint operators in $\mathcal{H}$. For simplicity we assume A_0 and B to be bounded. One can even assume that the space $\mathcal{H}$ is finite dimensional. Consider a perturbed operator

$$A_\epsilon = A_0 + \epsilon B.$$

Let λ_0 be a simple eigenvalue of A_0, with corresponding eigenvector e_0, $\|e_0\| = 1$. We look for an eigenvalue λ_e of A_ϵ in a neighborhood of λ_0. It is natural to use power series expansions

$$\lambda_\epsilon = \lambda_0 + \epsilon\lambda_1 + \epsilon^2\lambda_2 + \dots, \tag{5.1}$$

$$e_\epsilon = e_{0_\epsilon} + e_1 + \epsilon^2 e_2 + \dots. \tag{5.2}$$

Substituting (5.1) and (5.2) into the eigenvalue equation

$$(A_0 + \epsilon B)e_\epsilon = \lambda_\epsilon e_\epsilon, \tag{5.3}$$

and comparing equal powers of ϵ, we obtain the following sequence of equations:

$$A_0 e_0 = \lambda_0 e_0, \tag{5.4}$$

$$A_0 e_1 - \lambda_0 e_1 = \lambda_1 e_0 - B e_0, \tag{5.5}$$

$$A_0 e_2 - \lambda_0 e_2 = \lambda_2 e_0 + \lambda_1 e_1 - B e_1, \tag{5.6}$$

etc. To determine an eigenvector uniquely we have to normalize it. The natural normalization is $(e_\epsilon, e_0) = 1$ which implies $(e_k, e_0) = 0$, $k > 1$. Equation (5.4) is trivially satisfied due to our choice of λ_0 and e_0.

Now let us recall that in our situation the image $\operatorname{im}(A_0 - \lambda_0 I)$ coincides with with the orthogonal complement of e_0. Therefore, for equation (5.5) to be solvable it is necessary and sufficient that

$$(\lambda_1 e_0 - B e_0, e_0) = 0.$$

Hence
$$\lambda_1 = (Be_0, e_0).$$
With this λ_1, equation (5.5) has one and only one solution $e_1 \perp e_0$. In the same way choosing
$$\lambda_2 = (Be_1, e_0)$$
one can find a unique solution $e_2 \perp e_0$ of (5.6), etc.

Exercise 5.2. Calculate eigenvalues and eigenvectors of
$$A_\epsilon = \begin{pmatrix} 1+\epsilon & \epsilon \\ \epsilon & 2 \end{pmatrix}$$
up to the second order of ϵ.

Now we consider a simplest example with degeneration.

Example 5.3. Let
$$A_\epsilon = a_0 + \epsilon B = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \epsilon \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}.$$
Here $\lambda_0 = 1$ is a multiple eigenvalue of A_0, with multiplicity 2, and all vectors are eigenvectors. However, B has two simple eigenvalues. Let μ be one such an eigenvalue, with the eigenvector e_0. Then e_0 is an eigenvector of A_ϵ, with corresponding eigenvalue $1 + \epsilon\mu$.

Exercise 5.4. Find eigenvalues and eigenvectors of
$$A_\epsilon = \begin{pmatrix} 1+\epsilon^2 & \epsilon \\ \epsilon & 1 \end{pmatrix}$$
up to second order of ϵ.

5.2 The Riesz projector

Let us introduce a powerful tool of operator theory, the so-called Riesz projector. Let A be a closed linear operator in $\mathcal{H}$ such that its spectrum $\sigma(A)$ is a union of two disjoint closed subsets σ_0 and σ_1 one of them, say σ_0, is compact. Then there exists an (counterclockwise) oriented piecewise smooth closed contour $\Gamma \subset \mathbb{C}$ such that $\sigma(A) \cap \Gamma = \emptyset$ and a part of $\sigma(A)$ inside Γ is just σ_0. (Such a contour may contain more than one component). The operator

$$P = \frac{1}{2\pi i} \int_\Gamma R_z dz, \qquad (5.7)$$

where $R_z = (A - zI)^{-1}$ is the resolvent of A, is called the Riesz projector associated with σ_0. Since R_z is an analytic function outside $\sigma(A)$, the operator P does not depend on choice of Γ. One can prove that P is indeed a projector. However, we do not discuss here the general situation. Instead, we consider the case of self-adjoint operators.

Proposition 5.5. *Let A be a self-adjoint operator, E_λ its decomposition of identity. Assume that $\sigma_0 = \sigma(A) \cap (a, b), a, b \notin \sigma(A)$. Then $P = E(a, b) = E_b - E_a$.*

Proof. There exist $\epsilon > 0$ such that $a - \epsilon$, $b + \epsilon \notin \sigma(A)$ and $\sigma_0 = \sigma(A) \cap (a - \epsilon, b + \epsilon)$. Choose Γ such that $\Gamma \cap \mathbb{R} = \{a - \epsilon, a + \epsilon\}$. Now

$$R_z = \int_{\mathbb{R}} \frac{dE_\lambda}{\lambda - z} = \int_{\sigma(A)} \frac{dE_\lambda}{(\lambda - z)}.$$

Hence

$$P = \frac{1}{2\pi i} \int_\Gamma \left[\int_{\mathbb{R}} \frac{dE_\lambda}{(\lambda - z)} \right] dz.$$

It is not difficult to verify that one can change the order of integrals here. Therefore,

$$P = \int_{\mathbb{R}} \left[\frac{1}{2\pi i} \int_\Gamma \frac{dz}{(\lambda - z)} \right] dE_\lambda.$$

Due to the Cauchy integral formula, the internal integral is equal to 1 if $\lambda \in (a - \epsilon, b + \epsilon)$, and 0 if $\lambda \notin [a - \epsilon, b + \epsilon]$. In other words, this integral is just $\chi_{(a-\epsilon,b+\epsilon)}(\lambda)$, the characteristic function of $(a - \epsilon, b + \epsilon)$. Hence,

$$P = \int_{\mathbb{R}} \chi_{(a-\epsilon,b+\epsilon)}(\lambda) dE_\lambda = E_{b+\epsilon} - E_{a-\epsilon}.$$

Since $\sigma(A) \cap (a - \epsilon, a) = \sigma(A) \cap (b, b + \epsilon) = \emptyset$, we see that $P = E_b - E_a$. $\square$

Corollary 5.6. *Let A be a self-adjoint operator and $\sigma_0 = \{\lambda_0\}$, where λ_0 is an isolated point of $\sigma(A)$. Then the Riesz projector P is an orthogonal projector onto the eigenspace corresponding to λ_0.*

5.3 The Kato lemma

Let A be a self-adjoint (in general, unbounded) operator in $\mathcal{H}$, $D(A)$ its domain and $R_z(A)$ its resolvent. We want to understand which operators may be considered as small perturbations of A. First we fix a point $z_0 \in \mathbb{C} \setminus \sigma(A)$.

Proposition 5.7. *(i) There exists $\epsilon > 0$ with the following property: If B is a symmetric operator such that the operator $R = BR_{z_0}(A) = B(A - z_0 I)^{-1}$ is everywhere defined, bounded and $\|R\| < \epsilon$, then the operator $A + B$, with $D(A + B) = D(A)$, is self-adjoint.*

(ii) Let K be a compact subset of $\mathbb{C}\backslash\sigma(A)$. If ϵ is small enough ($\epsilon < \epsilon_0(K)$), then $\sigma(A + B) \cap K = \emptyset$ and

$$\|R_z(A + B) - R_z(A)\| < \delta, z \in K,$$

where $\delta = \delta(\epsilon) \to 0$, as $\epsilon \to 0$.

Proof. Since $R = B(A - z_0 I)^{-1}$ is everywhere defined, and $\operatorname{im}(A - z_0 I)^{-1} = D(A)$, we see that $D(B) \supset D(A)$. On $D(A)$ we have $B = R(A - z_0 I)$. Therefore,

$$\begin{aligned} A + B - zI &= A + R(A - z_0 I) - zI \\ &= [I + R(A - z_0 I)(A - zI)^{-1}](A - zI) \\ &= [I + R((A - zI) + (z - z_0)I)(A - zI)^{-1}](A - zI) \\ &= [I + R + (z - z_0)R(A - zI)^{-1}](A - zI). \end{aligned} \tag{5.8}$$

Due to the spectral theorem,

$$\|(A - zI)^{-1}\| = [\operatorname{dist}(z, K)]^{-1} = [\inf_{z' \in \sigma(A)} |z - z'|]^{-1}$$

(prove it). Let K be a compactum such that $K \cap \sigma(A) = \emptyset$. Then there is $c > 0$ such that $\|(A - zI)^{-1}\| \le c$, $z \in K$. Now let

$$\epsilon < [\sup_{z \in K}(1 + |z - z_0| \, \|(a - zI)^{-1}\|)]^{-1}.$$

Then

$$\|R + (z - z_0)R \cdot (A - z)^{-1}\| < 1 \tag{5.9}$$

and, hence, the operator

$$I + R + (z - z_0)R \cdot (A - z_0 I)^{-1} I$$

has a bounded inverse operator. This implies that $\sigma(A + B) \cap K = \emptyset$. Moreover, the norm in (5.9) goes to 0, as $\epsilon \to 0$. Hence,

$$I + R + (z - z_0)R \cdot (A - z_0 I)^{-1} \to I$$

in $L(\mathcal{H})$ uniformly with respect to $z \in K$. This proves statement (ii).

Let us now prove (i). Due to (ii), $R_z(A+B)$ is defined for $z = \pm i$ provided ϵ is small enough. Since $A+B$ is obviously symmetric, this implies that $R_{-i}(A+B) = R_i(A+B)^*$ (verify it). Now we have

$$\begin{aligned}(A+B)^* - iI - (A+B-iI)^* &= [R_{-i}(A+B)^{-1}]^* \\ &= [R_{-i}(A+B)^*]^{-1} = [R_i(A+B)]^{-1} = A - B - iI,\end{aligned}$$

which implies $(A+B)^* = A+B$. $\square$

5.4 Perturbation of eigenvalues

Let us consider a family of (in general, unbounded) operators $A(\epsilon)$ parametrized by $\epsilon \in (-\epsilon_0, \epsilon_0)$. We assume that

$$A(\epsilon) = A_0 + G(\epsilon),$$

where A is a self-adjoint operator and $G(\epsilon)$ is a symmetric operator such that $G(0) = 0$, and for some $z_0 \notin \sigma(A_0)$ the operator $G(\epsilon)(A_0 - z_0 I)^{-1}$ is everywhere defined, bounded and depends analytically on $\epsilon \in (-\epsilon_0, \epsilon_0)$. The last means that

$$G(\epsilon)(A_0 - z_0 I)^{-1} = \sum_{k=0}^{\infty} \epsilon^k B_k,$$

where $B_k \in L(\mathcal{H})$ and the series converges in $L(\mathcal{H})$ for all $\epsilon \in (-\epsilon_0, \epsilon_0)$. Due to Proposition 5.7., $A(\epsilon)$ is a self-adjoint operator provided $|\epsilon|$ is small enough (say $|\epsilon| < \epsilon_1$).

Now assume that $\lambda_0 \in \mathbb{R}$ is an isolated eigenvalue of finite multiplicity for the operator A_0. This means that

$$\sigma(A_0) \cap (\lambda_0 - \delta, \lambda_0 + \delta) = \{\lambda_0\}$$

for some $\delta > 0$ and the eigenspace

$$\{\Psi \in D(A_0) : A_0 \Psi = \lambda_0 \Psi\}$$

is finite dimensional.

Theorem 5.8. *There exist analytic vector functions $\Psi_j(\epsilon), j = 1, 2, \ldots, m$, and scalar analytic functions $\lambda_j(\epsilon), j = 1, 2, \ldots, m$, defined in a neighborhood of $0 \in \mathbb{R}$, such that*

$$A(\epsilon)\Psi_j(\epsilon) = \lambda_j(\epsilon)\Psi_j(\epsilon) \tag{5.10}$$

and $\{\Psi_j(\epsilon)\}$ is an orthonormal basis in the space $E^{(\epsilon)}(\lambda_0 - \delta, \lambda_0 + \delta)$, where $E^{(\epsilon)}_\lambda$ is the decomposition of identity for $A(\epsilon)$.

Proof.

1) Let $\Gamma \subset \mathbb{C}$ be a contour around λ_0 such that there are no points of $\sigma(A_0)$ inside Γ, and

$$P(\epsilon) = \frac{1}{2\pi i} \int_\Gamma R_z(A(\epsilon))dz$$

the Riesz projector. Proposition 5.7 (ii) implies that $\Gamma \cap k\sigma(A(\epsilon)) = \emptyset$ provided $|\epsilon|$ is small enough. Now we apply (5.8) with $A = A_0, B = G(\epsilon)$ and

$$R = R(\epsilon) = G(\epsilon)(A_0 - z_0 I)^{-1}.$$

We obtain

$$R_z(A(\epsilon)) = R_z(A_0)[I + R(\epsilon) + (z - z_0)R(\epsilon)R_z(A_0)]^{-1},$$

which implies that $R_z(A(\epsilon))$ is analytic in ϵ uniformly with respect to $z \in \Gamma$. Hence, $P(\epsilon)$ depends analytically on ϵ, provided ϵ is close to 0. $P(\epsilon)$ is an orthogonal projector, since it coincides with the spectral projector $E^{(\epsilon)}(\lambda_0 - \delta, \lambda_0 + \delta)$ of $A(\epsilon), \delta > 0$ small enough.

Consider a subspace $L_\epsilon = P(\epsilon)\mathcal{H}$, the image of $P(\epsilon)$. We want to prove that $\dim L_\epsilon$ does not depend on ϵ. Let $Q(\epsilon) = I - P(\epsilon)$,

$$C(\epsilon) = Q(\epsilon)Q(0) + P(\epsilon)P(0),$$
$$C_1(\epsilon) = Q(0)Q(\epsilon) + P(0)P(\epsilon).$$

All these operators depend analytically on ϵ and, clearly, $C(0) = C_1(0) = I$. Hence, $C(\epsilon)$ and $C_1(\epsilon)$ are invertible operators for all ϵ close to 0. However, $C(\epsilon)$ maps L_0 into L_ϵ, while $C_1(\epsilon)$ maps L_ϵ into L_0. Since $C(\epsilon)$ and $C_1(\epsilon)$ are invertible, this implies that $\dim L_\epsilon = \dim L_0 = m$.

Moreover, if $\{\Psi_1, \dots, \Psi_m\}$ is an orthonormal basis in L_0, then $\{C(\epsilon)\Psi_1, \dots, C(\epsilon)\Psi_m\}$ is a basis in L_ϵ which depends analytically on ϵ. Applying the orthogonalization procedure, we obtain an orthonormal basis $\{\varphi_1, (\epsilon), \dots, \varphi_m(\epsilon)\}$ in L_ϵ such that $\varphi_j(\epsilon) = \Psi_j$ and all $\Psi_j(\epsilon)$ depend analytically on ϵ. The space L_ϵ is invariant under action of $A(\epsilon)$. Hence, the restriction of $A(\epsilon)$ to L_ϵ is represented in this basis by an Hermitian matrix $(a_{jk}(\epsilon))$ depending analytically on ϵ. Moreover, $a_{jk}(0) = \lambda_0\delta_{jk}$, where δ_{jk} is the Kronecker symbol. Thus, we have reduced the problem to the case of Hermitian $(m \times m)$-matrix $D(\epsilon)$ which is analytic in ϵ and $D(0) = \lambda_0 I$.

2) Now we consider the reduced problem about the matrix $D(\epsilon)$. The case $m = 1$ is clear. Suppose we have proved the assertion for all such matrices of size $< m$, and consider the case of $(m \times m)$-matrix $D(\epsilon)$. We can write

$$D(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k D_k,$$

where all D_k are Hermitian matrices, $D_0 = D(0) = \lambda_0 I$.

If all D_k are scalar multiples of the identity matrix, $D_k = \lambda^{(k)} I$, then $D(\epsilon) = \lambda(\epsilon) I$, where

$$\lambda(\epsilon) = \sum_{k=0}^{\infty} \lambda^{(k)} \epsilon^k$$

is an analytic function. We can choose an arbitrary basis $\{\Psi_1, \dots, \Psi_m\}$ (not depending on ϵ) and the required assertion is evident.

Assume now that not all D_k are scalar matrices, and D_s is the first one which is not a scalar matrix, i. e. $D_k = \lambda^{(k)}$ for $k < s$ and $D_s \notin \{\lambda I\}_{\lambda \in \mathbb{C}}$. Let

$$C(\epsilon) = D_s + \epsilon D_{s+1} + \epsilon^2 D_{s+2} + \dots$$

Then

$$D(\epsilon) = \sum_{k=o}^{s-1} \lambda^{(k)} \epsilon^k I + \epsilon^s C(\epsilon).$$

Therefore, if $\Psi(\epsilon)$ is an eigenvector of $C(\epsilon)$ with the eigenvalue $\mu(\epsilon)$, i. e. $C(\epsilon)\Psi(\epsilon) = \mu(\epsilon)\Psi(\epsilon)$, then the same $\Psi(\epsilon)$ is an eigenvector of $D(\epsilon)$ with the eigenvalue

$$\lambda(\epsilon) = \sum_{k=0}^{s-1} \lambda^{(k)} \epsilon^k + \epsilon^s \mu(s).$$

Thus suffices to prove the assertion for the matrix $C(\epsilon)$.

Now remark, that not all eigenvalues of $D_s = C(0)$ coincide. Hence, as on step 1), we can use the Riesz projector and reduce the problem to the case of a matrix of the size $< m$.

$\square$

Proposition 5.9. *Let $\Psi_j(\epsilon)$ be a normalized analytic vector function satisfying (5.10). Then $\lambda_j'(\epsilon) = d\lambda_j(\epsilon)/d\epsilon$ satisfies the following relation*

$$\lambda_j'(\epsilon) = (A'(\epsilon)\Psi_j(\epsilon), \Psi_j(\epsilon)), \tag{5.11}$$

where $A'(\epsilon)$ is understood as

$$A'(\epsilon) = \left\{ \frac{d}{d\epsilon}[G(\epsilon)(A_0 - z_0 I)^{-1}] \right\} (A_0 - z_0 I).$$

We present here only formal calculations which lead to (5.11), not a rigorous proof. Differentiation of (5.10) gives

$$A'(\epsilon)\Psi_j(\epsilon) + A(\epsilon)\Psi_j(\epsilon) = \lambda_j'(\epsilon)\Psi_j(\epsilon) + \lambda_j(\epsilon)\Psi_j'(\epsilon). \tag{5.12}$$

On the other hand,

$$(A(\epsilon)\Psi_j'(\epsilon), \Psi_j(\epsilon)) = (\Psi_j'(\epsilon), A(\epsilon)\Psi_j(\epsilon)) = \lambda_j(\epsilon)(\Psi_j'(\epsilon), \Psi_j(\epsilon)).$$

Multiplying (5.12) by $\varphi_j(\epsilon)$, we get

$$(A'(\epsilon)\Psi_j(\epsilon), \Psi_j(\epsilon)) = \lambda_j'(\epsilon)(\Psi_j(\epsilon), \Psi_j(\epsilon) = \lambda_j'(\epsilon)$$

which is required.

6 Variational principles

6.1 The Glazman lemma

In many cases so-called variational principles are useful to study perturbation of eigenvalues, as well as for numerical calculation of them. Glazman's lemma is one of such principles.

Let A be a self-adjoint operator in a Hilbert space $\mathcal{H}$, E_λ its decomposition of identity. Recall that $E_{\lambda+0} = E_\lambda$ in the sense of strong operator topology. Set $E_{\lambda-0} = \lim_{\mu\to\lambda-0} E_\mu$ in the strong operator topology. We introduce the so-called distribution function $N(\lambda)$ of the spectrum of A by the formula

$$N(\lambda) = \dim(E_\lambda \mathcal{H});$$

this value may be equal to $+\infty$. Letting

$$N(\lambda - 0) = \lim_{\mu\to\lambda-0} N(k\mu),$$

we see that

$$N(\lambda - 0) = \dim(E_{\lambda-0}\mathcal{H}).$$

In general, $N(\lambda + 0) = \lim_{\mu\to\lambda+0} N(\mu)$ may be not equal to $N(\lambda)$.

Example 6.1. Let A be the operator of multiplication by the independent variable x in $L^2(0,1)$. Then $N(+0) = +\infty$, while $N(0) = 0$.

However, let us point out that $N(\lambda+0) = N(\lambda)$ provided $N(\lambda+0) < +\infty$.

Now we are able to state the Glazman lemma.

Proposition 6.2. *Let $D \subset D(A)$ be a linear subspace (not closed) such that A is essentially self-adjoint on D. Then for every $\lambda \in \mathbb{R}$ we have*

$$N(\lambda - 0) = \sup\{\dim L : L \subset D, (Au, u) < \lambda(u, u) \quad \forall u \in L \setminus \{0\}\} \tag{6.1}$$

Proof.

1) Suppose that $L \subset D$ and

$$(Au, u) < \lambda(u, u) \quad \forall u \in L \setminus \{0\} \tag{6.2}$$

Then $\dim L \le N(\lambda - 0)$. Assume not, i.e.

$$\dim L > N(\lambda - 0).$$

Then

$$L \cap (E_{\lambda-0}\mathcal{H})^\perp \ne \{0\}.$$

(Indeed, if $L \cap (E_{\lambda-0}\mathcal{H})^{\perp} = \{0\}$, then the projector $E_{\lambda-0}$ maps L into $E_{\lambda-0}\mathcal{H}$ injectively, which implies that

$$\dim L \leq \dim(E_{\lambda-0}\mathcal{H}) = N(\lambda - 0)).$$

Now let $0 \neq u \in (E_{\lambda-0}\mathcal{H})^{\perp} \cap L$. Then, clearly,

$$(Au, u) \geq \lambda(u, u),$$

which contradicts our assumption (6.2). Thus,

$$\dim L \leq N(\lambda - 0)$$

and we see that the right-hand side of (6.1), g_λ, is not greater then the left-hand side.

2) Let us prove that the left-hand side of inequality (6.1) is not greater then g_λ. First, remark that $E_{\lambda-0} = \lim_{N\to-\infty} E(N,\lambda)$ in the strong operator topology, where $E(N,\lambda) = E_{\lambda-0} - E_N$. Hence,

$$N(\lambda - 0) = \lim_{N\to-\infty} \dim[E(N,\lambda)\mathcal{H}].$$

Therefore, it suffices to prove that

$$\dim E(N,\lambda)\mathcal{H} \leq g_\lambda \quad \forall N < \lambda.$$

With this aim, choose in $E(N,\lambda)\mathcal{H}$ an arbitrary orthonormal basis (finite or infinite), and let $\{e_1,\dots,e_p\}$ be a finite number of its elements. We prove now that $p \leq g_\lambda$, which implies the required.

Since $E(N,\lambda) \subset D(A)$, then $e_j \in D(A), j = 1,\dots,p$. Hence, for every $\epsilon > 0$, there exists $\overline{e}_1,\dots,\overline{e_p} \in D$ such that

$$\|e_j - \overline{e_j}\| < \epsilon, \|Ae_j - A\overline{e_j}\| < \epsilon, j = 1\dots,p\_$$

(essential self-adjointness of A implies that D is dense in $D(A)$ with respect to the graph norm).

Let L be a linear hull of $\{\overline{e_1},\dots,\overline{e_p}\}$. Then $\dim L = p$, provided $\epsilon > 0$ is small enough (prove this statement!). Moreover, if $\epsilon > 0$ is small enough, then L satisfies condition (6.2). Hence, $p \leq g_\lambda$ and we conclude.

$\square$

Remark 6.3. In the proof above, we introduced $E(N, \lambda)$, since, in general, $E_{\lambda-0}\mathcal{H}$ may not lie in $D(A)$.

In the case of positive self-adjoint operator A, it is sometimes useful to associate with A a quadratic form. Assume first that $A \geq I$, i. e.

$$(Au, u) \geq (u, u) \quad u \in D(A).$$

Let us introduce a semi-linear form

$$A(u, v) = (Au, v), u, v \in D(A).$$

The form $A(\cdot, \cdot)$ is an inner product and, hence, generates a new norm

$$\|u\|_A = A(u, u)^{1/2}, \quad u \in D(A),$$

on $D(A)$. Obviously, $\|u\|_A \geq \|u\|$. Denote by $\mathcal{H}_A$ the completion of $D(A)$ with respect to the norm $\|\cdot\|_A$. Our claim is that there is a natural continuous embedding $\mathcal{H}_A \subset \mathcal{H}$. Indeed, if $\{x_n\} \subset D(A)$ is a Cauchy sequence in the norm $\|\cdot\|_A$, then it is also a Cauchy sequence in $\mathcal{H}$, and, hence, has a limit in $\mathcal{H}$. This limit is a member of $\mathcal{H}_A$. Moreover, $\|\cdot\|_A$ is equivalent to the norm

$$\|u\|'_A = (\|u\|^2 + \|A^{1/2}u\|^2)^{1/2},$$

since $(Au, u) = (A^{1/2}u, A^{1/2}u)$. The operator $A^{1/2}$ is closed and the last norm $\|\cdot\|'_A$ is just the graph norm on $D(A^{1/2})$. Moreover, $D(A)$ is dense in $D(A^{1/2})$ with respect to $\|\cdot\|'_A$ (prove this!). Therefore, up to norm equivalence, $\mathcal{H}_A$ coincides with $D(A^{1/2})$. By continuity, $A(u, v)$ is well defined on $\mathcal{H}_A$ and defines there an inner product

$$A(u, v) = (A^{1/2}u, A^{1/2}v).$$

This construction may be extended to the case of general self-adjoint operator A which is semi-bounded from below, i. e. $A \geq -\alpha I, \alpha \in \mathbb{R}$, or

$$(Au, u) \geq -\alpha(u, u), \quad u \in D(A).$$

Set $\hat{A} = A + (\alpha + 1)I$. Then $\hat{A} \geq I$ and the previous construction works. We get a new Hilbert space $\mathcal{H}_{\hat{A}}$ and a new form (inner product) $\hat{A}(\cdot, \cdot)$ on $\mathcal{H}_{\hat{A}}$. Now we set

$$A(u, v) = \hat{A}(u, v) - (\alpha + 1)(u, v).$$

on $\mathcal{H}_{\hat{A}}$. In fact, $A(u, v)$ is an extension of (Au, v) from $D(A)$ to $\mathcal{H}_{\hat{A}}$ by continuity.

Now we have the following version of Glazman's lemma.

Proposition 6.4. *Let A be a semi-bounded from below self-adjoint operator, D a dense linear subspace of $\mathcal{H}_A$. Then for every $\lambda \in \mathbb{R}$*

$$N(\lambda - 0) = \sup\{\dim L : L \subset D,\ A(u,u) < \lambda(u,u)\ \forall u \in L \setminus \{0\}\}. \tag{6.3}$$

The proof is similar to that of Proposition 6.2. The only difference is that now one does not need to approximate e_j by $\overline{e_j} \in D$. (Complete the details!)

Another (simplified) version of Glazman's lemma is also useful.

Proposition 6.5. *For every self-adjoint A and $\lambda \in \mathbb{R}$ we have*

$$N(\lambda) = \sup\{\dim L : L \subset D(A),\ (Au,u) \le \lambda(u,u)\ \forall u \in L\}. \tag{6.4}$$

Exercise 6.6. Prove the last statement.

Now we give some applications of previous results.

Proposition 6.7. *Let A_1 and A_2 be self-adjoint operators. Assume that there is a dense linear subspace D of $\mathcal{H}$ such that A_1 and A_2 are essentially self-adjoint on D and*

$$(A_1u,u) \le (A_2u,u), \quad u \in D.$$

Then

$$N_1(\lambda + 0) \ge N_2(\lambda + 0), \quad \lambda \in \mathbb{R}, \tag{6.5}$$

$$N_1(\lambda - 0) \ge N_2(\lambda - 0), \quad \lambda \in \mathbb{R}, \tag{6.6}$$

where N_1 and N_2 are the distribution functions of spectra for A_1 and A_2. If, in addition, $D(A_1) = D(A_2)$, then

$$N_1(\lambda) \ge N_2(\lambda), \quad \lambda \in \mathbb{R}. \tag{6.7}$$

Proof. Inequality (6.6) follows immediately from Proposition 6.2. Since the set of jumps of each monotone function is at most countable, (6.6) implies (6.5). To prove the last statement, we remark that, by continuity, the inequality

$$(A_1u,u) \le (A_2u,u)$$

holds true for $u \in D(A_1) = D(A_2)$. Then, Proposition 6.5. works. $\square$

Exercise 6.8. Complete the details in the last proof and show that $N(\lambda)$ is non-decreasing.

Corollary 6.9. *Let A_1, A_2 be as in Proposition 6.7. Assume that A_1 is semi-bounded from below and, for some $\lambda \in \mathbb{R}$, $\sigma(A_1) \cap (-\infty, \lambda)$ is discrete, i. e. consists of isolated eigenvalues of finite multiplicity. Then so is for A_2. Moreover,*

$$N_1(\lambda - 0) \geq N_2(\lambda - 0).$$

Remark 6.10. In fact, $N_1(\lambda-0)$ and $N_2(\lambda-0)$ are just sums of multiplicities of eigenvalues in $(-\infty, \lambda)$ for A_1 and A_2, respectively.

Proof. If $A_1 \geq CI$, then $A_2 \geq CI$ and $\sigma(A_1), \sigma(A_2) \subset [C, +\infty)$. Therefore, for each $\lambda' \subset \lambda$ the set $\sigma(A_1) \cap (-\infty, \lambda') = \sigma(A_1) \cap [C, \lambda')$ consists of eigenvalues of finite multiplicity or, equivalently, $N_1(\lambda' - 0) < +\infty$. By Proposition 6.7, so is for A_2, and we conclude, since $\lambda' < \lambda$ is arbitrarily chosen. □

Corollary 6.11. *Let A_1 and A_2 be as in Corollary 6.9. Denote by $\lambda'_1 \leq \lambda'_2 \leq \ldots$ and $\lambda''_1 \leq \lambda''_2 \leq \ldots$ their eigenvalues in $(-\infty, \lambda)$, counting multiplicity (any such a sequence, or both of them, may be finite). If λ''_k is well-defined for some k, then so is for λ'_k and $\lambda'_k \leq \lambda''_k$.*

Proof. If λ''_k is defined, then $\lambda''_k < \lambda$ and, hence, $N_2(\lambda_k) \geq k$. By (6.5), $N_1(\lambda''_k) \geq k$, which implies that $\lambda'_k \leq \lambda''_k$. □

Corollary 6.12. *Let A be a semi-bounded from below self-adjoint operator and B a bounded self-adjoint operator. Assume that $\sigma(A) \cap (-\infty, \lambda)$ is discrete. Then, for $\lambda' < \lambda$, $\sigma(A + \epsilon B) \cap (-\infty, \lambda')$ is discrete, provided $|\epsilon|$ is small enough. Moreover, the eigenvalues $\lambda_n(\epsilon) \in (-\infty, \lambda')$ of $A + \epsilon B$, labeled in the increasing order, are continuous functions of ϵ.*

Proof. Let $M = \|B\|$. Then, obviously,

$$A - \epsilon MI \leq A + \epsilon B \leq A + \epsilon MI.$$

If $\lambda_n \in (-\infty, \lambda')$ are eigenvalues of A, then the eigenvalues of $A \pm \epsilon MI$ are $\lambda_n \pm \epsilon M$. By Corollary 6.11.,

$$\lambda_n - \epsilon M \leq \lambda_n(\epsilon) \leq \lambda_n + \epsilon M.$$

This implies continuity of $\lambda_n(\epsilon)$ at $\epsilon = 0$. Replacing A by $A + \epsilon_0 B$, we obtain continuity of $\lambda_n(\epsilon)$ at the point ϵ_0. □

6.2 The minimax principle

First we introduce more general "eigenvalues" λ_n for a semi-bounded from below self-adjoint operator A. If $\sigma(A) \cap (-\infty, \lambda)$ is discrete, then $\lambda_1 \leq \lambda_2 \leq \ldots$ are corresponding eigenvalues (counting multiplicity). If for some $\lambda \leq +\infty$ we have infinitely many such eigenvalues, then λ_n is well-defined for all natural n. In general, we set

$$\lambda_n = \sup\{\lambda : N(\lambda) < n\}.$$

This, in fact, generalizes the previous definition. If, for example, the bottom μ_0 of $\sigma(A)$ is not an eigenvalue, then, clearly, $\lambda_n = \mu_0$ for all n. More generally, if $\sigma(A)$ consists of $[\alpha, +\infty)$ and of a finite number of eigenvalues below α, then $\lambda_n = \alpha$ for $n \geq n_0$.

Now we can state the following minimax principle of Courant.

Theorem 6.13. *Let A be a self-adjoint semi-bounded from below operator , $D \subset \mathcal{H}$ a dense linear subspace on which A is essentially self-adjoint. Then*

$$\lambda_1 = \inf_{f \in D \setminus \{0\}} \frac{(Af, f)}{(f, f)}, \tag{6.8}$$

$$\lambda_{n+1} = \sup_{\substack{L \subset D \\ \dim L = n}} \inf_{\substack{f \in D \cap L^\perp \\ f \neq 0}} \frac{(Af, f)}{(f, f)}. \tag{6.9}$$

Proof. Clearly, (6.8) is a particular case of (6.9). First, we prove that the right-hand side of (6.9) does not depend on D and, therefore, we can assume that $D = D(A)$. For each $L \subset D$, we have $D = L \oplus (D \cap L^\perp)$ and $D(A) = L \oplus (D(A) \cap L^\perp)$. This implies that $A|_{D(A) \cap L^\perp}$ is the closure of $A|_{D \cap L^\perp}$. Hence,

$$\inf_{\substack{f \in D \cap L^\perp \\ f \neq 0}} \frac{(Af, f)}{(f, f)} = \inf_{\substack{f \in D(A) \cap L^\perp \\ f \neq 0}} \frac{(Af, f)}{(f, f)}. \tag{6.10}$$

Recall that D is dense in $D(A)$ with respect to the graph norm

$$\|f\|_A^2 = \|f\|^2 + \|Af\|^2.$$

Let $L \subset D(A)$ and $\dim L = n$. Choose an orthonormal basis $\{e_1, \ldots, e_n\} \subset L$. Approximate each e_j by a vector form D and then orthogonalize approximating vectors. As a result, we get an orthonormal system $\{\overline{e}_1, \ldots, \overline{e}_n\} \subset D$ such that

$$\|e_j - \overline{e}_j\| < \delta,$$

δ is small. Let $\overline{L} = \text{span}\{\overline{e}_1, \dots \overline{e}_n\} \subset D$. Consider orthogonal projectors P_L and $P_{\overline{L}}$ onto L and $\overline{L}$, respectively. They are defined by

$$P_L f = \sum_{j=1}^{n} (f, e_j) e_j,$$
$$P_{\overline{L}} f = \sum_{j=1}^{n} (f, \overline{e}_j) \overline{e}_j.$$

These formulas imply that

$$\|P_L f - P_{\overline{L}} f\|_A < \epsilon \|f\|_A,$$

where $\epsilon = \epsilon(\delta) \to 0$ as $\delta \to 0$. From the last inequality it follows that

$$\|P_{L^\perp} f - P_{\overline{L}^\perp} f\|_A < \epsilon \|f\|_A,$$

where $P_{L^\perp} = I - P_L$ and $P_{\overline{L}^\perp} = I - P_{\overline{L}}$ are orthogonal projectors onto $L^\perp$ and $\overline{L}^\perp$, respectively. Hence, given $f \in D(A) \cap L^\perp$, letting $\overline{f} = P_{\overline{L}^\perp} f$ we get $\overline{f} \in D(A) \cap \overline{L}^\perp$ and $\|\overline{f} - f\|_A < \epsilon$. Therefore, replacing L by $\overline{L}$ in the right-hand part of (6.9), we change it by a value which tends to 0, as $\delta \to 0$.

Thus, we can assume that $D = D(A)$. By definition of λ_n, we have

$$m = \dim(E_{\lambda_n} \mathcal{H}) = N(\lambda_n) = N(\lambda_n + 0) \geq n$$

and

$$\dim(E_{\lambda_n - 0} \mathcal{H}) = N(\lambda_n - 0) < n.$$

(m may be finite or infinite). Hence, there exists a subspace $L \subset E_{\lambda_n} \mathcal{H}$ such that $\dim L = n$ and $L \supset E_{\lambda_n - 0} \mathcal{H}$.

First, consider the case $m > n$. Then it is not difficult to verify that $\lambda_{n+1} = \lambda_n$. Now we have

$$L^\perp \subset (E_{\lambda_n - 0} \mathcal{H})^\perp = (I - E_{\lambda_n - 0}) \mathcal{H} = H$$

Obviously, $\sigma(A|_M) \subset [\lambda_n, +\infty)$. Hence

$$(Af, f) \geq \lambda_n (f, f) = \lambda_{n+1} (f, f), \quad f \in L^\perp.$$

Assume, that $m = n$. In this case $L = E_{\lambda_n} \mathcal{H}$. If $\lambda_{n+1} > \lambda_n$, then $L = E_{\lambda_{n+1} - 0} \mathcal{H}$, and, therefore,

$$(Af, f) \geq \lambda_{n+1} (f, f), \quad f \in L^\perp. \tag{6.11}$$

The case $\lambda_{n+1} = \lambda_n$ is already considered. This implies that the right-hand part of (6.9) is not less then λ_{n+1}.

Now let us prove the opposite inequality. In fact, for every $L \subset D(A)$, $\dim L = m$, we have to prove the existence of a nonzero vector $f \in D(A) \cap L^\perp$ such that

$$(Af, f) \le \lambda_{n+1}(f, f).$$

However, one can take as such an f any nonzero vector in $E_{\lambda_{n+1}}\mathcal{H} \cap L^\perp$. The last intersection is nontrivial, since

$$\dim(E_{\lambda_{n+1}}\mathcal{H}) = N(\lambda_{n+1}) \ge n + 1.$$

$\square$

7 One-dimensional Schrödinger operator

7.1 Self-adjointness

Consider an operator H_0 defined on $D(H_0) = C_0^\infty(\mathbb{R})$ by the formula

$$H_0 u = -u'' + V(x)u, \tag{7.1}$$

where $V(x) \in L^\infty_{\text{loc}}(\mathbb{R})$ is a real valued function. Clearly, H_0 is a symmetric operator in $L^2(\mathbb{R})$. Recall that H_0 is said to be essentially self-adjoint if its closure H_0^{**} is a self-adjoint operator. In this case H_0 has one and only one self-adjoint extension.

Theorem 7.1. *Assume that*

$$V(x) \geq -Q(x), \tag{7.2}$$

where $Q(x)$ is a nonnegative continuous even function which is nondecreasing for $x \geq 0$ and satisfies

$$\int_{-\infty}^{\infty} \frac{dx}{\sqrt{Q(2x)}} = \infty. \tag{7.3}$$

Then H_0 is essentially self-adjoint.

Proof. As we have already seen in previous lectures, to prove self-adjointness of H_0^{**} it is enough to show that H_0^* is a symmetric operator. Hence, first we have to study the domain $D(H_0^*)$.

(i) *If $f \in D(H_0^*)$, then $f'(x)$ is absolutely continuous and $f'' \in L^2_{\text{loc}}(\mathbb{R})$.*

Indeed, let $g = H_0^* f$. For every $\varphi \in C_0^\infty(\mathbb{R})$ we have

$$\int_{-\infty}^{\infty} \overline{f(x)}\varphi''(x) = \int_{-\infty}^{\infty} (V(x)\overline{f(x)} - \overline{g(x)})\varphi(x)dx.$$

Denote by $F(x)$ the second primitive function of $V(x) \cdot f(x) - g(x)$. Then the previous identity and integration by parts imply

$$\int_{-\infty}^{\infty} \overline{f} \cdot \varphi'' dx = \int_{-\infty}^{\infty} \overline{F} \cdot \varphi'' dx.$$

Hence, $(F - f)'' = 0$ in the sense of distributions, i. e. $F - f$ is a linear function of x. This implies immediately the required claim.

Now we have to examine the behavior of $f \in D(H_0^*)$ as $x \to \infty$.

(ii) *If $f \in D(H_0^*)$, then*

$$\int_{-\infty}^{\infty} \frac{|f'(x)|^2}{Q(2x)} dx < \infty. \tag{7.4}$$

To prove the last claim, consider the integral

$$\begin{aligned} J &= \int_{-w}^{w} (1 - \frac{|x|}{w})(f''(x)\overline{f(x)} + f(x)\overline{f''(x)}) \\ &= \int_{-w}^{w} (1 - \frac{|x|}{w})(f' \cdot \overline{f} + f \cdot \overline{f'})' dx - 2\int_{-w}^{w} (1 - \frac{|x|}{w})|f'|^2 dx. \end{aligned}$$

Integrating by parts, we obtain

$$\begin{aligned} J &= (f' \cdot \overline{f} + f \cdot \overline{f'})(1 - \frac{|x|}{w})\Big|_{x=-w}^{w} - 2\int_{-w}^{w} (1 - \frac{|x|}{w})|f'|^2 dx \\ &\qquad + \frac{1}{w}\int_{-w}^{w} (f' \cdot \overline{f} + f \cdot \overline{f'}) \operatorname{sgn} x dx \\ &= \frac{1}{w}\int_{-w}^{w} (f' \cdot \overline{f} + f \cdot \overline{f'}) \operatorname{sgn} x dx - 2\int_{-w}^{w} (1 - \frac{|x|}{w})|f'|^2 dx \\ &= \frac{1}{w}\int_{-w}^{w} (|f|^2)' \operatorname{sgn} x dx - 2\int_{-w}^{w} (1 - \frac{|x|}{w})|f'|^2 dx \\ &= \frac{1}{w}[|f(w)|^2 + |f(-w)|^2 - 2|f(0)|^2] - 2\int_{-w}^{w} (1 - \frac{|x|}{w})|f'|^2 dx. \end{aligned}$$

Thus, we get the following identity

$$\begin{aligned} \int_{-w}^{w} (1 - \frac{|x|}{x})|f'(x)|^2 dx &= -\frac{1}{2}\int_{-w}^{w} (f'' \cdot \overline{f} + f \cdot \overline{f}'') \cdot (1 - \frac{|x|}{w}) dx \\ &\qquad + \frac{1}{2w}[|f(w)|^2 + |f(-w)|^2 - 2|f(0)|]. \end{aligned}$$

Multiplying the last identity by w, integrating over $w \in [0, t]$, and taking into account the identity

$$\int_0^T (\int_{-w}^{w} (w - |x|)h(x)dx)dw = \frac{1}{2}\int_{-T}^{T} (T - |x|)^2 h(x)dx$$

(prove it!), we get

$$\begin{aligned} \int_{-T}^{T} (T - |x|)^2 |f'|^2 dx &= -\frac{1}{2}\int_{-T}^{T} (T - |x|)^2 (f'' \cdot \overline{f} + f \cdot \overline{f}'') dx \\ &\qquad + \int_0^T (|f(w)|^2 + |f(-w)|^2) dw - 2|f(0)|^2 T, \end{aligned}$$

or, dividing by T^2,

$$\int_{-T}^{T}(1-\frac{|x|}{T})^2|f'|^2dx = -\frac{1}{2}\int_{-T}^{T}(1-\frac{|x|}{T})^2(f''\cdot\overline{f}+f\cdot\overline{f}'')dx$$
$$+\frac{1}{T^2}(\int_{-T}^{T}|f(x)|^2dx-2|f(0)|^2\cdot T).$$

Letting $g=-f''+V(x)f$, we obtain

$$\begin{aligned}&\int_{-T}^{T}(1-\frac{|x|}{T})^2|f'|^2dx\\ &=\frac{1}{2}\int_{-T}^{T}(1-\frac{|x|}{T})^2(g\cdot\overline{f}+\overline{g}\cdot f)dx-\int_{-T}^{T}(1-\frac{|x|}{T})^2V(x)|f(x)|^2dx\\ &\qquad+\frac{1}{T^2}(\int_{-T}^{T}|f(x)|^2dx-2|f(0)|^2T)\end{aligned}$$

Now remark that $f,g\in L^2(\mathbb{R})$ and $0\le 1-|x|/T\le 1$ for $x\in(T,-T)$. Hence, estimating $-V(x)$ by $Q(x)$, we get

$$\int_{-T}^{T}(1-\frac{|x|}{T})^2|f'|^2dx\le\int_{-T}^{T}(1-\frac{|x|}{T})^2Q(x)|f|^2dx+c,$$

where c is independent of T. The last inequality implies clearly

$$\frac{1}{4}\int_{-T/2}^{T/2}|f'(x)|^2dx\le\int_{-T}^{T}Q(x)|f|^2dx+c \tag{7.5}$$

Let

$$\omega(T)=\frac{1}{4}\int_{-T/2}^{T/2}|f'|^2dx,$$
$$\chi(T)=\int_{-T}^{T}Q(x)|f|^2dx+c$$

Consider the integral

$$\int_0^T\frac{\omega'(x)-\chi'(x)}{Q(x)}dx$$

and apply the following theorem on mean value: *if $f(x)$ is a continuous function and $K(x)\ge 0$ is a nondecreasing continuous function, then there exists $\xi\in[a,b]$ such that*

$$\int_a^b f(x)K(x)dx=K(a)\int_a^\xi f(x)dx.$$

Then, due to (7.5) we obtain

$$\begin{aligned}\int_0^T \frac{\omega'\chi'}{Q}dx &= \frac{1}{Q(0)}\int_0^\xi (\omega' - \chi')dx \\ &= \frac{1}{Q(0)}[\omega(\xi) - \chi(\xi) - \omega(0) + \chi(0)] \\ &\le \frac{1}{Q(0)}[\chi(0) - \omega(0)] = C.\end{aligned}$$

Since

$$\begin{aligned}\omega'(x) &= \frac{1}{2}[|f'(\frac{x}{2})|^2 + |f'(-\frac{x}{2})|^2], \\ \chi'(x) &= Q(x)[|f(x)|^2 + |f(-x)|^2],\end{aligned}$$

we get immediately

$$\begin{aligned}\frac{1}{8}\int_0^T & \frac{|f'(x/2)|^2 + |f'(-x/2)|^2}{Q(x)}dx \\ &\le \int_0^T (|f(x)|^2 + |f(-x)|^2)dx + C.\end{aligned}$$

Since $f \in L^2(\mathbb{R})$, the last inequality implies the required claim.

End of proof of Theorem 7.1. Let $f_1, f_2 \in D(H_0^*)$ and

$$g_i = -f_i'' + V(x)f_i, \;\; i = 1, 2.$$

We have to show that

$$\int_{-\infty}^{\infty} f_1\overline{g}_2 dx = \int_{-\infty}^{\infty} g_1\overline{f}_2 dx.$$

First we observe that

$$\begin{aligned}\int_{-t}^{t} (f_1\overline{g}_2 - g_1\overline{f}_2)dx &= \int_{-t}^{t} (f_1\overline{f}_2'' - f_1''\overline{f}_2)dx \\ &= \int_{-t}^{t} \frac{d}{dx}(f_1\overline{f_2'} - f_1'\overline{f_2})dx \qquad (7.6)\\ &= [f_1\overline{f_2}' - f_1'\overline{f_2}]|_{-t}^{t}.\end{aligned}$$

Let

$$\rho(t) = \frac{1}{\sqrt{Q(2t)}}, \quad P(x) = \int_0^x \rho(t)dt.$$

Multiplying (7.6) by $\rho(t)$ and integrating over $[0,T]$, we obtain

$$\int_0^T \rho(t)[\int_{-t}^{t}(f_1\overline{g}_2 - g_1\overline{f}_2)dx]dt = \int_0^T \rho(t)[f_1 - \overline{f}_2' - f_1'\overline{f}_2]|_{-t}^{t}dt. \tag{7.7}$$

For the left-hand part we have (changing the order of integration)

$$\begin{aligned}\int_0^T \rho(t)[\int_{-t}^{t}(f_1\overline{g}_2 - g_1\overline{f}_2)dx]dt \\ &= \int_{-T}^{T}[(f_1\overline{g}_2 - g_1\overline{f}_2)\int_{|x|}^{T}\rho(t)dt]dx \\ &= \int_{-T}^{T}(f_1\overline{g}_2 - g_1\overline{f}_2)(P(T)-P(|x|))dx.\end{aligned}$$

Now we estimate the right-hand part of (7.7) (more precisely, its typical term):

$$|\int_0^T f_1(t)\overline{f_2'(t)}\rho(t)dt| \le [\int_0^T |f_1(t)|^2dt \int_0^T |f_2'(t)|^2\rho^2(t)dt]^{1/2} \le C,$$

where, due to claim 2), the constant C is independent of T. Therefore,

$$|\int_T^T (P(T)-P(|x|))[f_1\cdot\overline{g_2} - g_1\cdot\overline{f_2}]dx| \le C.$$

Dividing by $P(T)$ and letting $T\to+\infty$ (hence, $P(T)\to+\infty$), we get

$$\lim_{t\to+\infty}|\int_{-T}^{T}(1-\frac{P(|x|)}{P(T)})[f_1\overline{g_2} - g_1\overline{f_2}]dx| = 0. \tag{7.8}$$

Now we have to prove that

$$\lim_{T\to+\infty}|\int_{-T}^{T}[f_1\overline{g_2} - g_1\overline{f_2}]dx| = 0 \tag{7.9}$$

To end this we fix $\epsilon>0$. Since $f_i, g_i \in L^2(\mathbb{R})$,

$$\int_{|x|\ge w}(|f_1||g_2| + |g_1||f_2|)dx \le \epsilon$$

for all w large enough. Then, for each $T\ge w$ we have

$$\begin{aligned}|\int_{-w}^{w}(1-\frac{P(|x|)}{P(T)})[f_1\overline{g_2} - g_1\overline{f_2}]dx| \\ &\le |\int_{-T}^{T}(1-\frac{P(|x|)}{P(T)})[f_1\overline{g_2} - g_1\overline{f_2}]dx| + \epsilon.\end{aligned}$$

Letting $T \to +\infty$ and using (7.8), we obtain

$$|\int_{-w}^{w} (f_1\overline{g_2} - g_1\overline{f_2})dx| \leq \epsilon,$$

which implies (7.9). $\square$

Example 7.2. $V(x) = a(1+|x|)^\alpha$. If either $a \geq 0$, $\alpha \in \mathbb{R}$, or $a < 0$, $\alpha \leq 2$, then the assumptions of Theorem 7.1 are satisfied. Hence, H_0 is essentially self-adjoint. It is known that in the case $a < 0$, $\alpha > 2$, H_0 is not an essentially self-adjoint operator.

7.2 Discreteness of spectrum

Consider the operator H_0 defined by (7.1). Assume that $V(x) \in L^\infty_{\mathrm{loc}}(\mathbb{R})$ is a real valued function and

$$\lim_{x\to\infty} V(x) = +\infty. \tag{7.10}$$

Clearly, Theorem 7.1 implies that H_0 is essentially self-adjoint (take as $Q(x)$ and appropriate constant). Denote by H the closure of H_0.

Theorem 7.3. *Assume (7.10). Then the spectrum $\sigma(H)$ of H is discrete, i.e. there exists an orthonormal system $y_k(x), k = 0, 1, \ldots$, of eigenfunctions, with eigenvalues $\lambda_k \to +\infty$ as $k \to \infty$.*

Proof. Without loss of generality, one can assume that $V(x) \geq 1$. Then, we have

$$(Hu, u) \geq (u, u), \quad u \in D(H),$$

which implies the existence of bounded inverse operator H^{-1}. The conclusion of theorem is equivalent to compactness of H^{-1}. We will prove that $H^{-1/2}$ is a compact operator. (Prove that this implies compactness of H^{-1}). To end this, we consider the set

$$M = \{y | y \in D(H), (Hy, y) \leq 1\}$$

and prove that M is precompact in $L^2(\mathbb{R})$.

Let us also consider the set

$$M_N = \{y : y \in M, y(x) = 0 \text{ if } |x| \geq N\}.$$

Integration by parts implies that

$$(Hy, y) = \int_{-\infty}^{\infty} (|y'|^2 + V(x)|y|^2)dx, y \in M_N. \tag{7.11}$$

Let us fix a function $\varphi(x) \in C_0^\infty(\mathbb{R})$ such that $0 \le \varphi(x) \le 1$, $\varphi(x) = 1$ if $|x| \le 1/2$, $\varphi(x) = 0$ if $|x| \ge 1$, and $|\varphi'(x)| \le B$.

If $y \in M$ and $N \ge 2B$, then

$$y_N(x) = \varphi(\frac{x}{N})y(x) \in 2M_N,$$

where

$$2M_n = \{y|y(x) = 2z(x), z \in M_N\}.$$

Indeed, due to (7.11), we have

$$\begin{aligned}(Hy_N, y_N) &= \int_{-\infty}^{\infty} [|\frac{1}{N}\varphi'(\frac{x}{N})y(x) + \varphi(\frac{x}{N})y'(x)|^2 \\ &\qquad + V(x)|\varphi(\frac{x}{N})y(x)|^2]dx \\ &= \int_{-\infty}^{\infty} [\frac{1}{N^2}\varphi'^2(\frac{x}{N})|y(x)|^2 + \varphi^2(\frac{x}{N})|y'(x)|^2 + \\ &\quad + \frac{2}{N}\varphi(\frac{x}{N})\varphi'(\frac{x}{N})\mathrm{Re}(\overline{y(x)}y'(x)) + V(x)\varphi^2(\frac{x}{N}|y(x)|^2]dx.\end{aligned}$$

Estimate separately the terms under the integral as follows:

$$\begin{gathered}\frac{1}{N^2}\varphi'^2(\frac{x}{N})|y(x)|^2 \le \frac{B^2}{N^2}|y(x)|^2 \le \frac{1}{4}|y(x)|^2 \le \frac{V(x)}{4}|y(x)|^2, \\ \varphi^2(\frac{x}{N})|y'(x)|^2 \le |y'(x)|^2, \\ \frac{2}{N}\varphi(\frac{x}{N})\varphi'(\frac{x}{N}\mathrm{Re}(\overline{y}(x)\varphi'(x)) \le \frac{B}{N}(|y(x)|^2 + |y'(x)|^2) \le \\ \le \frac{1}{2}(V(x)|y(x)|^2 + |y'(x)|^2), \\ V(x)\varphi^2(\frac{x}{N})|y(x)|^2 \le V(x)|y(x)|^2.\end{gathered}$$

Putting all this together, we get

$$(Hy_N, y_N) \le 2,$$

which is required.

Now, for every $y \in M$, we have

$$(Hy_N, y_N) = \int_{-\infty}^{\infty} |y(x) - \varphi(\frac{x}{N})y(x)|^2 dx \le$$

$$\le \int_{|x|\ge N/2} |y(x)|^2 dx \le (\min_{|x|\ge N/2} V(x))^{-1},$$

since
$$\int_{-\infty}^{\infty} V(x)|y(x)|^2 dx \le (Hy, y) \le 1, \quad y \in M.$$
Assumption (7.10) implies that, for each $\epsilon > 0$ there exists $N > 0$ such that M is contained in the ϵ-neighborhood of $2M_N$. Thus, it suffices to prove the compactness of M_N.

In fact, we will prove even that M_N is precompact in the space $C([-N, N])$. To do this we use the Arzela theorem. First we verify the equicontinuity of M_N. This follows from the estimate

$$|y(x_2) - y(x_1)| = |\int_{x_1}^{x_2} y'(t)dt| \le \tag{7.12}$$

$$\le |x_2 - x_1|^{1/2} (\int_{x_1}^{x_2} |y'(t)|^2 dt) \le |x_2 - x_1|^{1/2}.$$

Moreover, (7.12) implies that
$$|y(x)| \le |y(t)| + (2N)^{1/2}, \quad x, t \in [-N, N].$$
Integrating the last inequality with respect to $t \in [-N, N]$ and using the Cauchy inequality, we see that M_N is bounded in $C([-N, N])$. The proof is complete.

$\square$

Remark 7.4. In fact, for discreteness of $\sigma(H)$ the following condition is necessary and sufficient:

$$\int_r^{r+1} V(x)dx \to +\infty \text{ as } r \to \infty. \tag{7.13}$$

Exercise 7.5. Prove the statement of Remark 7.4.

Now we supplement Theorem 7.3 by some additional information about eigenvalues and corresponding eigenfunctions.

Theorem 7.6. *Under the assumption of Theorem 7.3, all the eigenvalues are simple. If $\lambda_0 < \lambda_1 < \lambda_2 < \dots$ are the eigenvalues, then any (nontrivial) eigenfunction corresponding to λ_k has exactly k nodes, i.e. takes the value 0 exactly k times. All the eigenfunctions decay exponentially fast at infinity.*

For the proof we refer to [2].

Except of exponential decay, all the statements of Theorem 7.6 have purely 1-dimensional character. In particular, multidimensional Schrödinger operators may have multiple eigenvalues.

Exercise 7.7. Let $V(x) \geq \epsilon > 0$ for $x \geq a$. Then the equation

$$-y'' + v(x)y = 0$$

has at most one (up to a constant factor) nontrivial solution such that $y(x) \to 0$ as $x \to +\infty$.

7.3 Negative eigenvalues

a. Dirichlet boundary condition

Consider the operator

$$Hy = -y'' + V(x)y \tag{7.14}$$

on the half-axis $\mathbb{R}_+ = \{x|x \geq 0\}$ with the Dirichlet boundary condition

$$y(0) = 0. \tag{7.15}$$

We assume that $V \in L^\infty_{\text{loc}}(\mathbb{R}_+)$ and

$$V(x) \geq -C_0, \quad x \in \mathbb{R}_+. \tag{7.16}$$

All the previous results hold in this case, with obvious changes. In particular, H is a self-adjoint operator in $L^2(\mathbb{R}_+)$. More precisely, due to corresponding version of Theorem 7.1, operator (7.14) is essentially self-adjoint on the subspace consisting of all $y \in C^\infty(\mathbb{R}_+)$ such that $y(0) = 0$ and $y(x) = 0$ for all sufficiently large x.

In addition to (7.16), we assume that

$$\lim_{x \to +\infty} V_-(x) = 0, \tag{7.17}$$

where $V_-(x) = \min(V(x), 0)$, $V_+(x) = \max(V(x), 0)$. For the sake of simplicity we will also assume that V_- is continuous. In this case one can show that $\sigma(H) \cap \{\lambda < 0\}$ consists of isolated eigenvalues of finite multiplicity. However, in fact, we will prove more strong result.

Denote by $N_-(H)$ the number of negative eigenvalues of H counting multiplicities. We set $N_-(H) = +\infty$ if either the number of negative eigenvalues is infinite, or there is at least one non-isolated point of $\sigma(H)$ in $(-\infty, 0)$. (In our previous notation, $N_-(H) = N(-0)$).

Theorem 7.8. *Under the previous assumptions*

$$N_-(H) \leq \int_0^\infty x|V_-(x)|dx. \tag{7.18}$$

Proof. First, due to comparison results discussed in previous lectures, without loss of generality we can assume that $V_+(x) = 0$ and, hence, $V(x) = V_-(x)$. Moreover, we assume that $V(x) \not\equiv 0$, since the last case is trivial.

Consider a family of operators

$$H_\tau y = -y'' + \tau V(x) y, \quad 0 \le \tau \le 1.$$

Assumption (7.17) and Exercise 7.7 imply that the negative part of $\sigma(H_\tau)$ consists of simple eigenvalues

$$\lambda_1(\tau) < \lambda_2(\tau) < \ldots < \lambda_n(\tau) < \ldots$$

From the perturbation theory we know that $\lambda_n(\tau)$ is an analytic function of τ and, moreover,

$$\lambda_n'(\tau) = \int_0^\infty V(x)|\varphi_n(\tau, x)|^2 dx < 0, \tag{7.19}$$

where $\varphi_n(\tau, x)$ is the normalized eigenfunction of H_τ with the eigenvalue $\lambda_n(\tau)$. In fact, for any fixed τ, $\lambda_n(\tau)$ is defined only on a subinterval $(\tau_0(n), 1] \subset [0, 1]$.

Given $\mu_0 < 0$, denote by N_{μ_0} the number of eigenvalues of H in $(-\infty, \mu_0)$. Clearly, $N_{\mu_0} \to N_-(H)$ as $\mu_0 \to 0$. Fix such μ_0.

Varying τ from 1 to 0, we see that for each n there is τ_n such that $\lambda_n(\tau_n) = \mu_0$ provided $\lambda_n(1) < \mu_0$ (and only in this case). Thus, the eigenvalues $\lambda_n = \lambda_n(1) < \mu_0$ are in $1-1$ correspondence with values $\tau \in (0, 1]$ such that there exists a non-zero $y \in L^2(\mathbb{R}_+)$ satisfying

$$-y'' - \mu_0 y = -\tau V(x) y \tag{7.20}$$

and boundary condition (7.15).

Denote by L the differential operator

$$-\frac{d^2}{dx^2} - \mu_0$$

in $L^2(\mathbb{R}_+)$, with boundary condition (7.15). Since $\mu_0 < 0$, L is an invertible operator and

$$(L^{-1} f)(x) = \int_0^\infty K(x, \xi) f(\xi) d\xi.$$

A direct calculation (using variation of constants, the boundary condition and assumption $y \in L^2(\mathbb{R}_+)$) gives rise to the formula

$$K(x, \xi) = \theta(\xi - x) \frac{\sinh \sqrt{-\mu_0} x}{\sqrt{-\mu_0}} e^{-\sqrt{-\mu_0}\xi} + \theta(x - \xi) \frac{\sinh \sqrt{-\mu_0}\xi}{\sqrt{-\mu_0}} e^{-\sqrt{-\mu_0} x},$$

where $\theta(x) = 1$ if $x \geq 0$, and $\theta(x) = 0$ if $x < 0$.

Now equation (7.20) is equivalent to

$$y = \tau L^{-1}[(-V)y].$$

Hence, the numbers τ_n are inverse eigenvalues of the integral operator K_1 with the kernel function

$$K_1(x,\xi) = -K(x,\xi)V(\xi).$$

Claim 7.9. *K_1 has at most countable number of non-zero eigenvalues λ_k. All they are simple, positive, and*

$$\sum \lambda_k = \int_0^\infty K_1(x,x)dx.$$

Let us postpone the proof of Claim and first finish the proof of theorem. Using an easy inequality $1 - e^{-t} \leq t, t \geq 0$, we have

$$\begin{aligned} N_{\mu_0} &\leq \sum_{\tau_k \leq 1} \tau_k^{-1} = \sum_{\lambda_k \geq 1} \lambda_k \leq \sum \lambda_k \\ &= \int_0^\infty \frac{\sinh \sqrt{-\mu_0}x}{\sqrt{-\mu_0}} e^{-\sqrt{-\mu_0}x} |V(x)| \\ &= \int_0^\infty \frac{1 - e^{-2\sqrt{-\mu_0}x}}{2\sqrt{-\mu_0}} |V(x)| dx \leq \int_0^\infty x|V(x)|dx. \end{aligned}$$

□

Proof of Claim. Denote by K the integral operator with the kernel function $K(x,\xi)$, i.e. L^{-1}, and by V the operator of multiplication by $|V|$. Obviously, $K_1 = KV$. Now consider the operator $K_2 = V^{1/2}KV^{1/2}$, with the kernel function

$$K_2(x,\xi) = |V(x)|^{1/2}K(x,\xi)|V(\xi)|^{1/2}.$$

It is easily seen that

$$\int_0^\infty K_1(x,x)dx = \int_0^\infty K_2(x,x)dx.$$

Now let $\lambda \in \mathbb{C}$, $\lambda \neq 0$, $H_\lambda(K_1)$ and $H_\lambda(K_2)$ be eigenspaces of K_1 and K_2 with the eigenvalue λ. If $f \in H_\lambda(K_1)$, then $V^{1/2}f \in H_\lambda(K_2)$ (check this). Thus, we have a well-defined linear map

$$V^{1/2} : H_\lambda(K_1) \to H_\lambda(K_2). \tag{7.21}$$

We prove that this map is an isomorphism. Indeed, let $f \in H_\lambda(K_1)$ and $V^{1/2}f = 0$. Then $Vf = 0$. Hence, $K_1 f = KVf = 0$, which contradicts the assumption $\lambda \neq 0$. Thus, (7.21) hat a trivial kernel. Now let $g \in H_\lambda(K_2)$. Then $V^{1/2}KV^{1/2}g = \lambda g$. Setting $f = \lambda^{-1}KV^{1/2}g$, we have $V^{1/2}f = g$ and $f \in H_\lambda(K_1)$, which implies that (7.21) is onto.

Since $K_1 \geq 0$, its eigenvalues are nonnegative. Since the equation $KVf = \lambda f$ is equivalent to the equation $\lambda Lf = Vf$, we see that all the eigenvalues are simple. Moreover, since $K_2(x, \xi) \geq 0$ is continuous, K_2 is a nuclear operator and

$$trK_2 = trK_1 = \int_0^\infty K_2(x,x)dx = \int_0^\infty K_1(x,x)dx.$$

$\square$

b. Neumann boundary condition.

First we show by a counterexample that estimate (7.18) fails in the case of Neumann boundary condition

$$y'(0) = 0, \tag{7.22}$$

as well as in the case of operator (7.14) on the whole axis.

Example 7.10. Let $V(x) = 0$ if $|x| \geq a$ and $V(x) = -\epsilon$, $\epsilon > 0$, if $|x| < a$. We show that operator H with boundary condition (7.22) has a negative eigenvalue for all $\epsilon > 0$, $a > 0$, which implies obviously that estimate (7.18) is impossible. To do this consider the equation on eigenfunctions on $\mathbb{R}$ with negative eigenvalue λ

$$\begin{aligned} -y'' - \epsilon y &= \lambda y, \qquad |x| < a, \\ -y'' &= \lambda y, \qquad |x| \geq a. \end{aligned}$$

At $x = \pm a$ the functions y and y' have to be continuous. Obviously, for corresponding operator H we have $H \geq -\epsilon I$. Hence, $\lambda \geq -\epsilon$. Since the potential V is an even function, we see that $y(-x)$ is an eigenfunction, provided so is y. Since all the eigenvalues are simple, we have $y(-x) = \pm y(x)$. If $y(x)$ is odd, then $y(0) = 0$ and y is an eigenfunction of the Dirichlet problem with negative λ, which is impossible. Consider the case of even y. Then $y'(0) = 0$ and

$$\begin{aligned} y(x) &= C_1 \cos\sqrt{\epsilon + \lambda}x, \qquad |x| < a, \\ y(x) &= C_2 e^{-\sqrt{-\lambda}|x|}, \qquad |x| > a. \end{aligned}$$

Due to compatibility conditions at $x = \pm a$, we have

$$C_1 \cos \sqrt{\epsilon+\lambda}a - C_2 e^{-\sqrt{-\lambda}}a = 0,$$
$$-C_1\sqrt{\epsilon+\lambda}\sin\sqrt{\epsilon+\lambda}a + C_2\sqrt{-\lambda}e^{-\sqrt{-\lambda}a} = 0.$$

Now λ is an eigenvalue iff there exists a nontrivial solution (C_1, C_2) of the last system. Equivalently, the determinant

$$e^{-\sqrt{-\lambda}}[\sqrt{-\lambda}\cos(\sqrt{\epsilon+\lambda}a) - \sqrt{\epsilon+\lambda}\sin(\sqrt{\epsilon+\lambda}a)]$$

should vanish. This gives rise to the equation

$$\tan[a\sqrt{\epsilon+\lambda}] = \sqrt{\frac{-\lambda}{\epsilon+\lambda}}.$$

The last equation always has a solution $\lambda \in (-\epsilon, 0)$ (draw a plot).

Now we consider the operator H_N in $L^2(\mathbb{R}_+)$ generated by the differential expression $-y'' + V(x)y$ and Neumann boundary condition $y'(0) = 0$. We assume that the potential is bounded below and locally bounded measurable function. Denote by $N_-(H_N)$ the number of negative eigenvalues of H_N. Then we have

Theorem 7.11. *$N_-(H_N) \le 1 + \int_0^\infty x|V_-(x)|dx$.*

Proof. Due to Theorem 7.4, it suffices to prove that

$$N_-(H_N) \le 1 + N_-(H).$$

In fact, we have

$$N(\lambda - 0, H_N) \le 1 + N(\lambda - 0, H), \quad \lambda \in \mathbb{R}.$$

Let

$$D = \{u \in C^\infty(\mathbb{R}_+) : u(0) = 0,\ \operatorname{supp} u \ \text{ is bounded}\},$$
$$D_N = \{u \in C^\infty(\mathbb{R}_+) : u'(0) = 0,\ \operatorname{supp} u \ \text{ is bounded}\}.$$

The operators H and H_N are essentially self-adjoint on D and D_N, respectively. We want to use the Glazman lemma discussed in previous lectures. For H and H_N, this lemma reads

$$N(\lambda - 0, H_N) = \sup\{\dim L : L \subset D_N, (Hu, u) < \lambda(u, u), u \in L \setminus \{0\}\}.$$
$$N(\lambda - 0, H) = \sup\{\dim \tilde{L} : \tilde{L} \subset D, (Hu, u) < \lambda(u, u), u \in \tilde{L} \setminus \{0\}\}.$$

Hence, we have to show that, given $L \subset D_N$ such that

$$(Hu, u) < \lambda(u, u), \quad u \in L \setminus \{0\},$$

there exists $\tilde{L} \subset D$ such that

$$(Hu, u) < \lambda(u, u), u \in \tilde{L} \setminus \{0\},$$

and

$$\dim L \leq 1 + \dim \tilde{L}.$$

But the last is evident: set

$$\tilde{L} = \{u \in L : u(0) = 0\}.$$

□

c. The case of whole axis.

Consider the operator

$$Hy = -y'' + V(x)y, \quad x \in \mathbb{R},$$

assuming that $V \in L^\infty_{\mathrm{loc}}(\mathbb{R})$ and $V(x) \geq -C_0$. Then H is a self-adjoint operator in $L^2(\mathbb{R})$. Let $N_-(H)$ be the number of negative eigenvalues.

Theorem 7.12. $N_-(H) \leq 1 + \int_{-\infty}^{\infty} |x||V_-(x)|dx$.

The proof is based on the Glazman lemma. We omit it here (see, e.g., [2]).

8 Multidimensional Schrödinger operator

8.1 Self-adjointness

Consider the operator

$$H_0 u = -\Delta u + V(x)u \tag{8.1}$$

with $D(H_0) = C_0^\infty(\mathbb{R}^n)$. We want to know whether H_0 is an essentially self-adjoint operator in $L^2(\mathbb{R})$. If this is the case, we denote by H the closure of H_0, i.e. $H = H_0^{**}$. We have the following result which is similar to Theorem 7.1.

Theorem 8.1. *Assume that $V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^n)$ and*

$$V(x) \geq -Q(|x|),$$

where $Q(r)$ is a nonnegative, nondecreasing, continuous function of $r \geq 0$ such that

$$\int_0^\infty \frac{dr}{\sqrt{Q(2r)}} = \infty.$$

Then H_0 is essentially self-adjoint.

The proof goes along the same lines as that of Theorem 7.1, but is more sophisticated. We omit it. Instead, we want to discuss another way to obtain essential self-adjointness.

We start with the following criterion of self-adjointness.

Proposition 8.2. *Let A be a closed, symmetric operator in a Hilbert space $\mathcal{H}$. The following statements are equivalent:*

(i) *A is self-adjoint;*

(ii) $\ker(A^* \pm iI) = \{0\}$*;*

(iii) $\operatorname{im}(A \pm iI) = \mathcal{H}$*.*

Outline of Proof. 1) First, $\operatorname{im}(A \pm iI)$ is a closed subspace of $\mathcal{H}$ (prove it). 2) Since $\ker A^* \oplus \operatorname{im} A = \mathcal{H}$ and $\operatorname{im} A$ is closed, (ii) and (iii) are equivalent. 3) Obviously, $(i) \Rightarrow (ii)$, since $\sigma(a) \subset \mathbb{R}$ for every self-adjoint A. Thus, we have to show that (ii) and $(iii) \Rightarrow (i)$. Since $D(A) \subset D(A^*)$, we have to prove that $D(A^*) \subset D(A)$. Let $f \in D(A^*)$ and $\varphi = (A^* + iI)f$. By (iii), there exists $g \in D(A)$ such that $(A + iI)g = \varphi$. Since A is symmetric, $Ag = A^*g$. Hence,

$$(A^* + iI)f = \varphi = (A^* + iI)g$$

or

$$(A^* + iI)(f - g) = 0.$$

By (ii), $f = g$ and $f \in D(A)$. Thus $D(A) = D(A^*)$ and A is self-adjoint. $\square$

Corollary 8.3. *Let A be a symmetric operator. Then A is essentially self-adjoint if and only if* $\ker(A^* \pm iI) = \{0\}$.

We have also the following version of Proposition 8.2.

Proposition 8.4. *Let A be a closed, nonnegative, symmetric operator. Then A is self-adjoint if and only if* $\ker(H^* + bI) = \{0\}$ *for some $b > 0$.*

Corollary 8.5. *Let A be a nonnegative symmetric operator. Then H is essentially self-adjoint if and only if* $\ker(H^* + bI) = \{0\}$ *for some $b > 0$.*

In what follows we will use the so-called Kato inequality. For any function u, we define $\operatorname{sgn} u$ by

$$(\operatorname{sgn} u)(x) = \begin{cases} 0, & u(x) = 0, \\ \overline{u}(x)|u(x)|^{-1}, & u(x) \neq 0, \end{cases}$$

and a regularized absolute value of u by

$$u_\epsilon(x) = (|u(x)|^2 + \epsilon^2)^{1/2}.$$

Clearly, $\lim u_\epsilon(x) = |u(x)|$ pointwise and $|u(x)| = (\operatorname{sgn} u) \cdot u$.

Theorem 8.6. *Let $u \in L^1_{\text{loc}}(\mathbb{R}^n)$. Suppose that the distributional Laplacian $\Delta u \in L^1_{\text{loc}}(\mathbb{R}^n)$. Then*

$$\Delta|u| \geq \operatorname{Re}[(\operatorname{sgn} u)\Delta u] \tag{8.2}$$

in the sense of distributions.

Proof. First, let $u \in C^\infty(\mathbb{R}^n)$. We want to prove that (8.2) holds pointwise except where $|u|$ is not differentiable.

For such $u(x)$ we have

$$u_\epsilon \nabla u_\epsilon = \operatorname{Re} \overline{u} \nabla u. \tag{8.3}$$

Since $u_\epsilon \geq |u|$, we get

$$|\nabla u_\epsilon| \leq u_\epsilon^{-1}|u||\nabla u| \leq |\nabla u|. \tag{8.4}$$

Next, take the divergence of (8.3), to obtain

$$|\nabla u_\epsilon|^2 + u_\epsilon \nabla u_\epsilon = |\nabla u|^2 + \operatorname{Re} \overline{u} \Delta u.$$

Together with (8.4), this implies

$$u_\epsilon \Delta u_\epsilon \geq \operatorname{Re} \overline{u} \Delta u,$$

or

$$\Delta u_\epsilon \geq \operatorname{Re}[(\operatorname{sgn}_\epsilon u) \Delta u], \tag{8.5}$$

where $\operatorname{sgn}_\epsilon u = \overline{u} u_\epsilon^{-1}$. Prove that $\Delta u_\epsilon \to \Delta |u|$ pointwise (except where $|u|$ is not smooth) and $\operatorname{sgn}_\epsilon u \to \operatorname{sgn} u$ pointwise.

The next step is based on regularization. Let $\varphi \in C_0^\infty(\mathbb{R}^n)$, $\varphi \geq 0$, and $\int \varphi dx = 1$. We define $\varphi_\delta(x) = \delta^{-n} \varphi(x/\delta)$ and

$$(I_\delta u)(x) = (\varphi_\delta * u)(x) = \int_{\mathbb{R}^n} \varphi_\delta(x-y) u(y) dy.$$

I_δ is called an *approximate identity.*

We list some properties of approximate identity:

(i) *if* $u \in L^1_{\text{loc}}(\mathbb{R}^n)$, *then* $I_\delta U \in C^\infty(\mathbb{R}^n)$;

(ii) I_δ *commutes with partial derivatives* $\partial | \partial_{x_i}$;

(iii) *the map* $I_\delta : L^p(\mathbb{R}^n) \to L^p(\mathbb{R}^n)$ *is bounded, with the norm* ≤ 1;

(iv) *for any* $u \in L^p(\mathbb{R}^n)$, $\lim_{\delta \to 0} \|I_\delta u - u\|_{L^p} = 0$;

(v) *for any* $u \in L^1_{\text{loc}}(\mathbb{R}^n)$, $I_\delta u \to u$ *in* $L^1_{\text{loc}}(\mathbb{R}^n)$.

Exercise 8.7. Prove (i)-(v).

Let $u \in L^1_{\text{loc}}(\mathbb{R}^n)$. Inserting $I_\delta u$ into (8.5) in place of u, we obtain

$$\Delta (I_\delta u)_\epsilon \geq \operatorname{Re}[\operatorname{sgn}_\epsilon (I_\delta u) \Delta (I_\delta u)].$$

Now one can pass to the limit as $\delta \to 0$ and next as $\epsilon \to 0$, to get (8.2). $\square$

Exercise 8.8. Justify the passage to the limit in the proof of Theorem 8.6.

As an application we state the following

Theorem 8.9. *Let* $V \in L^2_{\text{loc}}(\mathbb{R}^n)$ *and* $V \geq 0$. *Then* H_0 *is essentially self-adjoint.*

Proof. Clearly, H_0 is nonnegative symmetric operator. By Corollary 8.5, it is sufficient to show that $\ker(H_0^* + I) = \{0\}$. Thus, let us assume that

$$-\Delta u + Vu + u = 0 \tag{8.6}$$

for some $u \in L^2(\mathbb{R}^n)$ (in the sense of distributions). We have to prove that $u = 0$.

We note that $u \in L^2(\mathbb{R}^n)$ and $V \in L^2_{\mathrm{loc}}(\mathbb{R}^n)$ imply that $Vu \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$. Furthermore, $u \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$. By (8.6), $\Delta u \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$.

Now we apply the Kato inequality to get

$$\Delta|u| \geq \mathrm{Re}[(\operatorname{sgn} u)\Delta u] = \mathrm{Re}[(\operatorname{sgn} u)(V+1)u] = |u|(V+1) \geq 0.$$

As consequence,

$$\Delta I_\delta |u| = I_\delta \Delta |u| \geq 0.$$

Obviously, $I_\delta |u| \geq 0$.

On the other hand $I_\delta |u| \in D(\Delta)$. Indeed, this follows from $|u| \in L^2(\mathbb{R}^n)$ and

$$(\frac{\partial}{\partial x_i} I_\delta f) = \int \frac{\partial \varphi_\delta}{\partial x_i}(x-y) f(y) dy.$$

Now

$$(\Delta(I_\delta|u|), (I_\delta|u|)) = -\|\nabla(I_\delta|u|)\|^2_{L^2} \leq 0.$$

Since the left side here is nonnegative, we see that $\nabla(I_\delta|u|) = 0$. Hence, $I_\delta|u| = c \geq 0$. Since $|u| \in L^2(\mathbb{R}^n)$, we have $c = 0$. Therefore, $I_\delta|u| = 0$, hence, $|u| = 0$. ☐

Another approach to the problem relies on the notion of relatively bounded operators and the Kato-Rellich theorem.

Let A and B be closed operators in $\mathcal{H}$. One says that B is A-bounded if $D(A) \subset D(B)$. Obviously, any $B \in L(\mathcal{H})$ is A-bounded for any A.

Proposition 8.10. *If $\sigma(A) \neq \mathbb{C}$ and B is A-bounded, then there exist $a \geq 0$ and $b \geq 0$ and such that*

$$\|Bu\| \leq a\|Au\| + b\|u\| \tag{8.7}$$

for all $u \in D(A)$.

Proof. Let

$$\|u\|_A = (\|u\|^2 + \|Au\|^2)^{1/2}$$

be the graph norm on $D(A)$. We know that A is closed if and only if $D(A)$ is complete with respect to $\|\cdot\|_A$. Moreover, $\|\cdot\|_A$ is induced by an inner product

$$\langle u, v\rangle_A = \langle u, v\rangle + \langle Au, Av\rangle.$$

Denote by $\mathcal{H}_A$ the space $D(A)$ endowed with this inner product. Then $\mathcal{H}_A$ is a Hilbert space.

Exercise 8.11. If $z \notin \sigma(A)$, then $R_A(z) = (A - zI)^{-1}$ a bounded operator from $\mathcal{H}$ onto $\mathcal{H}_A$.

Since B is A-bounded, we see that $BR_A(z)$ is everywhere defined on H.

Exercise 8.12. $BR_A(z)$ is closed operator on $\mathcal{H}$.

Now the closed graph theorem implies that $BR_A(z)$ is bounded. Hence, there exists $a \leq 0$ such that

$$\|BR_A(z)f\| \leq a\|f\|, \quad f \in \mathcal{H}. \tag{8.8}$$

For any $f \in \mathcal{H}$, we have $u = R_A(z)f \in D(A)$ and each $u \in D(A)$ can be written in this form. Thus $f = (A - z)u$. Now (8.8) implies

$$\|Bu\| = \|BR_A(z)f\| \leq a\|(A - z)u\| \leq a\|Au\| + b\|u\|,$$

with $b = |z|a$. □

The infimum of all a in (8.7) is called the A-*bound* of B. Note that b in (8.7) depends, in general, on a. If B is A-bounded, then it follows from (8.7) that there exists a constant $c > 0$ such that

$$\|Bu\| \leq c\|u\|_A, \quad u \in \mathcal{H}_A,$$

i. e. $B : \mathcal{H}_A \to \mathcal{H}$ is bounded. Conversely, if B is a bounded operator from $\mathcal{H}_A$ into $\mathcal{H}$, then B is A-bounded.

Now we prove the following Kato-Rellich theorem.

Theorem 8.13. *Let A be self-adjoint, and let B be a closed, symmetric, A-bounded operator with A-bound less then 1. Then $A+B$, with $D(A+B) = D(A)$, is a self-adjoint operator.*

Proof. First, we have the following

Lemma 8.14. *Let A be self-adjoint and B be A-bounded with A-bound a. Then*

$$\|B(A - i\lambda I)^{-1}\| \leq a + b|\lambda|^{-1}$$

for all real $\lambda \neq 0$ and for some $b > 0$. The A-bound of B is given by

$$a = \lim_{|\lambda|\to\infty} \|BR_A(i\lambda)\|.$$

Proof of Lemma 8.14. Since A is self-adjoint, we have

$$\|(A - i\lambda I)u\|^2 = \|Au\|^2 + |\lambda|^2\|u\|^2,$$

hence,

$$\|Au\| \le \|(A - i\lambda I)u\|.$$

Setting $u = R_A(i\lambda)v$ yields

$$\|AR_A(i\lambda)\| \le 1.$$

Exercise 8.15. If A is self-adjoint, then

$$\|R_A(i\lambda)\| \le |\lambda|^{-1}.$$

Now we have

$$\|BR_A(i\lambda)u\| \le a\|AR_A(i\lambda)u\| + b\|R_A(i\lambda)u\| \le (a + b|\lambda|^{-1})\|u\|,$$

which implies the first statement.

The last inequality also shows that

$$\lim \sup_{|\lambda|\to\infty} \|BR_A(i\lambda)\| \le a.$$

On the other hand,

$$\|Bu\| = \|BR_A(i\lambda)(A - i\lambda I)u\| \le \|BR_A(i\lambda)\|[\|Au\| + |\lambda|\|u\|].$$

This inequality and the definition of A-bound imply that the A-bound is not greater then

$$\lim \inf_{|\lambda|\to\infty} \|BR_A(i\lambda)\|.$$

□

Exercise 8.16. $A + B$ is closed on $D(A)$.

Proof of Theorem 8.13 continued. Since $a < 1$, we have

$$\|BR_A(i\lambda)\| < 1 \tag{8.9}$$

for λ large enough. Now

$$A + B - i\lambda I = [I + BR_A(i\lambda)](A - i\lambda I).$$

Due to (8.9), $I+BR_A(i\lambda)$ is an invertible operator. Since $A-i\lambda I$ is invertible, it follows that $(A+B-i\lambda I)$ is invertible. In particular, $\mathrm{im}(A+B-i\lambda I) = \mathcal{H}$, and, by Proposition 8.1, $A + B$ is self-adjoint. □

As an application we have

Theorem 8.17. *Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and real. Then the operator $H = -\Delta + V$, with $D(H) = D(\Delta) = H^2(\mathbb{R}^3)$, is self-adjoint.*

Remark 8.18. Recall that

$$H^m(\mathbb{R}^n) = \{u \in L^2(\mathbb{R}^n) : \partial^\alpha u \in L^2(\mathbb{R}^3), |\alpha| \le m\}.$$

Remark 8.19. Suppose $V \in L^p(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)$, with $p > 2$ if $n = 4$ and $p > n/2$ if $n \ge 5$. Then the conclusion of Theorem 8.17 holds.

Proof. Let $V = V_1 + V_2$, with $V_1 \in L^2(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$. Since

$$\|V_2 u\|_{L^2} \le \|V_2\|_{L^\infty} \|u\|_{L^2},$$

we see that multiplication by V_2 is Δ-bounded with Δ-bound 0.

Consider $V = V_1 \in L^2(\mathbb{R}^3)$. Since Δ is self-adjoint, $i\lambda \notin \sigma(\Delta)$ for all $\lambda \in \mathbb{R}, \lambda \ne 0$. We have

$$\|V R_\Delta(i\lambda) f\|_{L^2} \le \|V\|_2 \|R_\Delta(i\lambda) f\|_{L^\infty},$$

provided the L^∞-norm here is finite. Thus, it is enough to prove this.

In fact, on $\mathbb{R}^3$ we have the following integral representation for $R_\Delta(i\lambda)$

$$(R_\Delta(i\lambda) f)(x) = (4\pi)^{-1} \int_{\mathbb{R}^3} e^{-(i\lambda)^{1/2}|x-y|} |x-y|^{-1} f(y) dy.$$

Using the Young inequality, this implies

$$\|R_\Delta(i\lambda) f\|_{L^\infty} \le \|f\|_{L^2} \|G_\lambda\|_{L^2},$$

where $G_\lambda(x) = (4\pi)^{-1} \exp[-(i\lambda)^{1/2}|x|]|x|^{-1}$ and

$$\|G_\lambda\|_{L^2}^2 = (4\pi)^{-2} \int_{\mathbb{R}^3} \exp[-2 \operatorname{Re}(i\lambda)^{1/2}|x|]|x|^{-2} dx$$

is finite. Moreover, it is easy to check that $\lim_{\lambda\to\infty} \|G_\lambda\|_{L^2} = 0$. Therefore, for any $\epsilon > 0$ we can find $\lambda > 0$ such that

$$\|G_\lambda\|_{L^2} \le \epsilon \|V\|_{L^2}^{-1}.$$

Now it follows that for all λ large enough

$$\|V R_\Delta(i\lambda) f\|_{L^\infty} \le \epsilon \|f\|_{L^2}.$$

Since (8.8) implies (8.7), we have

$$\|Vu\| \le \epsilon \|\Delta u\| + \epsilon\lambda \|u\|, \quad u \in D(A).$$

This implies that V is Δ-bounded with Δ-bound 0.

Applying the Kato-Rellich theorem, we conclude. $\square$

8.2 Discrete spectrum

We assume here that $V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^n)$ and

$$\lim_{|x|\to\infty}\inf V(x) = \lim_{R\to\infty}\inf_{|x|\geq R} V(x) \geq a. \tag{8.10}$$

Theorem 8.20. *Under assumption (8.10) the operator H is bounded below and, for each $a' < a$, $\sigma(H)\cap(-\infty, a')$ consists of a finite number of eigenvalues of finite multiplicity.*

Corollary 8.21. *If $\lim_{|x|\to\infty} V(x) = +\infty$, then $\sigma(H)$ is discrete.*

Proof of Theorem 8.20. Clearly, $V(x) \geq -C$ for some C and, hence, H is bounded below. Remark also that the conclusion of Theorem means that the spectral projector $E_{a'}$ of H is finite dimensional for all $a' < a$.

1) Let us consider

$$(H\psi,\psi) = \int_{\mathbb{R}^n} [-\Delta\psi + V(x)\psi]\overline{\psi}dx, \quad \psi\in D(H).$$

We want to show that

$$(H\psi,\psi) = \int_{\mathbb{R}^N} [|\nabla\psi|^2 + V(x)|\psi|^2]dx, \quad \psi\in D(H). \tag{8.11}$$

Identity (8.11) is obvious for $\psi \in C_0^\infty(\mathbb{R}^n)$. In general case we show first that

$$\int_{\mathbb{R}^n} [|\nabla\psi|^2 + V(x)|\psi|^2]dx < \infty, \quad \psi\in D(H). \tag{8.12}$$

Local elliptic regularity implies that if $\psi \in D(H)$, then $\psi \in H^2_{\mathrm{loc}}(\mathbb{R}^n)$. Hence, the integral in (8.12), with $\mathbb{R}^n$ replaced by each ball, is finite. Let $b \leq \inf V(x) - 1$. Since $\psi \in L^2(\mathbb{R}^n)$, inequality (8.12) is equivalent to the following one:

$$H_b(\psi,\psi) = \int [|\nabla\psi|^2 + (V(x)-b)|\psi|^2]dx < \infty, \psi\in D(H).$$

Finiteness of the quadratic form $H_b(\psi,\psi)$ means that

$$\int |\nabla\psi|^2 dx < \infty, \int (1+|V(x)|)|\psi|^2 dx < \infty. \tag{8.13}$$

The form $H_b(\psi,\psi)$ is generated by an Hermitian form

$$H_b(\psi_1,\psi_2) = \int [\nabla\psi_1\overline{\nabla\psi_2} + (V(x)-b)\psi_1\overline{\psi_2}dx,$$

which is finite provided ψ_1 and ψ_2 satisfy (8.13).

For $\psi \in C_0^\infty(\mathbb{R}^n)$ one has

$$((H-bI)\psi,\psi) = H_b(\psi,\psi). \tag{8.14}$$

Here the left-hand part is continuous with respect to the graph norm

$$(\|\psi\|^2 + \|H\psi\|^2)^{1/2}.$$

on $D(H)$. Hence, same is for $H_b(\psi,\psi)$ and, by continuity, H_b is well-defined on $D(H)$.

We have an obvious inequality

$$\|\psi\|_1^2 \le H_b(\psi,\psi), \quad \psi \in C_0^\infty(\mathbb{R}^n),$$

where $\|\cdot\|_1$ is the norm in $H^1(\mathbb{R}^n)$. Therefore, convergence of elements of $C_0^\infty(\mathbb{R}^n)$ with respect to the graph norm implies their convergence in $\|\cdot\|_1$. Since the space $H^1(\mathbb{R}^n)$ is complete, it follows that $\psi \in D(H)$ implies $\psi \in H^1(\mathbb{R}^n)$, i.e. $\psi \in L^2(\mathbb{R}^n)$ and the first inequality in (8.13) holds.

Similarly, the weighted L^2space

$$L^2(\mathbb{R}^n, 1+|V(x)|) = \{\psi \in L^2(\mathbb{R}^n) : \int_{\mathbb{R}^n} (1+V(x))|\psi(x)|^2 dx < \infty\}$$

is complete, which implies that $\psi \in L^2(\mathbb{R}^n, 1+|V(x)|)$ provided $\psi \in D(H)$.

Thus, for every $\psi \in D(H)$ satisfies (8.13) and (8.11) (which is equivalent to (8.14)) follows by continuity.

2) Now we recall a version of Glazman's lemma:

$$N(\lambda) = \sup\{\dim L : L < D(H), (Hu,u) \le \lambda(u,u), \quad u \in L\},$$

where $N(\lambda) = \#$ eigenvalues below λ.

Thus, to prove the theorem we have to show that if $a' < a$ and L is a subspace of $D(H)$ (not necessary closed) such that

$$(H\psi,\psi) \le a'(\psi,\psi), \quad \psi \in L, \tag{8.15}$$

then L is finite dimensional.

Due to step 1), we can rewrite (8.15) as

$$\int_{\mathbb{R}^N} [|\nabla\psi|^2 + (V(x) - a')|\psi|^2] dx \le 0, \quad \psi \in L. \tag{8.16}$$

Fix $\delta \in (0, a - a')$ and $R > 0$ such that $V(x) \ge a' + \delta$ for $|x| \ge R$. Let $M = -\inf V(x)$. If $C > 0$ and $C > M + a'$, then (8.16) implies

$$\int_{|x|\le R} |\nabla\psi|^2 dx + \int_{|x|\ge R} [|\nabla\psi|^2 + \delta|\psi|^2] dx \le C \int_{|x|\le R} |\psi|^2 dx, \psi \in L. \tag{8.17}$$

Let us consider an operator $A : L \to L^2(B_R)$, $A : \psi \mapsto \psi|_{B_R}$, where B_R is the ball of radius R centered at 0. The space L is considered with the topology induced form $L^2(\mathbb{R}^n)$. Clearly, A is continuous. Inequality (8.17) implies that $\ker A = \{0\}$. Now it suffices to show that $\tilde{L} = AL$ is a finite dimensional subspace of $L^2(B_R)$. Clearly, $\tilde{L} \subset H^1(B_R)$ and, due to (8.17),

$$\|\psi\|_{H^1(B_R)} \le C_1 \|\psi\|_{L^2(B_R)}, \quad \psi \in \tilde{L}.$$

Therefore, the identity operator I in $\tilde{L}$ can be represented as a composition of the embedding $\tilde{L} \subset H^1(B_R)$ which is continuous, as we already seen, and the embedding $H^1(B_R) \subset L^2(B_R)$ which is compact. Thus, I is a compact operator. Hence, $\tilde{L}$ is finite dimensional.

□

Remark 8.22. There exist various estimates for $N_-(H)$, the number of negative eigenvalues of H. In the case $n \ge 3$, the best known is the Lieb-Cwikel-Rozenblum bound

$$N_-(H) \le c_n \int_{\mathbb{R}^n} |V_-(x)|^{n/2} dx,$$

where $V_-(x) = \min[V(x), 0]$ and c_n is a constant depending only on n.

8.3 Essential spectrum

Recall that $\sigma_{\text{ess}}(H)$ consists of all non-isolated points of $\sigma(H)$ and eigenvalues of infinite multiplicity. In other words, $\lambda \in \sigma_{\text{ess}}(H)$ if and only if the space $E(\lambda - \epsilon, \lambda + \epsilon)\mathcal{H}$ is infinite dimensional for all $\epsilon > 0$. Here $E(\Delta)$ is the spectral projector associated with an interval $\Delta \subset \mathbb{R}$.

Theorem 8.23. *Assume that* $V \in L^\infty_{\text{loc}}(\mathbb{R}^n)$ *and* $\lim_{|x|\to\infty} V(x) = 0$. *Then* $\sigma_{\text{ess}}(H) = [0, +\infty)$.

Proof. By Theorem 8.20, $\sigma_{\text{ess}}(H) \cap (-\infty, 0) = \emptyset$. Therefore, we have to prove that $[0, +\infty) \subset \sigma(H)$.

Let $\lambda \geq 0$. Then $\lambda \in \sigma(H)$ if and only if there exists a sequence $\varphi_p \in D(H)$ such that

$$\lim_{p\to\infty} \frac{\|(H - \lambda I)\psi_p\|}{\|\varphi_p\|} = 0.$$

To construct such a function we start with the following observation. The function $e^{ik\cdot x}$, $|k| = \sqrt{\lambda}$, satisfies the equation

$$-\Delta e^{ik\cdot x} = \lambda e^{ik\cdot x}.$$

Therefore,

$$\lim_{|x|\to\infty} [-\Delta + V(x) - \lambda] e^{ik\cdot x} = 0.$$

Now let us fix a function $\chi \in C_0^\infty(\mathbb{R}^n)$ such that $\chi \geq 0$, $\chi(x) = 1$ if $|x| \leq 1/2$, and $\chi(x) = 0$ if $|x| \geq 2$. We set

$$\chi_p(x) = \chi(|p|^{-1/2}(x - p)), \quad p \in \mathbb{Z}^n.$$

Obviously,

$$\operatorname{supp} \chi_p \subset \{x \in \mathbb{R}^n : |x - p| \leq \sqrt{|p|}\}.$$

Therefore,

$$\lim_{p\to\infty} \sup_{x \in \operatorname{supp} \chi_p} |V(x)| = 0.$$

Now we set

$$\varphi_p(x) = \chi_p(x) e^{ik\cdot x}, \quad |k| = \sqrt{\lambda}.$$

First, we have

$$\|\varphi_p\|^2 = \int |\chi_p(x)|^2 dx = p^{n/2} \int |\chi(x)|^2 dx = C p^{n/2},$$

where $C > 0$.

Next,

$$H\varphi_p = -(\Delta\chi_p) \cdot e^{ik\cdot x} - (\nabla\chi_p)(\nabla e^{ik\cdot x}) + k^2 \chi_p e^{ik\cdot x} + V(x)\chi_p e^{ik\cdot x}.$$

Therefore,

$$(H - \lambda I)\varphi_p = e^{ik\cdot x}[H\chi_p - ik \cdot \nabla\chi_p]. \tag{8.18}$$

In addition,

$$|\nabla\chi_p| \leq C_1|p|^{-1/2}, \quad |\Delta\chi_p| \leq C_1|p|^{-1}.$$

Hence, (8.18) implies that

$$\lim_{p\to\infty}\sup_{x\in\mathbb{R}^n}|(H-\lambda I)\varphi_p(x)| = 0.$$

However,

$$\begin{aligned}\frac{\|(H-\lambda I)\varphi_p\|^2}{\|\varphi_p\|^2} &= C^{-1}p^{-n/2}\|(H-\lambda I)\psi\|^2\\ &\leq C_2 p^{-n/2}\cdot[\operatorname{meas}(\operatorname{supp}\chi_p)]^2\sup|(H-\lambda I)\varphi_p(x)|^2\\ &\leq C_3\sup|(H-\lambda I)\varphi_p(x)|^2 \to 0,\end{aligned}$$

and we conclude. □

Under further assumptions on the potential on can prove the absence of positive eigenvalues (with L^2-eigenfunctions). The following result is due to Kato.

Theorem 8.24. *Let $V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^n)$ and*

$$\lim_{|x|\to\infty}|x|V(x) = 0.$$

Then H has no positive eigenvalues, i.e. if $H\psi = \lambda\psi$ with $\lambda > 0$ and $\psi \in D(H)$, then $\psi = 0$.

Let us point out that $\lambda = 0$ may be an eigenvalue (not isolated).

Example 8.25. Let $\psi \in C^\infty(\mathbb{R}^n)$ be a function such that $\psi(x) = |x|^{2-n}$ if $|x| \geq 1$, and $\psi(x) > 0$ everywhere. Clearly, $\psi \in L^2(\mathbb{R}^n)$ provided $n \geq 5$. Set $V(x) = [\Delta\psi(x)]/\psi(x)$. Then $V \in C_0^\infty(\mathbb{R}^n)$ and ψ is an eigenfunction of $H = -\Delta + V$ with the eigenvalue 0.

We mention now a general result on location of essential spectrum — the so-called Persson theorem.

Theorem 8.26. *Let $V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^n)$ and $V(x) \geq -C$. Then*

$$\inf\sigma_{\mathrm{ess}}(H) = \sup[\inf\{\frac{(H,\psi,\psi)}{\|\psi\|^2} : \psi \in C_0^\infty(\mathbb{R}^n\setminus K), \psi \neq 0\}],$$

K runs over all compact subsets of $\mathbb{R}^n$.

Remark that here infimum is exactly the bottom of the spectrum of $-\Delta + V(x)$ in $L^2(\mathbb{R}^n \setminus K)$ with the Dirichlet boundary condition. The proof can be found in [6].

8.4 Decay of eigenfunctions

As usual, we assume here that $V \in L^\infty_{\text{loc}}(\mathbb{R}^n)$ and $V(x) \geq -C$.

Theorem 8.27. *Assume that*

$$\lim_{x\to\infty} \inf V(x) \geq a.$$

Let ψ be an eigenfunction of H with the eigenvalue $\lambda < a$. Then for every $\epsilon > 0$ there exists $C_\epsilon > 0$ such that

$$|\psi(x)| \leq C_\epsilon \exp[-\sqrt{\frac{a-\lambda-\epsilon}{2}}|x|]. \tag{8.19}$$

Corollary 8.28. *If $V(x) \to +\infty$ as $|x| \to \infty$, then*

$$|\psi(x)| \leq C_a e^{-a|x|}$$

for every $a > 0$.

Remark 8.29. Estimate (8.19) can be improved. In fact,

$$|\psi(x)| \leq C_2 \exp[-\sqrt{(a-\lambda-\epsilon)}|x|].$$

Proof of Theorem 8.27. First recall some facts about fundamental solution of $-\Delta + k^2$, i.e. a solution of

$$-\Delta\mathcal{E}_k + k^2\mathcal{E}_k = \delta(x).$$

There exists such a solution with the property that $\mathcal{E}_k \in C^\infty(\mathbb{R}^n \setminus \{0\})$ and the asymptotic behavior

$$\mathcal{E}_k(x) = c|x|^{-\frac{n-1}{2}} e^{-k|x|}(1 + O(1)), \quad x \to \infty,$$

where $c > 0$. Moreover, $\mathcal{E}_k$ is radially symmetric. In the case $n = 3$

$$\mathcal{E}_k(x) = \frac{1}{4\pi(x)} e^{-k|x|}.$$

Let ψ be a real valued eigenfunction

$$H\psi = \lambda\psi, \quad \lambda < a.$$

For the sake of simplicity, let us assume that V is smooth enough for large $|x|$. Then, due to the elliptic regularity, ψ is smooth for same x, i.e. ψ is a classical solution. One has

$$\Delta(\psi^2) = 2\Delta\psi \cdot \psi + 2(\nabla\psi)^2.$$

Therefore,
$$-\Delta(\psi^2) = 2(\lambda - V(x))\psi^2 - 2(\nabla\psi)^2.$$
Hence (add simply $2(b-\lambda)\psi^2$ to the both sides),
$$[-\Delta + 2(b-\lambda)]\psi^2 = -2(V(x)-b)\psi^2 - 2(\nabla\psi)^2.$$
We assume here that $b < a$ and, hence, the right hand part is nonnegative for $|x|$ large enough.

Set
$$u(x) = \psi^2 - M\mathcal{E}_k(x)$$
with $k = \sqrt{2(b-\lambda)}$ (here $\lambda < b < a$). Choose R such that $\mathcal{E}_k(x) \geq 0$, $V(x) > b$ and $\psi(x)$ is smooth for $|x| \geq R$. Next choose $M > 0$ such that
$$u(x) < 0, \quad |x| = R$$
(this is possible due to continuity of $\mathcal{E}(x)$ and $\psi(x)$ on the sphere $|x| = R$).

Obviously
$$-\Delta u + k^2 u = f \leq 0, \quad |x| \geq R.$$
Here
$$f = -2(V(x)-b)\psi^2 - 2(\nabla\varphi)^2.$$
Set
$$u_\epsilon(x) = \int_{\mathbb{R}^n} u(x-y)\varphi_\epsilon(u)dy,$$
where $\varphi_\epsilon(x) = \epsilon^{-n}\varphi(x/\epsilon)$, $\varphi \in C_0^\infty(\mathbb{R}^n)$, $\varphi \geq 0$ and
$$\int_{\mathbb{R}^n} \varphi dx = 1.$$
Enlarging R, if necessary, we have
$$(-\Delta + k^2)u_\epsilon = f_\epsilon \leq 0.$$
Since $u \in L^1(\mathbb{R}^n)$, $u_\epsilon(x) \to 0$ as $|x| \to \infty$ (check this). Let
$$\Omega_{R,\rho} = \{x : R \leq |x| \leq \rho\}$$
and
$$M_\rho(\epsilon) = \max_{|x|=\rho} |u_\epsilon(x)|.$$
Clearly, $u_\epsilon(x) < 0$ if $|x| = R$ and ϵ is small enough. By the maximum principle, we have
$$u_\epsilon(x) \leq M_\rho(\epsilon), \quad x \in \Omega_{R,\rho}$$
Letting $p\rho \to \infty$, we get $u_\epsilon(x) \leq 0$, if $|x| \geq \mathbb{R}$. Passing to the limit as $\epsilon \to 0$, we see that $u(x) \leq 0$ if $|x| \geq R$ and this implies the required. $\square$

Remark 8.30. Assume that the potential has a power growth of infinity:

$$V(x) \geq c|x|^{\alpha} - c_1,$$

where $c > 0$, $c_1 \in \mathbb{R}$ and $\alpha > 0$. Then for each eigenfunction ψ one has

$$|\psi(x)| \leq C \exp(-a|x|^{\frac{\alpha}{2}+1}).$$

with some $C > 0$ and $a > 0$ [2].

8.5 Agmon's metric

Let $x \in \mathbb{R}^n$ and $\xi, \eta \in \mathbb{R}^n$ (more precisely, we should consider ξ, η as tangent vectors at x). For the sake of simplicity we assume that the potential V is continuous. Define a (degenerate) inner product

$$\langle \xi, \eta \rangle_x = (V(x) - \lambda)_+ \langle \xi, \eta \rangle,$$

where $\langle \cdot, \cdot \rangle$ is the standard Euclidean inner product on $\mathbb{R}^n$ and $u(x)_+ = \max\{u(x), 0\}$. This is the *Agmon metric* on $\mathbb{R}^n$. Certainly, the Agmon metric is degenerate and depends on $V(x)$ and λ.

Let $\gamma : [0, 1] \to \mathbb{R}^n$ be a smooth path in $\mathbb{R}^n$. We define the Agmon length of γ as

$$L_A(\gamma) = \int_0^1 \|\gamma'(t)\|_{\gamma(t)} dt,$$

where $\|\xi\|_x = \langle \xi, \xi \rangle_x^{1/2}$. More explicitly,

$$L_A(\gamma) = \int_0^1 (V(\gamma|t|) - \lambda)_x^{1/2} \|\gamma'(t)\| dt$$

where $\|\xi\|$ is the standard Euclidean norm in $\mathbb{R}^n$. A path γ is a geodesic if it minimizes the length functional $L_A(\gamma)$.

Given a potential V and energy level λ, the distance between $x, y \in \mathbb{R}^n$ in the Agmon metric is

$$\rho_\lambda(x, y) = \inf\{L_A(\gamma) : \gamma \in P_{x,y}\},$$

where $P_{x,y} = \{\gamma : [0, 1] \to \mathbb{R}^n : \gamma(0) = x, \gamma(1) = y, \gamma \in C^1([0, 1])\}$.

Exercise 8.31. ρ_λ is a distance function.

Exercise 8.32. $\rho_\lambda(x, y)$ is locally Lipschitz continuous, hence, differentiable a. e. in x and y. At the points where it is differentiable

$$|\nabla_y \rho_\lambda(x, y)| \leq (V(y) - \lambda)_+.$$

Using Agmon metrics one can obtain an anisotropic estimate of decay of eigenfunctions. For simplicity we will prove such an estimate in L^2 form only.

Theorem 8.33. *Assume that $V \in C(\mathbb{R}^n)$ and $V(x) \geq -C$. Suppose λ is an eigenvalue of H and $\operatorname{supp}(\lambda - V(x))_+$ is a compact subset of $\mathbb{R}^n$. Let ψ be an eigenfunction with the eigenvalue λ. Then, for any $\epsilon > 0$ there exists a constant $c_\epsilon > 0$ such that*

$$\int_{\mathbb{R}^n} e^{2(1-\epsilon)\rho_\lambda(x)} |\psi(x)|^2 dx \leq c_\epsilon \tag{8.20}$$

where $\rho_\lambda(x) = \rho_\lambda(x, 0)$.

Remark 8.34. Our assumption on $(\lambda - V)_+$ implies that $\lambda < \inf \sigma_{\text{ess}}(H)$.

Lemma 8.35. *Let $f(x) = (1-\epsilon)\rho_\lambda(x), f_\alpha = f(1+\alpha f)^{-1}, \alpha > 0$, and $\varphi \in H^1(\mathbb{R}^n)$ be such that*

$$\int_{\mathbb{R}^n} |V(x)\varphi(x)|^2 dx < \infty$$

and

$$\operatorname{supp} \varphi \subset F_{\lambda,\delta} = \{x : V(x) - \lambda > \delta\}.$$

Then there exists $\delta_1 > 0$ such that

$$\operatorname{Re} \int_{\mathbb{R}^n} [\nabla(e^{f_\alpha}\varphi)\nabla(e^{-f_\alpha}\overline{\varphi}) + (V-\lambda)|\varphi|^2] dx \geq \delta_1 \|\varphi\|^2. \tag{8.21}$$

Proof. Direct calculation shows that the left-hand part of (8.2) is

$$\int_{\mathbb{R}^n} [|\nabla\varphi|^2 - |\nabla f_\alpha|^2 |\varphi|^2 + (V-\lambda)|\varphi|^2] dx \geq \ (\varphi, (V - \lambda - |\nabla f_\alpha|^2)\varphi^2).$$

Next

$$|\nabla f_\alpha|^2 = |\nabla f|^2 (1+\alpha f)^{-4} \leq |\nabla f|^2 = (1-\epsilon)^2 |\nabla \rho_\lambda(x)|^2$$
$$\leq (1-\epsilon)(V(x) - \lambda)_+.$$

Since $\operatorname{supp}\varphi \subset F_{\lambda,\delta}$, one has $V(x) - \lambda > \delta$ on $\operatorname{supp}\varphi$. Thus

$$\begin{aligned} (\varphi, (V - \lambda - |\nabla f_\alpha|^2)\varphi) &\geq (\varphi, (V-\lambda)\varphi - (1-\epsilon)(V-\lambda)_+\varphi) \\ &= (\varphi, (V-\lambda)\varphi - (1-\epsilon)(V-\lambda)\varphi) = (\varphi, \epsilon(V-\lambda)\varphi) \geq \epsilon\delta(\varphi,\varphi). \end{aligned} \tag{8.22}$$

∎

Lemma 8.36. *Let η be a smooth bounded function such that $|\nabla\eta|$ is compactly supported and*

$$\varphi = \eta\psi\exp(f_\alpha),$$

where $H\psi = \lambda\psi$. Then

$$\operatorname{Re}\int_{\mathbb{R}^n}[\nabla(e^{f_\alpha}\varphi)\nabla(e^{-f_\alpha}\overline{\varphi}) + (V-\lambda)|\varphi|^2]dx = \int_{\mathbb{R}^n}\xi e^{2f_\alpha}|\psi|^2dx, \tag{8.23}$$

where $\xi = |\nabla\eta|^2 + 2 < \nabla\eta, \nabla f_\alpha > \eta$.

Proof. Since $|f_\alpha(x)| \leq 1$, then $e^{f_\alpha}\varphi \in L^2(\mathbb{R}^n)$. One has

$$\begin{aligned}
&\int_{\mathbb{R}^n}[\nabla(e^{f_\alpha}\varphi)\nabla(e^{-f_\alpha}\overline{\varphi}) + V|\varphi|^2 - \lambda|\varphi|^2]dx \\
&\quad= \int_{\mathbb{R}^n}[\nabla(e^{2f_\alpha}\eta\psi)\nabla(\eta\overline{\psi}) + (V-\lambda)(e^{2f_\alpha}\eta\psi)(\eta\overline{\psi})]dx \\
&\quad= \int_{\mathbb{R}^n}[\nabla(e^{2f_\alpha}\eta^2\psi)\nabla\overline{\psi} + (V-\lambda)(e^{2f_\alpha}\eta^2\psi)\overline{\psi}]dx \\
&\qquad\qquad + \int_{\mathbb{R}^n}[(\nabla(e^{2f_\alpha}\eta\psi)\nabla\eta)\overline{\psi} - (e^{2f_\alpha}\eta\psi)\nabla\eta\nabla\overline{\psi}]dx.
\end{aligned} \tag{8.24}$$

We used here the identity

$$\nabla(e^{2f_\alpha}\eta\psi)\nabla(\eta\overline{\psi} = \nabla(e^{2f_\alpha}\eta^2\psi)\nabla\overline{\psi} + [\nabla(e^{2f_\alpha}\eta\psi)\nabla\eta]\overline{\psi} - (e^{2f_\alpha}\eta\psi)\nabla\eta\nabla\overline{\psi}.$$

Since $H\psi = \lambda\psi$, the first integral in the right since of (8.24) vanishes. Calculating $\nabla(e^{2f_\alpha}\eta\psi)$, we obtain from (8.24)

$$\begin{aligned}
&\int_{\mathbb{R}^n}[\nabla(e^{f_\alpha}\varphi)\nabla(e^{-f_\alpha}\overline{\varphi}) + V|\varphi|^2 - \lambda|\varphi|^2]dx \\
&\quad= \int_{\mathbb{R}^n}[2e^{2f_\alpha}\eta(\nabla\eta\cdot\nabla f_\alpha)\psi\overline{\psi} + e^{2f_\alpha}(\nabla\eta\cdot\nabla\eta)\psi\overline{\psi} \\
&\qquad\qquad + e^{2f_\alpha}\eta(\nabla\cdot\nabla\psi)\cdot\overline{\psi} - e^{2f_\alpha}\eta(\nabla\eta\cdot\nabla\overline{\psi})\cdot\psi]dx.
\end{aligned} \tag{8.25}$$

Taking the real part, we obtain the required. ☐

Proof of Theorem 8.33. We set

$$F_{\lambda,2\delta} = \{x \in \mathbb{R}^n : V(x) - \lambda > 2\delta\}, \tag{8.26}$$
$$A_{\lambda,\delta} = \{x \in \mathbb{R}^n : V(x) - \lambda < \delta\}. \tag{8.27}$$

Choose, $\eta \in C^\infty$ such that $\eta(x) = 1$ on $F_{\lambda,2\delta}$ and $\eta(x) = 0$ on $A_{\lambda,\delta}$. Clearly, $\mathrm{supp}|\nabla\eta|$ is compact. Take f, f_α and φ as before. By Lemmas 8.33 and 8.34,

$$
\begin{aligned}
\delta_1\|\varphi\|^2 &\leq \mathrm{Re}\int_{\mathbb{R}^n}[\nabla(e^{f_\alpha}\varphi)\nabla(e^{-f_\alpha}\overline{\varphi}) + (V-\lambda)|\varphi|^2]dx \\
&\leq |\int_{\mathbb{R}^n}\xi e^{2f_\alpha}|\psi|^2dx| \leq [\sup_{x\in\mathrm{supp}|\nabla\eta|}|\xi e^{2f_\alpha}|]\|\psi\|^2.
\end{aligned} \tag{8.28}
$$

Since $\mathrm{supp}|\nabla\eta| = \mathbb{R}^n \setminus (F_{\lambda,2\delta} \cup A_{\lambda,\delta})$ is compact, one can pass to the limit as $\alpha \to 0$ in (8.28). Thus

$$
\|e^{f_\alpha}\eta\psi\|^2 \leq c_\epsilon, \tag{8.29}
$$

where $c_\epsilon > 0$ is independent of $\alpha \geq 0$. Now we can take $\alpha = 0$ in (8.29).

Since $\mathrm{supp}|\nabla\eta| \cup \overline{A}_{\lambda,\delta}$ is compact, the integral

$$
\int_{\mathrm{supp}|\nabla\eta|\cup\overline{A}_{\lambda,\delta}} e^{2f}|\psi|^2dx < \infty.
$$

Hence, due to (8.29)

$$
\int_{\mathbb{R}^n} e^{2(1-\epsilon)\rho_\lambda(x)}|\psi(x)|^2dx \leq [\int_{\{\eta(x)=1\}} = \int_{\mathrm{supp}|\nabla\eta|\cup\overline{A}_{\lambda,\delta}}]e^{2f}|\psi|^2dx \leq c_\epsilon,
$$

with new c_ϵ. □

Remark 8.37. In fact, one can prove the following pointwise bound

$$
|\psi(x)| \leq c_\epsilon e^{-(1-\epsilon)\rho_\lambda(x)}.
$$

9 Periodic Schrödinger operators

We consider now Schrödinger operators $-\Delta + V(x)$, where V is a periodic function. That is, we assume that for some basis $\{e_i\} \subset \mathbb{R}^N$

$$V(x + e_i) = V(x), \quad i = 1, \ldots, N.$$

Such operators appear,e.g., in solid state physics. More details can be found in [10]. For classical theory of one-dimensional periodic operators see [5].

9.1 Direct integrals and decomposable operators

Let $\mathcal{H}'$ be a separable Hilbert space and (M, μ) a σ-finite measure space. Let $\mathcal{H} = L^2(M, d\mu, \mathcal{H}')$ be the Hilbert space of square integrable $\mathcal{H}'$-valued functions. Now we rename this space by *constant fiber direct integral* and write as

$$\mathcal{H} = \int_M^{\oplus} \mathcal{H}' d\mu.$$

If μ is a sum of point measures at points $m_1, m_2, \ldots, m_k$, then each $f \in L^2(M, d\mu, \mathcal{H}')$ is completely determined by $(f(m_1), f(m_2), \ldots, f(m_k))$ and, in fact, $\mathcal{H}$ is isomorphic to the direct sum of k copies of $\mathcal{H}'$. In a sense, $L^2(M, d\mu, \mathcal{H}')$ is a kind of "continuous direct sum".

A function $A(\cdot)$ from M to $L(\mathcal{H}')$ is called *measurable* if for each $\varphi, \psi \in \mathcal{H}'$ the scalar valued function $(\varphi, A(m)\psi)$ is measurable. $L^\infty(m, d\mu, L(\mathcal{H}'))$ stands for the space of such functions with

$$\|A\|_\infty = \text{ess sup} \|A(m)\|_{L(\mathcal{H}')} < \infty.$$

A bounded linear operator A in $\mathcal{H}$ is said to be a *decomposable operator* (by means of direct integral) if there is an $A(\cdot) \in L^\infty(M, d\mu, L(\mathcal{H}'))$ such that

$$(A\psi)(m) = A(m)\psi(m).$$

We write in this case

$$A = \int_M^{\oplus} A(m) d\mu(m).$$

The $A(m)$ are called the *fibers* of A.

Notice that every $A(\cdot) \in L^\infty(M, d\mu, L(\mathcal{H}))$ is associated with some decomposable operator. Moreover,

$$\|A\|_{L(\mathcal{H})} = \|A(\cdot)\|_\infty.$$

In fact, we have an isometric isomorphism of the algebra $L^\infty(M, d\mu, L(\mathcal{H}'))$ and the algebra of all decomposable operators. $L^\infty(M, d\mu, \mathbb{C})$ is a natural subalgebra of $L^\infty(M, d\mu, L(\mathcal{H}'))$. Its image $\mathcal{A}$ consists of those decomposable operators whose fibers are all multiples of the identity.

Proposition 9.1. *$A \in L(\mathcal{H})$ is decomposable iff A commutes with each operator in $\mathcal{A}$.*

A function $A(\cdot)$ from M to the set of all (not necessary bounded) self-adjoint operators in $\mathcal{H}'$ is called *measurable* if the function $(A(\cdot) + iI)^{-1}$ is measurable. Given such $A(\cdot)$, we define an operator A on $\mathcal{H}$ with domain

$$D(A) = \{\psi \in \mathcal{H} : \psi(m) \in D(A(m)) \text{ a. e. } ; \int_M \|A(m)\psi(m)\|^2 d\mu(m) < \infty\}$$

by

$$(A\psi)(m) = A(m)\psi(m)$$

We write

$$A = \int_M^\oplus A(m) d\mu$$

Let us summarize some properties of such operators

Theorem 9.2. *Let$A = \int_M^\oplus A(m)d\mu$, where $A(\cdot)$ is measurable and $A(m)$ is self-adjoint for each m. Then:*

(a) A is self-adjoint.

(b) For any bounded Borel function F on $\mathbb{R}$

$$F(A) = \int_M^\oplus F(A(m)) d\mu.$$

(c) $\lambda \in \sigma(A)$ if and only if for all $\epsilon > 0$

$$M(\{m : \sigma(A(m)) \cap (\lambda - \epsilon, \lambda + \epsilon) \neq \emptyset\}) > 0.$$

(d) λ is an eigenvalue of A if and only if

$$M(\{m : \lambda \text{ is an eigenvalue of } A(m)\}) > 0.$$

(e) If each $A(m)$ has purely absolutely continuous spectrum, then so does A.

(f) *Suppose that $B = \int_M^{\oplus} B(m)d\mu$ with each $B(m)$ self-adjoint. If B is A-bounded with A-bound a, then $B(m)$ is $A(m)$ bounded with $A(m)$-bound $a(m) \leq a$. If $a < 1$, then*

$$A + B = \int_M^{\oplus} (A(m) + B(m))d\mu$$

is self-adjoint on $D(A)$.

We explain here only some points of the theorem.

(a) It is easy to verify that A is symmetric. So, by Proposition 8.2, we need only to check that $\operatorname{im}(A \pm iI) = \mathcal{H}$. Let $C(m) = (A(m) + iI)^{-1}$. $C(m)$ is measurable and $\|C(m)\| \leq 1$ (prove it). Hence, $C = \int_M^{\oplus} C(m)d\mu$ is a well-defined bounded operator. Let $\psi = C\eta$, $\eta \in \mathcal{H}$. Then, $\psi(m) \in \operatorname{im} C(m) = D(A(m))$ a. e. and

$$\|A(m)\psi(m)\| = \|A(m)C(m)\eta(m)\| \leq \|\eta(m)\| \in L^2(d\mu)$$

(the last inclusion is not trivial!). So, $\psi \in D(A)$. Moreover, $(A + iI)\psi = \eta$. Similarly, one checks that $\operatorname{im}(A - iI) = \mathcal{H}$.

(c) Let $P_\Delta(A)$ be the spectral projector of A associated with an interval Δ. We know that $P_\Delta(A) = \chi_\delta(A)$, where $\chi_\Delta(\lambda)$ is the characteristic function of Δ. By (b), we have

$$P_\Delta(A) = \int_M^{\oplus} P_\Delta(A(m))d\mu.$$

Now we need only to remark that $\lambda \in \sigma(A)$ iff $P_{(\lambda-\epsilon,\lambda+\epsilon)}(A) \neq 0$.

(d) Similar to (c).

9.2 One dimensional case

Consider the operator

$$H = -\frac{d}{dx^2} + V(x),$$

where $V(x)$ is a 2π-periodic function, $V \in L^\infty(\mathbb{R})$. Let $\mathcal{H}' = L^2(0, 2\pi)$ and

$$\mathcal{H} = \int_{[0,2\pi)}^{\oplus} \mathcal{H}' \frac{d\theta}{2\pi}$$

Consider the operator $U : L^2(\mathbb{R}) \to \mathcal{H}$ defined by

$$(Uf)_\theta(x) = \sum_{n\in\mathbb{Z}} e^{-i\theta n} f(x + 2\pi n). \tag{9.1}$$

U is well-defined for $f \in C_0^\infty(\mathbb{R})$, since the sum is convergent. We have

$$\begin{aligned}
&\int_0^{2\pi} \Big(\int_0^{2\pi} |\sum_n e^{-in\theta} f(x+2\pi n)| dx\Big) \frac{d\theta}{2\pi} \\
&\quad = \int_0^{2\pi} [(\sum_n \sum_j \overline{f(x+2\pi n)} f(x+2\pi j)) \int_0^{2\pi} e^{-i(j-n)\theta} \frac{d\theta}{2\pi}] dx \\
&\qquad = \int_0^{2\pi} (\sum_n |f(x+2\pi n)|^2) dx = \int_{-\infty}^{\infty} |f(x)|^2 dx.
\end{aligned}$$

Thus, U has a unique extension to an isometric operator.

Next, we show that U is a unitary operator. By means of direct calculation we see that

$$(U^* g)(x+2\pi n) = \int_0^{2\pi} e^{in\theta} g_\theta(x) \frac{d\theta}{2\pi}$$

for $g \in \mathcal{H}$. It is also not difficult to verify that $\|U^* g\|^2 = \|g\|^2$.

The operator U is the so-called *Floquet transform*.

Denote by L the self-adjoint operator in $L^2(\mathbb{R})$ generated by $-d^2/dx^2$. For $\theta \in [0, 2\pi)$ we consider the self-adjoint operator L_θ in $L^2(0, 2\pi)$ generated by $-d^2/dx^2$ with the boundary conditions

$$\psi(2\pi) = e^{i\theta}\psi(0), \psi'(2\pi) = e^{i\theta}\psi'(0).$$

We have

$$ULU^{-1} = \int_{[0,2\pi)}^{\oplus} L_\theta \frac{d\theta}{2\pi}. \tag{9.2}$$

Let A be the operator on the right-hand side of (9.2). We shall show that if $f \in C_0^\infty(\mathbb{R})$, then $Uf \in D(A)$ and $U(-f'') = A(Uf)$. Since $-d^2/dx^2$ is essentially self-adjoint on C_0^∞ and A is self-adjoint, (9.2) will follow.

So, suppose $f \in C_0^\infty(\mathbb{R})$. Then Uf is given by the convergent sum (9.1). Hence, $Uf \in C^\infty$ on $(0, 2\pi)$ with $(Uf)'_\theta(x) = (Uf')_\theta(x)$ (similarly for higher derivatives). Moreover,

$$(Uf)_\theta(2\pi) = \sum_n e^{-i\theta n} f(2\pi(n+1)) = \sum_n e^{-i\theta(n-1)} f(2\pi n) = e^{i\theta}(Uf)_\theta(0).$$

Similarly, $(Uf)'(2\pi) = e^{i\theta}(Uf)'(0)$. Thus, for each θ, $(Uf) \in D(L_\theta)$ and

$$L_\theta(Uf) = U(-f'')_\theta.$$

Hence, $Uf \in D(A)$ and $A(Uf) = U(-f'')$.

Now let

$$H_\theta = L_\theta + V(x)$$

considered as an operator in $L^2(0, 2\pi)$

Theorem 9.3.

$$UHU^{-1} = \int_{[0,2\pi)}^{\oplus} H_\theta \frac{d\theta}{2\pi}$$

Proof. In view of (9.2), it is enough to show that

$$UVU^{-1} = \int_{[0,2\pi)}^{\oplus} V_\theta \frac{d\theta}{2\pi},$$

where V_θ is an operator (θ-independent) on the fiber $L^2(0, 2\pi)$ defined by

$$(V_\theta f)(x) = V(x)f(x), \quad x \in (0, 2\pi).$$

One has

$$\begin{aligned}(UVf)_\theta(x) &= \sum_n e^{-in\theta} V(x + 2\pi n) f(x + 2\pi n) \\ &= V(x) \sum_n e^{-in\theta} f(x + 2\pi n) = V_\theta (Uf)_\theta(x).\end{aligned}$$

Thus, we conclude. □

Now we remark that the operator $L_\theta + I$ is invertible. The inverse $K_\theta = (L_\theta + I)^{-1}$ can be found explicitly:

$$(K_\theta u)(x) = \int_0^{2\pi} G_\theta(x, y) u(y) dy,$$

where

$$\begin{aligned}G_\theta(x, y) = \frac{1}{2} e^{-|x-y|} + \alpha(\theta) e^{x-y} + \beta(\theta) e^{y-x},\\ \alpha(\theta) = \frac{1}{2}(e^{2\pi - i\theta} - 1)^{-1},\\ \beta(\theta) = \frac{1}{2}(e^{2\pi - i\theta} - 1)^{-1}.\end{aligned}$$

This implies that K_θ is compact and depends analytically on θ in a neighborhood of $[0, 2\pi]$.

Since L_θ depends analytically on θ, so does H_θ. Moreover, H_θ has a compact resolvent. Hence, the spectrum of H_θ is discrete and consists of eigenvalues $\lambda_1(\theta) \leq \lambda_2(\theta) \leq \ldots$. Due to Theorem 9.2(c), we see that $\sigma(H)$ is a union of intervals

$$[\inf \lambda_k(\theta), \sup \lambda_K(\theta)]$$

(this is the so-called *band structure* of spectrum). Since H is bounded below, $\sigma(H)$ the complement of the union intervals $(-\infty, a_0), (a_1, b_1), (a_2, b_2), \ldots$, with $b_i < a_{i+1}$. Finite intervals (a_1, b_1), $i \geq 1$, are called *spectral gaps*.

One can prove similar results in multidimensional case as well. However, in one dimensional case one can obtain much more information.

First, remark that $H(\theta)$ and $H(2\pi - \theta)$ are antiunitary equivalent under complex conjugation. Therefore $\lambda_k(\theta) = \lambda_k(2\pi - \theta)$. Next, one can prove that eigenvalues $\lambda_k(\theta), \theta \in (0, \pi)$, are nondegenerate, hence, depend analytically on $\theta \in (0, \pi)$. In fact, $\lambda_k(\theta)$ can be analytically continued through $\theta = 0$ and $\theta = \pi$. However, such the continuation may coincide with $\lambda_{n+1}(\theta)$ or $\lambda_{n-1}(\theta)$ if $\lambda(\theta)$ (resp. $\lambda(\pi)$) is a double eigenvalue (only double degeneration may occur).

Moreover, for k odd (resp. even) $\lambda_n(\theta)$ is strictly monotone increasing (resp. decreasing) on $(0, \pi)$. Therefore,

$$\begin{aligned}\lambda_1(0) < \lambda_1(\pi) \leq \lambda_2(\pi) < \lambda_2(0) \leq \ldots \\ \leq \lambda_{2n-1}(0) < \lambda_{2n-1}(\pi) \leq \lambda_{2n}(\pi) < \lambda_{2n}(0) \leq \ldots\end{aligned}$$

Intervals (bands) $[\lambda_{2n-1}(0), \lambda_{2n-1}(\pi)]$ and $[\lambda_{2n}(\pi), \lambda_{2n}(0)]$ form the spectrum. They can touch, but cannot overlap. In 1-dimensional case the following is also known:

(a) *If no gaps are present, then $V = const$.*

(b) *If precisely one gap opens up, then, V is a Weierstrass elliptic function.*

(c) *If all odd gaps are absent, then V is π-periodic.*

(d) *If only finitely many gaps are present, then V is a real analytic function.*

(e) *In the space of all 2π-periodic C^∞ functions the set of potentials V, for which all gaps are open, is a massive (hence, dense) set.*

9.3 Multidimensional case

Consider the operator $H = -\Delta + V(x)$ on $\mathbb{R}^N$. $V(x)$ is 2π-periodic in $x_i, i = 1, \ldots, N, V \in C(\mathbb{R}^N)$ (for the sake of simplicity), $V(x) \geq -C$. In this case one can define the Floquet transform

$$(Uf)_\theta(x) = \sum_{n \in \mathbb{Z}^N} e^{-i\theta \cdot n} f(x + 2\pi n),$$

where $\theta \in [0, 2\pi)^N, x \in (0, 2\pi)^N$. The operator L_θ in $L^2((0, 2\pi)^N)$ is now defined as $-\Delta$ with boundary conditions

$$\psi(x_1, \ldots, x_{k-1}, 2\pi, x_{k+1}, \ldots, x_N) = e^{i\theta_k}\psi(x_1, \ldots, x_{k-1}, 0, x_{k+1}, \ldots, x_N)$$
$$\psi_{x_k}(x_1, \ldots, x_{k-1}, 2\pi, x_{k+1}, \ldots, x_N) = e^{i\theta_k}\psi_{x_k}(x_1, \ldots, x_{k-1}, 0, x_{k+1}, \ldots, x_N).$$

Another way is to consider L_θ on the subspace of $L^2_{\mathrm{loc}}(\mathbb{R}^N)$ that consists of functions satisfying Bloch condition

$$\psi(x + 2\pi n) = e^{i\theta\cdot n}\psi(x), \quad n \in \mathbb{Z}^N.$$

The Floquet transform again decomposes H and gives rise to a band structure of the spectrum. However, H_θ may have multiple eigenvalues and the bands may overlap, in contrast to 1-dimensional case. Under some not so restrictive assumptions on V it is known that, in the case $N = 2, 3$, a generic H can have only a finite number of gaps. This is also in the contrast to 1-dimensional case.

Nevertheless, in all dimensions the spectrum of H is absolutely continuous.

Now let us discuss the so-called integrated density of states. First consider the spectral function $e(\lambda; x, y)$. The spectral projector E_λ turns out to be an integral operator. Its kernel function $e(\lambda; x, y)$ is just the *spectral function* of H. In the case of interest $e(\lambda; \cdot, \cdot)$ is a continuous function on $\mathbb{R}^N \times \mathbb{R}^N$. Moreover, it is periodic along the diagonal, i. e.

$$e(\lambda; x + 2\pi n, y + 2\pi n) = e(\lambda; x, y).$$

By definition, the *integrated density of states* $N(\lambda)$ is the mean value of $e(\lambda; x, x)$, i.e.

$$N(\lambda) = \frac{1}{\operatorname{meas} K}\int_K e(\lambda; x, x)dx,$$

where $K = [0, 2\pi]^N$. $N(\lambda)$ is a nondecreasing function which is equal to zero for $\lambda < \inf \sigma(H)$ and constant on each gap of the spectrum. Moreover, $\sigma(A)$ coincides with the set of growth points of $N(\lambda)$.

One can express $N(\lambda)$ in terms of band functions $\lambda_k(\theta)$:

$$N(\lambda) = (2\pi)^{-N}\sum_{k=1}^{\infty}\operatorname{meas}\{\theta \in K : \lambda_k(\theta) \le \lambda\} = (2\pi)^{-N}\int_K N_\theta(\lambda)d\theta.$$

Here $N_\theta(\lambda)$ is the ordinary distribution function for the discrete spectrum of H_θ,

$$N_\theta(\lambda) = \#\ \text{eigenvalues of } H_\theta \text{ below } \lambda.$$

If $V = 0$, then

$$N(\lambda) = (2\pi)^{-N} v_N \lambda^{N/2} \theta(\lambda),$$

where v_N is the volume of unit ball in $\mathbb{R}^N$ and $\theta(\lambda)$ is the Heaviside function.

One can give another description of $N(\lambda)$ as follows. Let

$$\Omega_n = \{x \in \mathbb{R}^N : |x_j| \leq \pi n, j = 1, \dots, N\}.$$

Consider the operator H_n defined on Ω_n by $-\Delta + V(x)$ with periodic boundary conditions (precisely, $2\pi n$-periodic). The operator H_n is self-adjoint in $L^2(\Omega_n)$ and has discrete spectrum. Denote by $N_n(\lambda)$ the ordinary distribution function for eigenvalues of H_n. Then

$$N(\lambda) = \lim_{n\to\infty} \frac{1}{\operatorname{meas} \Omega_n} N_n(\lambda). \tag{9.3}$$

Moreover, let $G_n(t, x, y)$ be the Green function of parabolic operator $\partial/\partial t - H_n$ on $(0, \infty) \times \Omega_n$ with periodic boundary conditions and $G(t, x, y)$ the fundamental solution of the Cauchy problem for $\partial/\partial t - H$. One can verify that

$$G(t, x + 2\pi k, y + 2\pi k) = G(t, x, y), \quad k \in \mathbb{Z}^N.$$

Consider the Laplace transforms of N and N_n:

$$\tilde{N}(t) = \int_{-\infty}^{\infty} e^{-\lambda t} dN(\lambda), \qquad t > 0,$$
$$\tilde{N}(t) = \int_{-\infty}^{\infty} e^{-\lambda t} dN_n(t), \qquad t > 0.$$

Then

$$\tilde{N}_n(t) = \frac{1}{\operatorname{meas} \Omega_n} \int_{\Omega_n} G_n(t, x, x) dx,$$
$$\tilde{N}(t) = \frac{1}{\operatorname{meas} K} \int_K G(t, x, x) dx =: M_x(G(t, x, x))$$

and $\tilde{N}_N(t) \to \tilde{N}(t)$.

9.4 Further results

Consider the case of almost periodic (a. p.) potential. A bounded continuous function $f(x)$ is said to be *almost periodic* if the set of its translations $\{f(\cdot + y)\}_{y \in \mathbb{R}^N}$ is precompact in the space $C_b(\mathbb{R}^N)$ of bounded continuous functions. The *mean value* of such f is defined by

$$M(f) = \lim_{R\to\infty} \frac{1}{R^N} \int_{|x_j| \leq R/2} f(x) dx.$$

(The existence of the limit here is a deep theorem). Denote by $CAP(\mathbb{R}^N)$ the space of all such functions.

If $V \in CAP(\mathbb{R}^N)$, then $-\Delta + V$ is essentially self-adjoint operator in $L^2(\mathbb{R}^N)$. Let H be the corresponding self-adjoint operator.

Let us consider another operator generated by $-\Delta + V(x)$. In the space $CAP(\mathbb{R}^N)$ we introduce an inner product $(f,g)_B = M(f \cdot \overline{g})$ and corresponding norm $\|\cdot\|_B$ (one can show that $\|f\|_B = 0, f \in CAP(\mathbb{R}^N)$, implies that $f = 0$.) The space $CAP(\mathbb{R}^N)$ is incomplete with respect to this norm. The completion $B^2(\mathbb{R}^N)$ is called the *space of Besicovitch a. p. functions.* It turns out to be that $-\Delta + V(x)$ generates (in a unique way) a self-adjoint operator H_B in $B^2(\mathbb{R}^N)$. A deep theorem by M. Shubin states that $\sigma(H) = \sigma(H_B)$. Remark that the structure of these two spectra is different. For example, $-\Delta$ has continuous spectrum in $L^2(\mathbb{R}^N)$, but purely point spectrum in $B^2(\mathbb{R}^N)$: each function $e^{i\xi \cdot x}$ is an eigenfunction of $-\Delta$ in $B^2(\mathbb{R}^N)$ with the eigenvalue $|\xi|^2$.

In a. p. case the structure of spectrum become much more complicated, than in periodic case. In particular, we cannot introduce band functions. Let us discuss only few results in this direction. Recall that a perfect Cantor set (not necessary of measure 0) is a closed subset of $\mathbb{R}$ without isolated points, the complement of which is everywhere dense in $\mathbb{R}$. A *limit periodic function* is a uniform limit of periodic functions (of different periods).

Theorem 9.4. *In the space of all limit periodic functions (with the standard* sup*-norm) on $\mathbb{R}$ there exists a massive (hence, dense) set consisting of potentials V such that the spectrum $\sigma(H)$ of $H = -d^2/dx^2 + V(x)$ is a perfect Cantor set. The same is true in the space of potentials of the form*

$$V(x) = \sum_{n=0}^{\infty} a_n \cos \frac{x}{2n}, \quad \sum |a_n| < \infty.$$

This theorem was obtained by Avron and Simon. Moreover, one can find a dense set of limit periodic potentials such that $\sigma(H)$ is a perfect Cantor set and the spectrum is absolutely continuous of the multiplicity 2.

However, the spectrum does not always have to be absolutely continuous. Chulaevskii and Molchanov demonstrated that there are limit periodic potentials with pure point Cantor spectrum of Lebesgue measure 0. Corresponding eigenfunctions decay faster than any power of $|x|$ as $|x| \to \infty$, but not exponentially! In some cases the spectrum is purely point with exponentially decaying eigenfunctions. The last phenomenon is called Anderson localization and is more typical for random operators.

Let us finish our discussion with considering of integrated density of states. Again one can consider the spectral function $e(\lambda; x, y)$. This function is almost periodic along the diagonal, i.e. $e(\lambda : x+z, y+z)$ is a. p. in $z \in \mathbb{R}^N$, uniformly with respect to $x, y \in \mathbb{R}^N$. Now we set

$$N(\lambda) = M_x(e(\lambda; , x, x)),$$

where M_x is the mean value of an a. p. function. One can also extend formula (9.3). Let Ω_n be a sequence of smooth bounded domains which blow up in a "regular" way, e.g., Ω_n is a ball of radius n centered at the origin. Let H_n be the operator generated by $-\Delta + V(x)$ on Ω_n with some self-adjoint (e.g., Dirichlet or Neumann) boundary condition and $N_n(\lambda)$ the distribution function for eigenvalues of H_n. Then

$$N(\lambda) = \lim_{n\to\infty} \frac{1}{\operatorname{meas} \Omega_n} N_n(\lambda).$$

Again, for the Laplace transform of $N(\lambda)$ one has

$$\tilde{N}(t) = M_x(G(t, x, x)),$$

where $G(t, x, x)$ is the fundamental solution of Cauchy problem for $\partial/\partial t - H$. This function is now a. p. along the diagonal.

For details we refer the reader to [9], [15] and references therein.

9.5 Decaying perturbations of periodic potentials

Consider the operator $H = -\Delta + V(x)$ with a potential of the form

$$V(x) + V_0(x) + V_1(x),$$

where $V_0(x)$ is periodic and $V_1(x)$ decays at infinity (we do not specify here precise assumptions). The operator H can be considered as a perturbation of the operator $H_0 = -\Delta + V_0(x)$. As we already know, the spectrum $\sigma(H_0)$ is absolutely continuous (at least, for continuous potentials) and may have gaps. If the perturbation $V_1(x)$ decays sufficiently fast, the multiplication by $V_1(x)$ is a Δ-compact (hence, H_0-compact) operator. This means ([10], vol. 4) that $V_1(-\Delta + 1)^{-1}$ and $V_1(H_0 + \alpha)^{-1}$, with $\alpha > 0$ large enough, are compact operators. It is known [10] that an essential spectrum is staple under relatively compact perturbations. Therefore, $\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(H_0) = \sigma(H_0))$. However, the perturbation $V_1(x)$ may introduce eigenvalues of finite multiplicity below the essential spectrum and/or into spectral gaps. Typically, corresponding eigenfunctions decay exponentially fast. See a survey [3].

Now we want to point out the following question. Is it possible that H has eigenvalues which belong to $\sigma_{\text{ess}}(H) = \sigma(H_0)$? Such eigenvalues are called *embedded* eigenvalues. If $V_0(x) \equiv 0$, then Theorem 8.24 shows that there are no positive eigenvalues. The point 0 may be an eigenvalue in the case $N > 1$. So, in higher dimensions we should justify our question as follows: can an interior point of the spectrum be an eigenvalue? In general case not so much is known. On the contrary, if $N = 1$ the situation is quite clear: if $(1 + |x|)V_1(x) \in L^1(\mathbb{R})$, then embedded eigenvalues cannot appear [11], [12] (this result is not trivial!). Moreover, the last works contain results on the number of eigenvalues introduced into spectral gaps. For instance, far gaps cannot contain more than two eigenvalues.

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