Geometrical aspects of spectral theory

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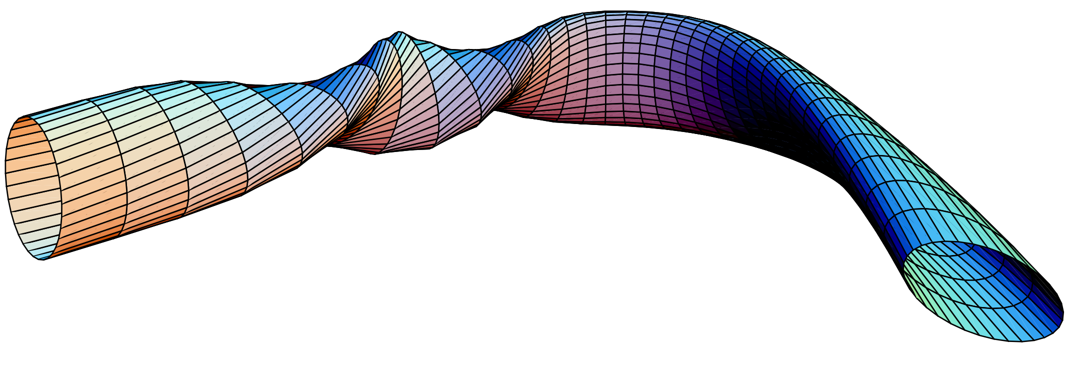


Contents

Chapter 0

Introduction

Spectral theory is an extremely rich field which has found its application in many areas of physics and mathematics. One of the reason which makes it so attractive on the formal level is that it provides a unifying framework for problems in various branches of mathematics, for example partial differential equations, calculus of variations, geometry, stochastic analysis, *etc.*

The goal of the lecture is to acquaint the students with spectral methods in the theory of linear differential operators coming both from modern as well as classical physics, with a special emphasis put on geometrically induced spectral properties. We give an overview of both classical results and recent developments in the field, and we wish to always do it by providing a physical interpretation of the mathematical theorems.

0.1 Why spectrum?

Most processes in Nature can be under first approximation described by one of the following linear differential equations:

- the wave equation $$\frac{\partial^2 u}{\partial t^2} - \Delta u = 0\,, \tag{1}$$
- the heat equation $$\frac{\partial u}{\partial t} - \Delta u = 0\,, \tag{2}$$
- the Schrödinger equation $$i\frac{\partial u}{\partial t} + \Delta u = 0\,. \tag{3}$$

One typically thinks of $t \in \mathbb{R}$ as the time variable and $-\Delta$ is the Laplacian in the d-dimensional Euclidean, *i.e.* $\Delta = \partial_{x_1}^2 + \cdots + \partial_{x_d}^2$ in the Cartesian coordinates $x = (x_1, \dots, x_d) \in \mathbb{R}^d$, with $d \geq 1$. (In this document, we adopt the geometric convention and call by the Laplacian the differential expression $-\Delta$ rather than Δ.) Qualitative properties of the respective solutions are very different, which of course reflects the variety of the physical systems.

- The wave equation is a classical model for a vibrating string, membrane or elastic solid, but it also models propagation of electromagnetic waves, moreover it arises in relativistic quantum mechanics and cosmology.
- The heat equation, also known as the diffusion equation, describes in typical applications the evolution in time of the density of some quantity such as the heat, chemical concentration, *etc*,. It also represents the simplest version of the Fokker-Planck equation describing the stochastic motion of a Brownian particle.
- Finally, the Schrödinger equation is the fundamental equation of quantum theory, which is probably the best physical theory mankind has ever had (at least from the point of view of the technological impact and the number of experiments confirming it).

The common denominator of the above equations is

- the Helmholtz equation $$-\Delta\psi = \lambda\psi\,, \tag{4}$$

which is obtained from (1)–(3) after a separation of the space x and time t variables. Indeed, (1)–(3) reduce to (4) after writing

- $u(x,t) = \psi(x)\, e^{-i\sqrt{\lambda}\, t}$,
- $u(x,t) = \psi(x)\, e^{-\lambda\, t}$,
- $u(x,t) = \psi(x)\, e^{-i\,\lambda\, t}$,

respectively, so it can be understood as a stationary counterpart of the evolution equations. Equation (4) can be understood as a *spectral problem for the Laplacian*, with eigenvalues λ and eigenfunctions ψ usually having direct physical interpretations. For instance, the numbers λ have the meaning of

- squares of resonant frequences for vibrating systems,
- decay rates for dissipative systems,
- bound-state energies for quantum systems.

More importantly, the solutions of the evolution equations (1)–(3) can be obtained on the basis of a complete spectral analysis of the Laplacian. (It follows from the linear nature of the differential equations: By the so-called *superposition principle*, if u_1, u_2 are solutions, then the sum $u_1 + u_2$ is also a solution.)

We use the Laplacian just to simplify the presentation in this introductory section; depending on the concrete physical problem in question, the Laplacian $-\Delta$ in (1)–(3) may need to be replaced by a general elliptic differential operator. The spectral theory of differential operators thus represents a unifying mathematical framework for various (possibly very different!) physical systems.

0.2 Why geometry?

As usual for evolution equations, (1)–(3) are subject to initial conditions at $t = 0$. In the physical problems mentioned above, the space variables x are typically restricted to a subdomain $\Omega \subset \mathbb{R}^d$. Then it is also necessary to equip (1)–(4) with boundary conditions on the boundary $\partial\Omega$.

The easiest situation is represented by

- *Dirichlet boundary conditions* $$\psi = 0 \qquad \text{on} \qquad \partial\Omega\,. \tag{5}$$

As well as being simple to treat, these boundary conditions are directly relevant to a number of physical problems, for instance:

- vibrations of an elastic membrane whose boundary is fixed, heat flow in a medium whose boundary is kept at zero temperature (a cooling mug), killing boundary conditions for the Brownian motion, the motion of a quantum particle which is confined to a region by the barrier associated with a large chemical potential (nanostructures), *etc.*

Intrinsically harder situation is represented by

- *Neumann boundary conditions* $$\frac{\partial\psi}{\partial n} = 0 \qquad \text{on} \qquad \partial\Omega\,, \tag{6}$$

where n denotes the outward unit normal vector field of $\partial\Omega$. However, these are also important in physical applications:

- the vibration of a membrane at those parts of the boundary which are free to move, the flow of a fluid through a channel or past an obstacle, the flow of heat in a medium with an insulated boundary (a vacuum flask), reflecting boundary conditions for the Brownian motion, *etc.*

Representing an interpolation between the Dirichlet and Neumann boundary conditions, it might be also sometimes relevant to employ

- *Robin boundary conditions* $$\frac{\partial\psi}{\partial n} + \alpha\,\psi = 0 \qquad \text{on} \qquad \partial\Omega\,, \tag{7}$$

where $\alpha : \partial\Omega \to \mathbb{R}$ is a function. The constant choices $\alpha = 0$ and $\alpha = \pm\infty$ (the latter understood in the sense of dividing (7) by α and taking the limit $\alpha \to \pm\infty$) correspond to Neumann and Dirichlet boundary conditions, respectively. In physical applications, these conditions arises for instance

- in electromagnetism as an approximation for materials with thin layers (*e.g.* stealth aircrafts) and in acoustics in connection with propagation of sonic waves through elastic cylinders.

Finally, it is also possible to consider the case of combined boundary conditions, where different kinds of boundary conditions are imposed on distinct parts of $\partial\Omega$.

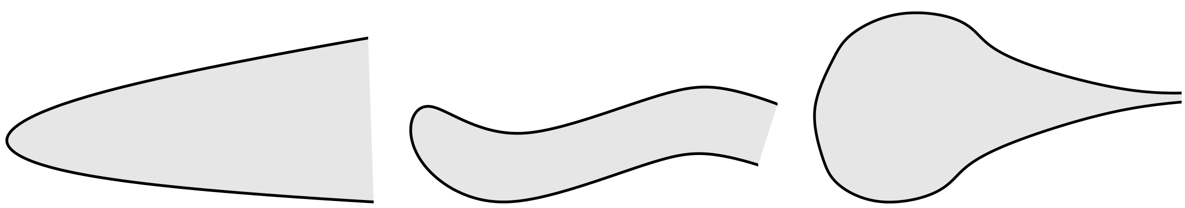
0.3 Which geometry?

Geometrically, we shall be interested in a (non-empty) *open* set, typically denoted by the symbol Ω. In [35], I. M. Glazman introduced the following useful classification (see also [25, Sec. X.6.1]).

Definition 0.1 (Glazman's classification of Euclidean open sets)**.** An open set $\Omega \subset \mathbb{R}^d$ is

- *quasi-conical* if it contains arbitrarily large balls;
- *quasi-cylindrical* if it is not quasi-conical but it contains infinitely many (pairwise) disjoint identical (*i.e.* of the same radius, congruent) balls;
- *quasi-bounded* if it is neither quasi-conical nor quasi-cylindrical.

Obviously, each open set $\Omega \subset \mathbb{R}^d$ belongs to one of the classes. Bounded sets represent a subset of quasi-bounded sets, but the latter class is much larger as we shall see below. The whole Euclidean space $\mathbb{R}^d$ or its conical sector are examples of quasi-conical domains. The infinite sequence of disjoint identical (respectively, expanding) balls is an example of a quasi-cylindrical (respectively, quasi-conical) set. Finally, an infinite (solid) cylinder $\mathbb{R} \times B_R$, where B_R is a $(d-1)$-dimensional ball of radius R, is a quasi-cylindrical domain. See Figure 1 for typical examples in $\mathbb{R}^2$.



quasi-conical quasi-cylindrical quasi-bounded

Figure 1: Examples of planar domains as regards the Glazman classification.

In the following chapters, we shall be interested in spectral properties of the Robin Laplacian as regards the above classification. Without loss of generality, we may assume that Ω is a *domain*, *i.e.* an open connected set. Indeed, the spectrum of Ω is obtained as the union of the spectra of individual connected components of Ω.

0.4 The plan

The objective of the present lecture is to study the interplay between the geometry of Ω and the spectrum of differential operators, subject to various boundary conditions. Because of the time constraint, we shall almost exclusively consider just the Laplace operator and Dirichlet boundary conditions. Before we start implementing the plan, let us begin with rather technical preliminaries.

Chapter 1

Preliminaries

First of all, let us properly interpret the Helmholtz equation (4), subject to Dirichlet boundary conditions, as a spectral problem. The spectrum is a property of an operator, so we have to specify what an operator is. An operator acts on a space, so we first need to specify what kind of spaces we are interested in. So our plan in this section is schematically as follows:

spectral problem	for an	operator	in a	vector space
3.		2.		1.

We follow the operator-theoretic approach of quantum mechanics.

1.1 The Lebesgue space as a Hilbert space

Let $\mathcal{H}$ be a *complex* vector space with inner product $(\cdot,\cdot)$. Our convention is that the inner product is linear (respectively, antilinear) in the second (respectively, first) component. If $\mathcal{H}$ is finite-dimensional (*i.e.* $\dim \mathcal{H} < \infty$), it is well known that every Cauchy sequence in $\mathcal{H}$ is convergent (the converse claim is elementary). This useful property is not necessarily true if $\mathcal{H}$ is infinite-dimensional (*i.e.* $\dim \mathcal{H} = \infty$). But we shall always restrict to vector spaces for which it is true; such vector spaces are called *complete*. A complete vector space with inner product is called a *Hilbert space*. Additionally, we shall assume that $\mathcal{H}$ is *separable*, meaning that $\mathcal{H}$ contains an (at most) countable subset which is dense in $\mathcal{H}$. In summary, we shall always assume:

$$\mathcal{H} := \text{separable complex Hilbert space.}$$

The separability is equivalent to the fact that $\mathcal{H}$ has an (at most) countable orthonormal basis. In quantum mechanics, the Hilbert space represents the space of states of a physical system. This explains the separability assumption, since countably many observations should be enough to determine a physical state. The Hilbert space must be assumed to be complex, because the Schrödinger equation (1.2) is intrinsically complex.

Let $\Omega \subset \mathbb{R}^d$ with $d \geq 1$ be any open set. A canonical example of infinite-dimensional complex Hilbert space is the *Lebesgue space*

$$L^2(\Omega) := \left\{ \underset{\text{measurable}}{\psi : \Omega \to \mathbb{C}} : \int_\Omega |\psi(x)|^2 \, \mathrm{d}x < \infty \right\}$$

equipped with the inner product

$$(\phi, \psi) := \int_\Omega \overline{\phi(x)}\, \psi(x) \, \mathrm{d}x \,, \qquad \text{where} \qquad \phi, \psi \in L^2(\Omega)\,.$$

The corresponding norm reads

$$\|\psi\| := \sqrt{\int_\Omega |\psi(x)|^2 \, \mathrm{d}x}\,.$$

In quantum mechanics, $L^2(\Omega)$ is the Hilbert space for describing an electron constrained to a nanostructure of shape Ω.

Here "measurable" and the integrals refer to the Lebesgue measure in $\mathbb{R}^d$. Following Schechter [64, Sec. 1.5], those of you who are unfamiliar with Lebesgue integration theory, do not despair. You can consider the integration in the sense of Riemann without serious misgivings. However, you should keep in mind that it is the Lebesgue integration which leads to the completeness of $L^2(\Omega)$.

It is a classical result of functional analysis (see, *e.g.*, [67]) that $L^2(\Omega)$ is complete and separable and that the space

$$C_0^\infty(\Omega) := \{\psi \in C^\infty(\Omega) : \ \operatorname{supp}\psi \text{ is compact in } \Omega\},$$

where $C^\infty(\Omega)$ is the space of infinitely smooth complex-valued functions $\psi : \Omega \to \mathbb{C}$, is dense in $L^2(\Omega)$. One has $\dim L^2(\Omega) = \infty$, because $L^2(Q)$ with $Q \subset \Omega$ being a cube can be regarded as a subspace of $L^2(\Omega)$ (by extending the functions of $L^2(Q)$ by zero outside Q) and $L^2(I)$ with I being a finite interval is clearly infinite-dimensional for it contains all monomials.

1.2 The Dirichlet Laplacian as a self-adjoint operator

A *(linear) operator* H in $\mathcal{H}$ is the linear map

$$H : \operatorname{dom} H \subset \mathcal{H} \to \mathcal{H},$$

where $\operatorname{dom} H$ is a linear subspace of $\mathcal{H}$ called the *domain* of H. Restricting the action of H to a subspace of $\mathcal{H}$ is necessary in infinite-dimensional Hilbert spaces.

Recall that an operator H in a Hilbert space $\mathcal{H}$ is called *self-adjoint* if

$$H = H^*$$

where H^* is the *adjoint* of H. As in finite-dimensional spaces, the adjoint H^* of any operator H is defined by means of the duality introduced via the inner product

$$\forall \psi \in \operatorname{dom} H,\ \phi \in \operatorname{dom} H^*, \qquad (\phi, H\psi) = (H^*\phi, \psi). \tag{1.1}$$

More specifically, since we have to be careful about domains, we set

$$\begin{aligned} \operatorname{dom} H^* &:= \big\{\phi \in \mathcal{H} : \ \exists \eta \in \mathcal{H},\ \forall \psi \in \operatorname{dom} H,\ (\phi, H\psi) = (\eta, \psi)\big\}, \\ H^*\phi &:= \eta. \end{aligned}$$

This operator is well (*i.e.* uniquely) defined provided that H is *densely defined* (*i.e.*, $\operatorname{dom} H$ is a dense subspace of $\mathcal{H}$). (Indeed, if $(\eta_1, \psi) = (\phi, H\psi) = (\eta_2, \psi)$ for all $\psi \in \operatorname{dom} H$, then $\eta_1 - \eta_2 \in (\operatorname{dom} H)^\perp$, consequently $\eta_1 = \eta_2$.)

It is usually easy to verify that H is *symmetric*, *i.e.*, H is densely defined and

$$\forall \phi, \psi \in \operatorname{dom} H, \qquad (\phi, H\psi) = (H\phi, \psi).$$

(Note carefully that here ϕ is taken from $\operatorname{dom} H$, contrary to (1.1) where it is assumed to belong to $\operatorname{dom} H^*$.) This is equivalent to saying that $H \subset H^*$, *i.e.* the adjoint H^* is an extension of H. The self-adjointness $H = H^*$ requires in addition that $\operatorname{dom} H = \operatorname{dom} H^*$, which is a much more delicate matter. (For an instructive example of a symmetric non-self-adjoint operator, see Exercise 3.)

In quantum mechanics, physical observables are represented by self-adjoint operators. The self-adjointness is unavoidable in this context (leaving aside the recent concept of quasi-self-adjoint representations in quantum mechanics [53]). Indeed, using a self-adjoint operator H as the Hamiltonian in the Schrödinger equation

$$i\,\frac{\mathrm{d}\psi}{\mathrm{d}t} = H\psi, \tag{1.2}$$

the solutions are given by the unitary propagator e^{-itH}. Conversely, by Stone's theorem [67, Thm. 7.38], the generators of unitary groups are necessarily self-adjoint operators. So there is no way out without abandoning the conservative (*i.e.* unitary) nature of quantum mechanics.

Let $\Omega \subset \mathbb{R}^d$ be an open set. We would like to introduce an operator H in $L^2(\Omega)$, which acts as the Laplacian and satisfies the Dirichlet boundary conditions (5) on $\partial\Omega$. Here it also becomes clear that the domain of such an operator must be a *proper* subset of $L^2(\Omega)$. Indeed, first, ψ should be differentiable in a sense to make $\Delta\psi$ meaningful and, second, $\Delta\psi$ should be an element of $L^2(\Omega)$. Moreover, ψ should vanish on $\partial\Omega$ in a sense.

An obvious choice is

$$\dot{H}\psi := -\Delta\psi\,, \qquad \psi \in \operatorname{dom}\dot{H} := C_0^\infty(\Omega)\,. \tag{1.3}$$

(Here we could take $C_0^2(\Omega)$ instead of $C_0^\infty(\Omega)$, but the difference in smoothness does not influence the subsequent analysis.) Now the action of the Laplacian is implemented in the classical sense and the Dirichlet boundary condition is realised in a very strong way, for the functions in the domain are actually required to vanish in a neighbourhood of $\partial\Omega$.

Proposition 1.1. *$\dot{H}$ is densely defined, symmetric and non-negative.*

Proof. $\dot{H}$ is densely defined because $C_0^\infty(\Omega)$ is dense in $L^2(\Omega)$. Integrating by parts (or, more specifically, using the divergence theorem), we easily get

$$\begin{aligned}
\forall\phi,\psi\in\operatorname{dom}\dot{H}\,, \qquad (\phi,\dot{H}\psi) &= -\int_\Omega \bar{\phi}\,\Delta\psi = -\int_\Omega \nabla\cdot(\bar{\phi}\,\nabla\psi) + \int_\Omega \nabla\bar{\phi}\cdot\nabla\psi \\
&= -\int_{\partial\Omega}\bar{\phi}\,\frac{\partial\psi}{\partial n} + \int_\Omega \nabla\bar{\phi}\cdot\nabla\psi \\
&= \int_\Omega \nabla\bar{\phi}\cdot\nabla\psi = \int_\Omega \nabla\cdot(\nabla\bar{\phi}\,\psi) - \int_\Omega \Delta\bar{\phi}\,\psi \\
&= \int_{\partial\Omega}\frac{\partial\bar{\phi}}{\partial n}\,\psi - \int_\Omega \Delta\bar{\phi}\,\psi \\
&= -\int_\Omega \Delta\bar{\phi}\,\psi = (\dot{H}\phi,\psi)\,.
\end{aligned} \tag{1.4}$$

The equalities on the second and fourth lines are due to the divergence theorem and the boundary terms vanish at the following equalities because $\phi,\psi = 0$ in a neighbourhood of $\partial\Omega$. Moreover, from the identity on the third line, we get

$$\forall\psi\in\operatorname{dom}\dot{H}\,, \qquad (\psi,\dot{H}\psi) = \|\nabla\psi\|^2 \geq 0\,,$$

so the operator $\dot{H}$ is non-negative. ☐

Although the operator $\dot{H}$ is symmetric, it is not self-adjoint. Indeed,

$$\operatorname{dom}\dot{H} \subsetneqq \{\phi\in L^2(\Omega)\cap C^\infty(\Omega) :\ \Delta\phi\in L^2(\Omega)\} \subset \operatorname{dom}\dot{H}^*\,,$$

where the latter inclusion holds because all the identities in (1.4) are actually verified for ϕ in this larger set (the functions in $\operatorname{dom}\dot{H}^*$ do not need to satisfy any kind of Dirichlet boundary condition!).

It is clear that the choice of the domain $\operatorname{dom}\dot{H}$ is too restrictive and one can justify the action of the operator on a much larger domain. How to choose the domain as large as possible? While still making $-\Delta\psi\in L^2(\Omega)$ and $\psi = 0$ on $\partial\Omega$ sensible, even if the price to pay would be to interpret the action of the Laplacian and boundary conditions in a weaker sense?

Given any symmetric extension H of a symmetric operator $\dot{H}$, we have the general inclusions:

$$\dot{H}\subset H\subset H^*\subset\dot{H}^*. \tag{1.5}$$

It follows that the problem of finding a self-adjoint realisation reduces to extending H till the central inclusion becomes sharp. This is the idea of the theory of self-adjoint extensions of symmetric operators originally developed by von Neumann [66]. This is not an easy task, however. Moreover, $\dot{H}$ could admit several self-adjoint extensions; how to choose the physically relevant one?

The correct choice of the domain is a delicate matter, which requires the knowledge of rather advanced techniques. The most effective way here is to implement the so-called *Friedrichs extension* that we explain now. Let us start with the sesquilinear form $\dot{h}$ associated with the operator $\dot{H}$, namely,

$$\dot{h}(\phi,\psi) := (\phi,\dot{H}\psi)\,, \qquad \phi,\psi\in\operatorname{dom}\dot{h} := \operatorname{dom}\dot{H} = C_0^\infty(\Omega)\,.$$

As a above, it is easy to check:

Proposition 1.2. *$\dot{h}$ is densely defined, symmetric and non-negative.*

In particular, the first integration by parts in (1.4) yields

$$\forall \phi, \psi \in \operatorname{dom} \dot{h}\,, \qquad \dot{h}(\phi,\psi) = (\nabla\phi, \nabla\psi)\,,$$

so the right-hand side would be a well defined form even in the larger space $C_0^1(\Omega)$, while still keeping the Dirichlet boundary conditions in the very restrictive sense. In any case, the subspace $\operatorname{dom} \dot{h}$ equipped with the inner product associated with the norm

$$|||\psi||| := \sqrt{\|\nabla\psi\|^2 + \|\psi\|^2} \tag{1.6}$$

is a pre-Hilbert space (its completion will be a Hilbert space).

To make the form domain as large as possible, we introduce the *closure* h of $\dot{h}$ by

$$\begin{aligned} \operatorname{dom} h &:= \overline{C_0^\infty(\Omega)}^{|||\cdot|||} = \left\{ \psi \in L^2(\Omega) : \ \exists \{\psi_n\}_{n\in\mathbb{N}} \subset C_0^\infty(\Omega),\ \psi_n \xrightarrow[n\to\infty]{} \psi \ \wedge \ \dot{h}[\psi_n - \psi_m] \xrightarrow[n,m\to\infty]{} 0 \right\}, \\ h(\phi,\psi) &:= \lim_{n,m\to\infty} \dot{h}(\phi_n, \psi_m)\,. \end{aligned}$$

To make the definition meaningful, however, we have to verify that the number $h(\phi,\psi)$ does not depend on the choice of the sequences $\{\phi_n\}_{n\in\mathbb{N}}$ and $\{\psi_n\}_{n\in\mathbb{N}}$. This is equivalent to the compatibility condition (known as the *closability* of $\dot{h}$) that:

$$\forall \{\psi_n\}_{n\in\mathbb{N}} \subset \operatorname{dom} \dot{h}\,, \qquad \left.\begin{aligned} \psi_n &\xrightarrow[n\to\infty]{} 0 \\ \dot{h}[\psi_n - \psi_m] &\xrightarrow[n,m\to\infty]{} 0 \end{aligned}\right\} \quad \Longrightarrow \quad \dot{h}[\psi_n] \xrightarrow[n\to\infty]{} 0\,. \tag{1.7}$$

Proposition 1.3. *$\dot{h}$ is closable.*

Proof. We could use the general fact [47, Corol. VI.1.28] that every form constructed from a densely defined symmetric operator which is bounded from below is closable. However, let us present a direct proof. Let $\{\psi_n\}_{n\in\mathbb{N}} \subset \operatorname{dom} \dot{h} = C_0^\infty(\Omega)$ be such that $\|\psi_n\| \to 0$ and $\|\nabla\psi_n - \nabla\psi_m\| \to 0$ as $n, m \to \infty$. Because of the completeness of $L^2(\Omega)$, it follows that there exists a vector-valued function $g \in L^2(\Omega; \mathbb{C}^d)$ such that $\|\nabla\psi_n - g\| \to 0$ as $n \to \infty$. Consequently,

$$\begin{aligned} \forall \varphi \in C_0^\infty(\Omega;\mathbb{C}^d)\,, \qquad (\varphi, g) &= \lim_{n\to\infty} (\varphi, \nabla\psi_n) = \lim_{n\to\infty} \int_\Omega \bar{\varphi}\cdot\nabla\psi_n = -\lim_{n\to\infty}\int_\Omega \operatorname{div}\bar{\varphi}\,\psi_n \\ &= \lim_{n\to\infty} (-\operatorname{div}\varphi, \psi_n) \\ &= (-\operatorname{div}\varphi, \psi) = 0\,. \end{aligned} \tag{1.8}$$

From the arbitrariness of φ, it follows that $g = 0$. So (1.7) holds. ☐

From the identity $(\varphi, g) = (-\operatorname{div}\varphi, \psi)$ of (1.8), it follows that g is a *weak* (or *distributional*) gradient of ψ. (By definition, every distribution is infinitely many differentiable, the weak differentiability requires that the obtained distribution after the differentiation is actually a function.) It is customary to denote the weak derivatives by the same symbols, so we are allowed to write $g = \nabla\psi$ in this generalised sense.

In summary, h acts in the same way as $\dot{h}$:

$$h(\phi,\psi) = (\nabla\phi,\nabla\psi)\,, \qquad \phi,\psi \in \operatorname{dom} h = \overline{C_0^\infty(\Omega)}^{|||\cdot|||} =: W_0^{1,2}(\Omega) \tag{1.9}$$

provided that the gradients on the right-hand side are interpreted as weak gradients. Here the functional space $W_0^{1,2}(\Omega)$ is called a *Sobolev space*.

If we were in a finite-dimensional Hilbert space $\mathcal{H}$, the Riesz representation theorem would ensure that there exists an operator H in $\mathcal{H}$ associated with the form h, *i.e.*,

$$\forall \phi \in \operatorname{dom} h,\ \psi \in \operatorname{dom} H\,, \qquad h(\phi,\psi) = (\phi, H\psi)\,. \tag{1.10}$$

The good news is that an analogue of the representation theorem holds in infinite-dimensional spaces provided that the form h is densely defined, symmetric, bounded from below (*i.e.* there exists a real number c such that $h[\psi] \geq c\|\psi\|^2$ for every $\psi \in \operatorname{dom} h$) and closed (*cf* [47, Sec. VI.2.1]). The *closedness* of h means that $\operatorname{dom} h$ equipped with the norm $|||\psi||| := \sqrt{h[\psi] + (1-c)\|\psi\|^2}$ is a Hilbert space, which is equivalent to the sequential criterion:

$$\forall \psi \in \mathcal{H},\ \{\psi_n\}_{n\in\mathbb{N}} \subset \operatorname{dom} h\,, \qquad \left.\begin{aligned} \psi_n &\xrightarrow[n\to\infty]{} \psi \\ h[\psi_n - \psi_m] &\xrightarrow[n,m\to\infty]{} 0 \end{aligned}\right\} \quad \Longrightarrow \quad \begin{cases} \psi \in \operatorname{dom} h \\ h[\psi_n - \psi] \xrightarrow[n\to\infty]{} 0 \end{cases}.$$

Moreover, the associated operator H is necessarily self-adjoint (because the adjoint operator H^* is associated with the adjoint form h^* defined by $h^*(\phi,\psi) := \overline{h(\psi,\phi)}$, $\operatorname{dom} h^* := \operatorname{dom} h$, which coincides with h by its symmetry) and bounded from below. By (1.10), the operator H acts as follows:

$$\begin{aligned} \operatorname{dom} H &:= \{\psi \in \operatorname{dom} h \ :\ \exists \eta \in \mathcal{H},\ \forall \phi \in \operatorname{dom} h,\ h(\phi,\psi) = (\phi,\eta)\}\,, \\ H\psi &:= \eta\,. \end{aligned} \tag{1.11}$$

In summary, there is a one-to-one correspondence between the set of all densely defined, symmetric, closed forms which are bounded from below and the set of all self-adjoint operators which are bounded from below; schematically:

operator		form
H	$\xleftrightarrow{1-1}$	h
self-adjoint		densely defined, symmetric, closed
bounded from below		bounded from below

Indeed, the direction $\longleftarrow$ follows by the aforementioned representation theorem of Kato's [47, Thm. VI.2.1]. To establish the opposite direction $\longrightarrow$, given a self-adjoint operator H which is bounded from below, let us define the form $\dot{h}[\psi] := (\psi, H\psi)$, $\operatorname{dom} \dot{h} := \operatorname{dom} H$. The form $\dot{h}$ is obviously densely defined, symmetric and bounded from below. It is not necessarily closed, but it is closable [47, Thm. VI.1.27]. (Here it is important that $\dot{h}$ arises as a form of an operator, since not every densely defined, symmetric form, bounded from below, is closable! See Exercise 1.) The closure h of $\dot{h}$ defined as above then satisfies all the desired properties.

In our case, when h is given by (1.9), the identity $h(\phi,\psi) = (\phi,\eta)$ for every $\phi \in \operatorname{dom} h$ and $\psi \in \operatorname{dom} H$ means

$$\forall \phi \in W_0^{1,2}(\Omega),\ \psi \in \operatorname{dom} H\,, \qquad \int_\Omega \nabla\bar{\phi} \cdot \nabla\psi = \int_\Omega \bar{\phi}\,\eta\,.$$

In particular, using the dense subspace $C_0^\infty(\Omega)$ of the form domain $W_0^{1,2}(\Omega)$,

$$\forall \phi \in C_0^\infty(\Omega),\ \psi \in \operatorname{dom} H\,, \qquad \int_\Omega -\Delta\bar{\phi}\,\psi = \int_\Omega \nabla\bar{\phi} \cdot \nabla\psi = \int_\Omega \bar{\phi}\,\eta\,, \tag{1.12}$$

where the first equality is just the definition of the weak gradient (motivated by an integration by parts). Hence $\eta = -\Delta\psi$ is the weak Laplacian of ψ. That is,

$$H\psi = -\Delta\psi\,, \qquad \operatorname{dom} H = \left\{\psi \in W_0^{1,2}(\Omega) :\ \Delta\psi \in L^2(\Omega)\right\}.$$

Now the action of the Laplacian is implemented in the generalised sense of distributions and the Dirichlet boundary condition is realised in a very weak sense. We set $-\Delta_D^\Omega := H$ and call the operator the *Dirichlet Laplacian*. Let us emphasise that this definition works for *any* open set (without any requirement on the regularity of the boundary; for example, Ω can have a fractal boundary!). The associated form will be denoted by $Q_D^\Omega := h$.

Definition 1.4. For every open set $\Omega \subset \mathbb{R}^d$, the *Dirichlet Laplacian* is the operator in $L^2(\Omega)$ defined by

$$-\Delta_D^\Omega \psi := -\Delta\psi\,, \qquad \mathrm{dom}(-\Delta_D^\Omega) := \left\{\psi \in W_0^{1,2}(\Omega) :\ \Delta\psi \in L^2(\Omega)\right\}.$$

It is the operator associated with the form

$$Q_D^\Omega[\psi] := \|\nabla\psi\|^2\,, \qquad \mathrm{dom}(Q_D^\Omega) := W_0^{1,2}(\Omega)\,.$$

If the domain Ω is "nice" (which involves both certain smoothness of the boundary $\partial\Omega$ as well as a control of a global behaviour of the domain geometry if Ω is unbounded; for example, a bounded domain with $\partial\Omega \in C^2$, which means that the boundary $\partial\Omega$ is locally a graph of a twice continuously differentiable function, is a nice domain), then

$$\mathrm{dom}(-\Delta_D^\Omega) = \left\{\psi \in W^{2,2}(\Omega) :\ \psi = 0 \text{ on } \partial\Omega\right\}. \tag{1.13}$$

Here

$$W^{2,2}(\Omega) := \left\{\psi \in L^2(\Omega) :\ \nabla\psi, \nabla^2\psi \in L^2(\Omega)\right\}$$

is yet another Sobolev space, with $\nabla^2\psi$ denoting the distributional Hessian of ψ, and the vanishing of ψ on the boundary should be interpreted in the sense of traces. (Strictly speaking, $\nabla\psi \in L^2(\Omega)$ means $\nabla\psi \in L^2(\Omega;\mathbb{C}^d)$, and similarly for the matrix $\nabla^2\psi$.) At the same time,

$$W_0^{1,2}(\Omega) = \left\{\psi \in W^{1,2}(\Omega) :\ \psi = 0 \text{ on } \partial\Omega\right\} \tag{1.14}$$

if Ω is a nice domain. As expected, $W^{1,2}(\Omega)$ is also a Sobolev space, defined by

$$W^{1,2}(\Omega) := \left\{\psi \in L^2(\Omega) :\ \nabla\psi \in L^2(\Omega)\right\}$$

for an arbitrary open set Ω.

Proposition 1.5. *For every open set $\Omega \subset \mathbb{R}^d$, $W_0^{1,2}(\Omega) \subset W^{1,2}(\Omega)$.*

Proof. Let us repeat the proof of Proposition 1.3. Let $\psi \in W_0^{1,2}(\Omega)$. Then there exists a sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset C_0^\infty(\Omega)$ such that $\psi_n \to \psi$ and $\|\nabla\psi_n - \nabla\psi_m\| \to 0$ as $n, m \to \infty$. Because of the completeness of $L^2(\Omega)$, it follows that there exists a vector-valued function $g \in L^2(\Omega^d;\mathbb{C}^d)$ such that $\|\nabla\psi_n - g\| \to 0$ as $n \to \infty$. Consequently,

$$\begin{aligned}
\forall\varphi \in C_0^\infty(\Omega;\mathbb{C}^d)\,, \qquad (\varphi, g) &= \lim_{n\to\infty} (\varphi, \nabla\psi_n) = \lim_{n\to\infty} \int_\Omega \bar\varphi \cdot \nabla\psi_n = -\lim_{n\to\infty} \int_\Omega \operatorname{div}\bar\varphi\,\psi_n \\
&= \lim_{n\to\infty} (-\operatorname{div}\varphi, \psi_n) \\
&= (-\operatorname{div}\varphi, \psi)\,.
\end{aligned}$$

Hence, g equals the weak gradient $\nabla\psi$ of ψ. It follows that $\psi \in W^{1,2}(\mathbb{R}^d)$. □

The spaces $W_0^{1,2}(\Omega)$ and $W^{1,2}(\Omega)$ become Hilbert spaces if equipped with the norm $|||\cdot|||$ introduced in (1.6).

More generally, in the notation $W_0^{k,p}(\Omega)$, p stands for the underlying Lebesgue space $L^p(\Omega)$ (in our case, we shall exclusively work with $p = 2$), k denotes the highest order of derivative involved and 0 refers to the weak realisation of the Dirichlet boundary conditions.

Do not despair! You do not need to understand all these advanced notions related to Sobolev spaces. The moral is that there is a sort of natural space to make the action of the Laplacian sensible and that the Dirichlet boundary conditions are in fact incorporated through the domain of the operator.

In quantum mechanics, the Dirichlet Laplacian $-\Delta_D^\Omega$ represents the kinetic energy of an electron constrained to a nanostructure of shape Ω with hard-wall boundaries.

Remark 1.6 (More on the Friedrichs extension)**.** Let us recall that the Dirichlet Laplacian $-\Delta_D^\Omega$ was introduced as a particular (so-called Friedrichs) extension of the operator $\dot{H}$ defined in (1.3). Let us recapitulate the general strategy: Given a densely defined, symmetric operator $\dot{H}$ which is bounded from below, we define the form $\dot{h}[\psi] := (\psi, H\psi)$, $\operatorname{dom}\dot{h} := \operatorname{dom} H$, which is also densely defined, symmetric and bounded from below. The form $\dot{h}$ is not necessarily closed, but it is closable [47, Corol. VI.1.28]. The closure h of $\dot{h}$ is associated with a self-adjoint operator H which is bounded from below.

It is quite possible that there exists another self-adjoint extension of the initial operator $\dot{H}$. What is the specialty and physical relevance of the Friedrichs extension? The Friedrichs extension is mathematically characterised by the property that among all self-adjoint extensions $\tilde{H} \supset \dot{H}$, the Friedrichs extension H has the smallest form-domain (*i.e.*, the domain of the associated form h is contained in the domain of the form associated with any other $\tilde{H}$). Moreover, H is the only self-adjoint extension of $\dot{H}$ with domain contained in $\operatorname{dom} h$. If H is to be the Hamiltonian of a quantum system, then the value of the associated quadratic form $h[\psi]$ has the physical meaning of an expectation value of energy of the system in the state ψ. The Friedrichs extension is thus the natural choice following the minimal energy constraints of Nature.

Finally, let us comment on why it is useful to proceed via forms. In principle, given a densely defined, symmetric operator $\dot{H}$ which is bounded from below, it is closable [47, Thm. V.3.4], so we could construct the operator closure $\tilde{H}$. The problem is that $\tilde{H}$ is in general just a *closed symmetric* operator, but not necessarily *self-adjoint*. On the other hand, for forms there is no distinction between "closed symmetric" and "self-adjoint" (the latter is not even being introduced).

Let us come back to (1.13). The inclusion $\supset$ of (1.13) is obvious, it is the opposite inclusion $\subset$ which is non-trivial. It can be established by standard elliptic regularity theory (see, *e.g.*, [26, Sec. 6.3]), for which certain regularity assumptions about Ω are necessary. In dimension one, however, elementary arguments are available.

Proposition 1.7. *If* $d = 1$ *and* Ω *is a bounded interval, then* (1.14) *and* (1.13) *hold true.*

Proof. Let us write $\Omega =: (a, b)$ with $0 < a < b < \infty$. First of all, note that [23, Lem. 7.1.1]

$$W^{1,2}((a,b)) = \left\{\psi \in L^2((a,b)) :\ \exists g \in L^2((a,b)),\, c \in \mathbb{C}\,,\ \forall x \in [a,b]\,,\quad \psi(x) = c + \int_a^x g(\xi)\,\mathrm{d}\xi\right\}. \tag{1.15}$$

So $W^{1,2}((a,b))$ consists of absolutely continuous functions on $[a,b]$. In particular, the function value $\psi(x)$ is well defined for every $x \in [a,b]$. (One important remark is in order here: Elements of L^2 or $W^{1,2}$ are not actually functions but equivalence classes of functions under the relation of almost everywhere equivality. When we say that $\psi \in W^{1,2}$ is continuous we mean that there exists a continuous function in the equivalence class. It is easy to show that there cannot be more than one such continuous function.)

To show that the right-hand side of (1.15) is a subset of the left-hand side, it is enough to notice that g is the weak derivative of ψ. Conversely, let $\psi \in W^{1,2}((a,b))$ and $\psi' =: g$. Defining $h(x) := \int_a^x g(\xi)\,\mathrm{d}\xi$, we observe that $\psi - h \in W^{1,2}((a,b))$ and $(\psi - h)' = 0$. Consequently, $(\varphi', \psi - h) = 0$ for every $\varphi \in C_0^\infty((a,b))$. Since also $(\varphi', 1) = 0$ for every $\varphi \in C_0^\infty((a,b))$, it follows that $\psi - h$ must be equal to a constant c, being orthogonal to the function φ' orthogonal to 1. Therefore ψ is of the form as described on the right-hand side of (1.15).

Now let us prove (1.14). If $\psi \in W_0^{1,2}((a,b))$, then there exists a sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset C_0^\infty((a,b))$ such that $\psi_n \to \psi$ and $\psi_n' \to \psi'$ as $n \to \infty$, where ψ' is the weak derivative of ψ. By (1.15), there exists a complex constant c such that $\psi(x) = c + \int_a^x \psi'(\xi)\,\mathrm{d}\xi$ for every $x \in [a,b]$. At the same time, $\psi_n(x) = \int_a^x \psi_n'(\xi)\,\mathrm{d}\xi$ for every $x \in [a,b]$ and $n \in \mathbb{N}$. Consequently,

$$\forall x \in [a,b]\,, \qquad \psi(x) - \psi_n(x) = c + \int_a^x [\psi'(\xi) - \psi_n'(\xi)]\,\mathrm{d}\xi\,.$$

Here the right-hand side tends to c for every $x \in [a,b]$ as $n \to \infty$ and the left-hand side tends to zero for almost every $x \in [a,b]$ as $n \to \infty$. Thus $c = 0$, so $\psi(a) = 0$. At the same time,

$$\psi(b) = \int_a^b \psi'(\xi)\,\mathrm{d}\xi = \lim_{n\to\infty} \int_a^b \psi_n'(\xi)\,\mathrm{d}\xi = 0\,.$$

Conversely, let $\psi \in W^{1,2}(a,b)$ be such that $\psi(a) = 0 = \psi(b)$. Then, by (1.15), there exists a function $g \in L^2((a,b))$ such that $\psi(x) = \int_a^x g(\xi)\,\mathrm{d}\xi$ and $\int_a^b g(\xi)\,\mathrm{d}\xi = 0$ for every $x \in [a,b]$. We have to show that there exists a sequence $\{\psi_n\}_{n\in\mathbb{N}^*} \subset C_0^\infty((a,b))$ such that $\psi_n \to \psi$ and $\psi_n' \to \psi' = g$ as $n \to \infty$. Given $\varepsilon < (b-a)/4$, let $f_n : \mathbb{R} \to [0,1]$ be such that, for every $n \geq 1$,

$$f_n(x) := \begin{cases} 0 & \text{if} \quad x \leq a + \varepsilon/n\,, \\ \eta_a(a + n(x-a)) & \text{if} \quad x \in (a+\varepsilon/n, a+2\varepsilon/n)\,, \\ 1 & \text{if} \quad x \in [a+2\varepsilon, b-2\varepsilon]\,, \\ \eta_b(b - n(b-x)) & \text{if} \quad x \in (b-2\varepsilon/n, b-\varepsilon/n)\,, \\ 0 & \text{if} \quad x \geq b - \varepsilon/n\,, \end{cases}$$

where $\eta_a \in C_0^\infty((a+\varepsilon, a+2\varepsilon])$ is such that $0 \leq \eta_a \leq 1$ and $\eta_a = 1$ on a left neighbourhood of $a+2\varepsilon$ and $\eta_a \in C_0^\infty([b-2\varepsilon, b-\varepsilon))$ is such that $0 \leq \eta_b \leq 1$ and $\eta_b = 1$ on a right neighbourhood of $b-2\varepsilon$. Noticing that $f_n \in C_0^\infty((a+\varepsilon/n, b-\varepsilon/n))$, define $g_n := f_n g$ and $\psi_n(x) := \int_a^x g_n(\xi)\,\mathrm{d}\xi$. By the dominated convergence theorem, it is easy to see that $\{\psi_n\}_{n\in\mathbb{N}^*}$ is the desired sequence.

Finally, to prove (1.13), we are inspired by [47, Ex. VI.2.16]. As mentioned above, the inclusion $\supset$ of (1.13) is obvious by the previously established facts. Conversely, to prove the inclusion $\subset$ of (1.13), let us assume that $\psi \in \operatorname{dom}(-\Delta_D^{(a,b)})$. Then $\psi \in W_0^{1,2}((a,b))$ and there exists a function $\eta \in L^2((a,b))$ such that

$$\forall \phi \in W_0^{1,2}((a,b))\,, \qquad \int_a^b \bar\phi'(\xi)\,\psi'(\xi)\,\mathrm{d}\xi = \int_a^b \bar\phi(\xi)\,\eta(\xi)\,\mathrm{d}\xi\,. \tag{1.16}$$

We have to show that $\psi'' \in L^2((a,b))$ and $\eta = -\psi''$. For every $x \in [a,b]$, define $H(x) := \int_a^x \eta(\xi)\,\mathrm{d}\xi$, a primitive of η. Noticing that $H' = \eta$ and integrating by parts on the right-hand side of (1.16), the identity becomes

$$\forall \phi \in W_0^{1,2}((a,b))\,, \qquad \int_a^b \bar\phi'(\xi)\,\psi'(\xi)\,\mathrm{d}\xi = -\int_a^b \bar\phi'(\xi)\,H(\xi)\,\mathrm{d}\xi\,.$$

In other words, $(\phi', \psi' + H) = 0$ for every $\phi \in W_0^{1,2}((a,b))$. Thus $\psi' + H$ must be equal to a constant c, being orthogonal to the function ϕ' orthogonal to 1. It follows that ψ' is absolutely continuous on $[a,b]$ and $-\psi'' = \eta$ as desired. □

Remark 1.8 (Lipschitz sets)**.** If Ω is a set with boundary $\partial\Omega$ which can be parameterised by a *finite* covering of Lipschitz maps, we have

$$\operatorname{dom}(-\Delta_D^\Omega) = \left\{\psi \in W^{1,2}(\Omega) \;:\; \Delta\psi \in L^2(\Omega) \;\wedge\; \psi = 0 \text{ on } \partial\Omega\right\},$$

where boundary trace can be interpreted as an element of $W^{1/2,2}(\partial\Omega)$. For bounded sets, the claim can be deduced from [56] and the method extends to unbounded sets because we assume that there are only a finite number of the Lipschitz maps. Moreover, if Ω is in addition *bounded*, it is a deep result of [45] that

$$\operatorname{dom}(-\Delta_D^\Omega) = \left\{\psi \in W^{3/2,2}(\Omega) \;:\; \Delta\psi \in L^2(\Omega) \;\wedge\; \psi = 0 \text{ on } \partial\Omega\right\} \tag{1.17}$$

and the extra regularity enables one to interpret the boundary trace as an element of $W^{1,2}(\partial\Omega)$. We are grateful to Jussi Behrndt for the references.

1.3 What is the spectrum?

Now we are in a position to properly interpret (4). If the Helmholtz equation (4) is equipped with the Dirichlet boundary conditions (5), then the left-hand side of (4) is understood as the action of the Dirichlet Laplacian $-\Delta_D^\Omega$ on a function $\psi \in \operatorname{dom}(-\Delta_D^\Omega)$. The boundary value problem (4)–(5) means that we are looking for complex numbers λ such that there exists a function $\psi \in \operatorname{dom}(-\Delta_D^\Omega)$ such that $-\Delta_D^\Omega\psi = \lambda\psi$ (both λ and ψ are unknown!). Of course, it is reasonable to exclude the trivial situation $\psi = 0$, which is always a solution for any $\lambda \in \mathbb{C}$.

In finite-dimensional spaces, this is precisely what you know as a spectral problem.

Definition 1.9. Let H be an operator in a Hilbert space $\mathcal{H}$. The *point spectrum* of H is defined by:

$$\sigma_{\mathrm{p}}(H) := \big\{\lambda \in \mathbb{C} : \ \exists \underset{\psi \neq 0}{\psi} \in \operatorname{dom} H \ , \quad H\psi = \lambda\psi\big\} \,.$$

Any element $\lambda \in \sigma_{\mathrm{p}}(H)$ is called an *eigenvalue* of H. Any non-zero vector $\psi \in \operatorname{dom} H$ satisfying $H\psi = \lambda\psi$ is called an *eigenvector* of H corresponding to the eigenvalue λ.

Given any operator T in $\mathcal{H}$, recall the definition of the *kernel*, $\ker T := \{\psi \in \operatorname{dom} T : \ T\psi = 0\}$. Given $\lambda \in \sigma_{\mathrm{p}}(H)$, the set of all eigenvectors corresponding to λ clearly coincides with $\ker(H-\lambda I) \setminus \{0\}$, where I is the identity operator on $\mathcal{H}$ (*i.e.*, $I\psi := \psi$, $\operatorname{dom} I := \mathcal{H}$). In particular, the number of all linearly independent eigenvectors corresponding to λ equals

$$m_{\mathrm{g}}(\lambda) := \dim\ker(H - \lambda I) \,.$$

This number is called the *(geometric) multiplicity* of the eigenvalue $\lambda \in \sigma_{\mathrm{p}}(H)$. If $m_{\mathrm{g}}(\lambda) = 1$, we say that the eigenvalue λ is *simple*. If $m_{\mathrm{g}}(\lambda) > 1$, we say that the eigenvalue λ is *degenerate*.

From Definition 1.9, it is clear that λ is in the point spectrum of H if, and only if, the operator $H - \lambda I : \operatorname{dom} H \to \mathcal{H}$ is not injective (recall that any operator T is injective, if, and only if, $\ker T = \{0\}$). If the Hilbert space $\mathcal{H}$ is finite-dimensional, then this is also equivalent to the fact that the operator $H - \lambda I$ is not surjective. This follows from the fundamental theorem

$$\dim\ker(H - \lambda I) + \dim\operatorname{ran}(H - \lambda I) = \dim\mathcal{H} \,, \tag{1.18}$$

where $\operatorname{ran} T := \{T\psi : \ \psi \in \operatorname{dom} T\}$ is the *range* of T. In infinite-dimensional spaces, however, injectivity is not equivalent to surjectivity (see Exercise 2).

If $\lambda \notin \sigma_{\mathrm{p}}(H)$, then the inverse operator $(H - \lambda I)^{-1}$ is well defined on $\operatorname{dom}(H - \lambda I)^{-1} := \operatorname{ran}(H - \lambda I)$. Since $H - \lambda I$ is not necessarily surjective, the operator $(H - \lambda I)^{-1}$ is *a priori* not defined on the entire space $\mathcal{H}$. Even if it happens to be defined on the entire space $\mathcal{H}$ (*i.e.* $\operatorname{ran}(H-\lambda I) = \mathcal{H}$) or its dense subspace (*i.e.* $\overline{\operatorname{ran}(H - \lambda I)} = \mathcal{H}$), it might not be bounded. To handle this situation, we are led to the following generalisation of eigenvalues.

Definition 1.10. Let H be an operator in a Hilbert space $\mathcal{H}$. The *continuous spectrum* of H is defined by:

$$\sigma_{\mathrm{c}}(H) := \Big\{\lambda \in \mathbb{C} \setminus \sigma_{\mathrm{p}}(H) : \ \exists \underset{\|\psi_n\|=1}{\{\psi_n\}_{n\in\mathbb{N}}} \subset \operatorname{dom} H, \quad \|H\psi_n - \lambda\psi_n\| \xrightarrow[n\to\infty]{} 0\Big\} \,.$$

Any element $\lambda \in \sigma_{\mathrm{c}}(H)$ is called an *approximate eigenvalue* of H. Any corresponding sequence $\{\psi_n\}_{n\in\mathbb{N}}$ is called the *approximate eigenvector* (or *quasi-mode*) of H corresponding to the approximate eigenvalue λ.

Proposition 1.11. *Let H be an operator in a Hilbert space $\mathcal{H}$. Let $\lambda \notin \sigma_{\mathrm{p}}(H)$. Then*

$$\lambda \in \sigma_{\mathrm{c}}(H) \quad \Longleftrightarrow \quad (H - \lambda I)^{-1} \ \textit{is unbounded.}$$

Proof.

$\boxed{\Longrightarrow}$ By definition of the inverse, for every $f \in \operatorname{ran}(H-\lambda I)$, there exists $\phi \in \operatorname{dom} H$ such that $(H-\lambda I)\phi = f$. Consequently,

$$\|(H - \lambda I)^{-1}\| := \sup_{\substack{f\in\operatorname{dom}(H-\lambda I)^{-1} \\ f\neq 0}} \frac{\|(H - \lambda I)^{-1} f\|}{\|f\|} = \sup_{\substack{\phi\in\operatorname{dom} H \\ \phi\neq 0}} \frac{\|\phi\|}{\|(H - \lambda I)\phi\|} \,.$$

If $\lambda \in \sigma_{\mathrm{c}}(H)$, then

$$\|(H-\lambda I)^{-1}\| \geq \frac{\|\psi_n\|}{\|(H-\lambda I)\psi_n\|} \xrightarrow[n\to\infty]{} \infty\,,$$

where $\{\psi_n\}_{n\in\mathbb{N}}$ is an approximate eigenvector of H corresponding to λ; hence $(H-\lambda I)^{-1}$ is unbounded.

$\boxed{\Longleftarrow}$ Conversely, if $(H-\lambda I)^{-1}$ is unbounded (*i.e.*, $\|(H-\lambda I)^{-1}\| = \infty$), then, for every $n \in \mathbb{N}$, there exists $\phi_n \in \operatorname{dom} H$ such that

$$\frac{\|\phi_n\|}{\|(H-\lambda I)\phi_n\|} \geq n\,.$$

Since necessarily $\phi_n \neq 0$, the normalised vector $\psi_n := \phi_n/\|\phi_n\|$ satisfies

$$\|(H-\lambda I)\psi_n\| \leq \frac{1}{n}\,;$$

hence $\lambda \in \sigma_{\mathrm{c}}(H)$ by Definition 1.10. □

We define the spectrum of any operator H as the union of its eigenvalues and approximate eigenvalues. Notice that, contrary the point spectrum, the definition of the continuous spectrum requires the norm structure of the Hilbert space $\mathcal{H}$.

Definition 1.12. Let H be an operator in a Hilbert space $\mathcal{H}$. The *spectrum* of H is defined by:

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

By definition of the individual components, it is the disjoint union. Finally, let us state a uniform characterisation of the points in the spectrum.

Proposition 1.13. *Let H be an operator in a Hilbert space $\mathcal{H}$. Then*

$$\sigma(H) = \Big\{\lambda \in \mathbb{C}:\ \exists \underset{\|\psi_n\|=1}{\{\psi_n\}_{n\in\mathbb{N}}} \subset \operatorname{dom} H, \quad \|H\psi_n - \lambda\psi_n\| \xrightarrow[n\to\infty]{} 0\Big\}\,.$$

Proof. Eigenvalues λ of H clearly satisfy the identity (choose for ψ_n the normalised eigenvector of H corresponding to λ, obtaining in this way a stationary sequence). Excluding the eigenvalues, we are back at the definition of the continuous spectrum. □

The reader is warned that our Definition 1.12 does not coincide with the usual definition of the spectrum of a general operator H in a Hilbert space $\mathcal{H}$. There is also the so-called *residual spectrum*, which is formed by those complex numbers $\lambda \notin \sigma_{\mathrm{p}}(H)$ for which the closure of $\operatorname{ran}(H-\lambda I)$ does not coincide with $\mathcal{H}$ (*i.e.* the inverse operator $(H-\lambda I)^{-1}$ is not densely defined). However, this pathological part of the spectrum is always empty in an important case, namely, when H is *self-adjoint*, which is always the case of the operators considered in this course.

1.4 Other boundary conditions

In the previous sections, we interpreted (4) with (5) as the spectral problem for the Dirichlet Laplacian. How to handle the Neumann (6) and Robin (7) boundary conditions? Schematically, we are interested in a rigorous interpretation of the boundary-value problem

$$\lambda \in \sigma(-\Delta_\alpha^\Omega) \qquad \longleftrightarrow \qquad \begin{cases} -\Delta\psi = \lambda\psi & \text{in} \quad \Omega\,, \\ \dfrac{\partial\psi}{\partial n} + \alpha\psi = 0 & \text{on} \quad \partial\Omega\,, \end{cases} \tag{1.19}$$

where $\alpha \in \mathbb{R}$ and n is the outward unit normal of $\partial\Omega$. The Neumann case corresponds to $\alpha = 0$ (in which case we usually use the index N). Since our definition of the spectrum in Section 1.3 is abstract, it remains to introduce suitable self-adjoint realisations of the Robin Laplacians $-\Delta_\alpha^\Omega$. The convenient Hilbert space is again the Lebesgue space $L^2(\Omega)$.

The classical interpretation of the boundary-value problem (1.19) requires certain smoothness of Ω, at least to define the normal n. Just for a moment(!), let us therefore assume that Ω is bounded and of class C^2 (*i.e.* the boundary $\partial\Omega$ is locally a graph of a twice continuously differentiable function). Consider the domain

$$\mathcal{D}_\alpha := \left\{ \psi \in C^2(\overline{\Omega}) \ : \ \frac{\partial\psi}{\partial n} + \alpha\psi = 0 \text{ on } \partial\Omega \right\}.$$

Motivated by the Dirichlet case, where we introduced the Dirichlet Laplacian through an associated sesquilinear form, let us see what the natural form associated with (1.19) is. Integrating by parts as in (1.4), we have

$$\begin{aligned} \forall \phi,\psi \in \mathcal{D}_\alpha\,, \qquad (\phi, -\Delta\psi) &= -\int_\Omega \bar{\phi}\,\Delta\psi = -\int_\Omega \nabla\cdot(\bar{\phi}\,\nabla\psi) + \int_\Omega \nabla\bar{\phi}\cdot\nabla\psi \\ &= -\int_{\partial\Omega} \bar{\phi}\,\frac{\partial\psi}{\partial n} + \int_\Omega \nabla\bar{\phi}\cdot\nabla\psi \\ &= \alpha\int_{\partial\Omega} \bar{\phi}\,\psi + \int_\Omega \nabla\bar{\phi}\cdot\nabla\psi =: Q_\alpha^\Omega(\phi,\psi). \end{aligned} \tag{1.20}$$

Actually, it is enough to assume that $\phi \in C^1(\Omega)\cap C^0(\overline{\Omega})$ and $\psi \in C^2(\Omega)\cap C^1(\overline{\Omega})$ plus the boundary condition for ψ, but these smoothness nuances are irrelevant for the subsequent analysis. What is more important to notice is that the last formula is well defined for $\phi,\psi \in C^1(\overline{\Omega})$, without requiring the second derivative whatsoever. Q_α^Ω is the natural form associated with the Robin Laplacian. Instead of following the procedure of Section 1.2, which would consist of taking the Friedrichs extension of the Laplacian initially defined on $\mathcal{D}_\alpha$, here we start directly with the form Q_α^Ω.

1.4.1 Neumann boundary conditions

The crucial observation is that the boundary term of Q_α^Ω vanishes in the Neumann case $\alpha = 0$. Then the form naturally extends to the Sobolev space $W^{1,2}(\Omega)$ and no(!) regularity hypotheses about Ω are needed.

Definition 1.14. For every open set $\Omega \subset \mathbb{R}^d$, the *Neumann Laplacian* is the operator $-\Delta_N^\Omega$ in $L^2(\Omega)$ associated with the form

$$Q_N^\Omega[\psi] := \|\nabla\psi\|^2\,, \qquad \operatorname{dom}(Q_N^\Omega) := W^{1,2}(\Omega)\,.$$

Note that the form Q_N^Ω acts as the Dirichlet form Q_D^Ω (see Definition 1.4), but its domain is larger. In fact, the functions in the form domain $\operatorname{dom}(Q_N^\Omega)$ do not satisfy any kind of boundary conditions! How can it be if this form is to be associated with the Neumann Laplacian? To explain this apparent paradox, let us see what the abstract representation formula (1.11) says in the present situation. The identity $Q_N^\Omega(\phi,\psi) = (\phi,\eta)$ for every $\phi \in \operatorname{dom}(Q_N^\Omega)$ and $\psi \in \operatorname{dom}(-\Delta_N^\Omega)$ means

$$\forall \phi \in W^{1,2}(\Omega),\ \psi \in \operatorname{dom}(-\Delta_N^\Omega)\,, \qquad \int_\Omega \nabla\bar{\phi}\cdot\nabla\psi = \int_\Omega \bar{\phi}\,\eta\,.$$

As in the Dirichlet case (1.12), using (*cf* Proposition 1.5) that $W_0^{1,2}(\Omega)$ is a subspace of $W^{1,2}(\Omega)$, we get that $\eta = -\Delta\psi$ is the weak Laplacian of ψ. That is,

$$\forall \phi \in W^{1,2}(\Omega),\ \psi \in \operatorname{dom}(-\Delta_N^\Omega)\,, \qquad \int_\Omega \nabla\bar{\phi}\cdot\nabla\psi = -\int_\Omega \bar{\phi}\,\Delta\psi\,.$$

Assume just for a moment(!) that we could integrate by parts in the integral on the left-hand side (which would require that ψ as well as Ω are sufficiently regular; for example, Ω is a bounded domain of class C^2 and $\psi \in W^{2,2}(\Omega)$), then

$$\forall \phi \in W^{1,2}(\Omega),\ \psi \in \operatorname{dom}(-\Delta_N^\Omega)\,, \qquad \int_{\partial\Omega} \bar{\phi}\,\frac{\partial\psi}{\partial n} - \int_\Omega \bar{\phi}\,\Delta\psi = -\int_\Omega \bar{\phi}\,\Delta\psi\,.$$

Using the arbitrariness of ϕ, it would follow that $\frac{\partial\psi}{\partial n} = 0$ on $\partial\Omega$. In summary,

$$-\Delta_N^\Omega \psi = -\Delta\psi\,, \qquad \mathrm{dom}(-\Delta_N^\Omega) = \left\{\psi \in W^{1,2}(\Omega) :\ \Delta\psi \in L^2(\Omega) \ \wedge\ \frac{\partial\psi}{\partial n} = 0 \text{ on } \partial\Omega\right\}. \tag{1.21}$$

It is the explanation of the aforementioned paradox: The Neumann boundary condition naturally appears in the operator domain despite the presence of no boundary condition in the form domain. For an arbitrary open set Ω, the specification of the operator domain (1.21) remains true, provided that we interpret the validity of the Neumann boundary condition in the following weak sense:

$$\frac{\partial\psi}{\partial n} = 0 \text{ on } \partial\Omega \qquad :\Longleftrightarrow \qquad \forall\phi,\psi \in W^{1,2}(\Omega),\ \Delta\psi \in L^2(\Omega)\,, \quad (\nabla\phi,\nabla\psi) = -(\phi,\Delta\psi)\,.$$

If Ω is nice (for example, bounded and of class C^2), then

$$\mathrm{dom}(-\Delta_N^\Omega) = \left\{\psi \in W^{2,2}(\Omega)\ :\ \frac{\partial\psi}{\partial n} = 0 \text{ on } \partial\Omega\right\}, \tag{1.22}$$

where the boundary condition $\frac{\partial\psi}{\partial n} = 0$ on $\partial\Omega$ can be interpreted in the sense of traces. Again, the inclusion $\supset$ is elementary, while the opposite inclusion $\subset$ requires further methods, namely elliptic regularity theory for the boundary-value Neumann problem (see, *e.g.*, [11, Thm. 9.26]).

Remark 1.15 (Lipschitz sets)**.** In analogy with Remark 1.8, we can say more for sets Ω whose boundary $\partial\Omega$ can be parameterised by a *finite* covering of Lipschitz maps. Then (1.21) still holds (*cf* [56]) if the boundary condition $\frac{\partial\psi}{\partial n} = 0$ on $\partial\Omega$ is interpreted as a trace in $W^{-1/2,2}(\partial\Omega)$. Moreover, if Ω is in addition *bounded*, it is a deep result of [44] that

$$\mathrm{dom}(-\Delta_N^\Omega) = \left\{\psi \in W^{3/2,2}(\Omega)\ :\ \Delta\psi \in L^2(\Omega)\ \wedge\ \frac{\partial\psi}{\partial n} = 0 \text{ on } \partial\Omega\right\} \tag{1.23}$$

and the extra regularity enables one to interpret the boundary trace as an element of $L^2(\partial\Omega)$.

1.4.2 Robin boundary conditions

It is customary to define general Robin boundary conditions with help of the form Q_α^Ω introduced in (1.20), where the boundary integral is understood as a perturbation of the Neumann form Q_N^Ω corresponding to $\alpha = 0$. To this purpose, we make the geometric hypothesis about the existence of the trace embedding $W^{1,2}(\Omega) \hookrightarrow L^2(\partial\Omega)$. More specifically, we assume that, for every $\delta > 0$ there exists a constant C_δ depending on δ and the geometry of Ω such that

$$\forall\psi \in W^{1,2}(\Omega)\,, \qquad \|\psi\|^2_{L^2(\partial\Omega)} \le \delta\,\|\nabla\psi\|^2 + C_\delta\,\|\psi\|^2\,. \tag{1.24}$$

Then the boundary integral of Q_α^Ω is relatively bounded with respect to Q_N^Ω with the relative bound equal to zero. Consequently, the symmetric form Q_α^Ω is closed and bounded from below [47, Thm. VI.1.33].

Definition 1.16. For every open set $\Omega \subset \mathbb{R}^d$ satisfying (1.24) and $\alpha \in \mathbb{R}$, the *Robin Laplacian* is the operator $-\Delta_\alpha^\Omega$ in $L^2(\Omega)$ associated with the form

$$Q_\alpha^\Omega[\psi] := \|\nabla\psi\|^2 + \alpha\|\psi\|^2_{L^2(\partial\Omega)}\,, \qquad \mathrm{dom}(Q_\alpha^\Omega) := W^{1,2}(\Omega)\,.$$

Hypothesis (1.24) is satisfied for nice domains Ω, for example, if Ω is bounded and of class C^2. Moreover, by means of the elliptic regularity theory, for such domains one has

$$\mathrm{dom}(-\Delta_\alpha^\Omega) = \left\{\psi \in W^{2,2}(\Omega)\ :\ \frac{\partial\psi}{\partial n} + \alpha\psi = 0 \text{ on } \partial\Omega\right\}, \qquad -\Delta_\alpha^\Omega\psi = -\Delta\psi\,.$$

To see that (1.24) holds for the nice domains, one can use a local straightening of the boundary $\partial\Omega$ by means of curvilinear coordinates and the following elementary one-dimensional bound.

Lemma 1.17. *For every $l > 0$, we have*

$$\forall \varphi \in W^{1,2}((-l,l))\,, \qquad \sup_{(-l,l)} |\varphi|^2 \leq 2\, \|\varphi\|_{L^2((-l,l))}\, \|\varphi'\|_{L^2((-l,l))} + \frac{1}{2l}\, \|\varphi\|^2_{L^2((-l,l))}\,. \tag{1.25}$$

Proof. By the density $C^\infty([-l,l])$ in $W^{1,2}((-l,l))$, it is enough to prove the estimate for $\varphi \in C^\infty([-l,l])$. For every $x \in [-l,l]$, we write

$$|\varphi(x)|^2 - |\varphi(l)|^2 = \int_l^x (|\varphi|^2)' = \int_l^x 2\,\Re(\overline{\varphi}\varphi') \leq \int_x^l 2|\varphi||\varphi'|\,,$$
$$|\varphi(x)|^2 - |\varphi(-l)|^2 = \int_{-l}^x (|\varphi|^2)' = \int_{-l}^x 2\,\Re(\overline{\varphi}\varphi') \leq \int_{-l}^x 2\,|\varphi||\varphi'|\,.$$

Summing up these two estimates and applying the Schwarz inequality, we arrive at

$$|\varphi(x)|^2 \leq \frac{|\varphi(l)|^2 + |\varphi(-l)|^2}{2} + \|\varphi\|_{L^2((-l,l))}\, \|\varphi'\|_{L^2((-l,l))}\,. \tag{1.26}$$

To estimate the boundary values of φ, we set $\xi(x) := x/l$ and write similarly as above

$$|\varphi(l)|^2 + |\varphi(-l)|^2 = \int_{-l}^l (\xi|\varphi|^2)' = \int_{-l}^l \xi\, 2\,\Re(\overline{\varphi}\varphi') + \int_{-l}^l \xi'\, |\varphi|^2 \leq \int_{-l}^l 2\,|\varphi||\varphi'| + \frac{1}{l}\int_{-l}^l |\varphi|^2\,,$$

where the inequality employs the facts that $|\xi| \leq 1$ and $|\xi'| \leq l^{-1}$. Applying the Schwarz inequality to the first term on the right-hand side as above and plugging the obtained estimate to (1.26), we obtain (1.25). $\square$

Remark 1.18. Inequality (1.25) is sharp, as can be verified for a constant choice of φ.

Remark 1.19 (Unifying convention)**.** Henceforth we use the common symbol $-\Delta_\alpha^\Omega$ to denote both the Robin Laplacian if $\alpha \in \mathbb{R}$ and the Dirichlet Laplacian if $\alpha = \infty$. In the special situation $\alpha = 0$ or $\alpha = \infty$ we also write $-\Delta_N^\Omega$ and $-\Delta_D^\Omega$, respectively. If $\alpha \in \{0, \infty\}$, no regularity about Ω is assumed, unless otherwise stated. If $\alpha \in \mathbb{R} \setminus \{0\}$ and the Robin Laplacian $-\Delta_\alpha^\Omega$ is to be considered, *we implicitly assume the validity of* (1.24). In the latter case we of course restrict the class of admissible Ω.

1.5 Homothetic transformations

Let $\Omega \subset \mathbb{R}^d$ be an arbitrary open set. By a *homothetic transformation* of Ω we understand a simultaneously translated and dilated image of Ω. More specifically, given any point $x_0 \in \mathbb{R}^d$ and a positive number ϵ, let us consider the mapping

$$\mathscr{L}_\epsilon : \mathbb{R}^d \to \mathbb{R}^d : \{x \mapsto x_0 + \epsilon x\}\,. \tag{1.27}$$

The action of x_0 is a **translation**, while the scaling by ϵ is a **dilation**. If $x_0 = 0$ and $\epsilon = 1$, then $\mathscr{L}_\epsilon$ is an identity. The image $\mathscr{L}_\epsilon(\Omega)$ is a **homothetic transformation** of Ω. Occasionally, we also write $x_0 + \Omega := \{x_0 + x : x \in \Omega\}$ and $\epsilon\Omega := \{\epsilon x : x \in \Omega\}$. Then $\mathscr{L}_\epsilon(\Omega) = x_0 + \epsilon\Omega$.

Theorem 1.20 (Change of the spectrum under homothety)**.** *Let $\Omega \subset \mathbb{R}^d$ be an open set and $\alpha \in L^\infty(\partial\Omega)$ or $\alpha = \infty$ (unless $\alpha \in \{0,\infty\}$, we assume* (1.24)*). For any $x_0 \in \mathbb{R}^d$ and $\epsilon > 0$, consider the homothety* (1.27)*. Then*

$$\sigma\left(-\Delta^{\mathscr{L}_\epsilon(\Omega)}_{\epsilon^{-1}\alpha\circ\mathscr{L}_\epsilon^{-1}}\right) = \epsilon^{-2}\,\sigma(-\Delta_\alpha^\Omega)\,. \tag{1.28}$$

In particular, $\sigma\big(-\Delta_D^{\mathscr{L}_\epsilon(\Omega)}\big) = \epsilon^{-2}\,\sigma(-\Delta_D^\Omega)$ and $\sigma\big(-\Delta_N^{\mathscr{L}_\epsilon(\Omega)}\big) = \epsilon^{-2}\,\sigma(-\Delta_N^\Omega)$.

Proof. By exchanging the role of $\mathscr{L}_\epsilon(\Omega)$ and Ω, it is enough to show that the set on the right-hand side of (1.28) is a subset of the left-hand side. For simplicity, let us set $\Omega_\epsilon := \mathscr{L}_\epsilon(\Omega)$ and $\alpha_\epsilon := \alpha \circ \mathscr{L}_\epsilon^{-1}$.

Let $\lambda \in \sigma(-\Delta_\alpha^\Omega)$. Then there exists a sequence $\{\psi_j\}_{j\in\mathbb{N}} \subset \mathrm{dom}(-\Delta_\alpha^\Omega)$ such that

$$\forall j \in \mathbb{N}\,, \qquad \|\psi_j\|_{L^2(\Omega)} = 1 \qquad \text{and} \qquad \lim_{j\to\infty} \| -\Delta\psi_j - \lambda\psi_j\|_{L^2(\Omega)} = 0\,. \tag{1.29}$$

Our strategy is to show that the transformed elements

$$\psi_j^\epsilon := \epsilon^{-d/2}\, \psi_j \circ \mathscr{L}_\epsilon^{-1} \tag{1.30}$$

form a sequence in $\mathrm{dom}(-\Delta_{\epsilon^{-1}\alpha_\epsilon}^{\Omega_\epsilon})$ that satisfies

$$\forall j \in \mathbb{N}\,, \qquad \|\psi_j^\epsilon\|_{L^2(\Omega_\epsilon)} = 1 \qquad \text{and} \qquad \lim_{j\to\infty} \| -\Delta\psi_j^\epsilon - \epsilon^{-2}\lambda\, \psi_j^\epsilon\|_{L^2(\Omega_\epsilon)} = 0\,. \tag{1.31}$$

This will prove the claim by Proposition 1.13.

First of all, it is easy to see that $\phi \in W^{1,2}(\Omega)$ implies $\phi^\epsilon \in W^{1,2}(\Omega_\epsilon)$, where ϕ^ϵ is defined in analogy with (1.30). At the same time, $\phi \in W_0^{1,2}(\Omega)$ implies $\phi^\epsilon \in W_0^{1,2}(\Omega_\epsilon)$. To see it, we recall that $\phi \in W_0^{1,2}(\Omega)$ means that there exists a sequence $\{\phi_k\}_{k\in\mathbb{N}} \subset C_0^\infty(\Omega)$ such that $\phi_k \to \phi$ in the norm of $W^{1,2}(\Omega)$ as $k \to \infty$. Then $\{\phi_k^\epsilon\}_{k\in\mathbb{N}} \subset C_0^\infty(\Omega_\epsilon)$ and, by a change of variables, $\phi_k^\epsilon \to \phi^\epsilon$ in the norm of $W^{1,2}(\Omega^\epsilon)$ as $k \to \infty$. Consequently, the transformed sequence (1.30) belongs to the form domain of $-\Delta_{\epsilon^{-1}\alpha_\epsilon}^{\Omega_\epsilon}$.

To show that (1.30) actually belongs to the domain of the operator $-\Delta_{\epsilon^{-1}\alpha_\epsilon}^{\Omega_\epsilon}$, we use the fact that $\psi_j \in \mathrm{dom}(-\Delta_\alpha^\Omega)$ means that $\psi_j \in \mathrm{dom}(Q_\alpha^\Omega)$ additionally satisfies

$$\forall \phi \in \mathrm{dom}(Q_\alpha^\Omega)\,, \qquad Q_\alpha^\Omega(\phi, \psi_j) = (\phi, -\Delta\psi_j)_{L^2(\Omega)}\,.$$

If $\alpha = \infty$, the condition reads

$$\forall \phi \in W_0^{1,2}(\Omega)\,, \qquad (\nabla\phi, \nabla\psi_j)_{L^2(\Omega)} = (\phi, -\Delta\psi_j)_{L^2(\Omega)}\,.$$

By a change of variables (using $\mathrm{d}\Omega^\epsilon = \epsilon^d \mathrm{d}\Omega$), it follows that

$$\forall \phi^\epsilon \in W_0^{1,2}(\Omega)\,, \qquad \epsilon^2\, (\nabla\phi^\epsilon, \nabla\psi_j^\epsilon)_{L^2(\Omega_\epsilon)} = \epsilon^2\, (\phi^\epsilon, -\Delta\psi_j^\epsilon)_{L^2(\Omega_\epsilon)}\,.$$

By dividing by ϵ^2, we get that $\{\psi_j^\epsilon\}_{n\in\mathbb{N}} \subset \mathrm{dom}(-\Delta_D^{\Omega_\epsilon})$, which settles the Dirichlet case. Let us now turn to Robin boundary conditions, assuming that $\alpha : \partial\Omega \to \mathbb{R}$ is a bounded function (which includes the Neumann case $\alpha = 0$). Then we know

$$\forall \phi \in W^{1,2}(\Omega)\,, \qquad (\nabla\phi, \nabla\psi_j)_{L^2(\Omega)} + (\phi, \alpha\psi_j)_{L^2(\partial\Omega)} = (\phi, -\Delta\psi_j)_{L^2(\Omega)}\,.$$

By a change of variables (using additionally $\mathrm{d}\partial\Omega^\epsilon = \epsilon^{d-1}\mathrm{d}\partial\Omega$), it follows that

$$\forall \phi^\epsilon \in W^{1,2}(\Omega)\,, \qquad \epsilon^2\, (\nabla\phi^\epsilon, \nabla\psi_j^\epsilon)_{L^2(\Omega_\epsilon)} + \epsilon\, (\phi^\epsilon, \alpha_\epsilon\, \psi_j^\epsilon)_{L^2(\partial\Omega_\epsilon)} = \epsilon^2\, (\phi^\epsilon, -\Delta\psi_j^\epsilon)_{L^2(\Omega_\epsilon)}$$

(recall the difference between the definition of α_ϵ and ϕ^ϵ). From this formula, it is clear that we need a non-trivial rescaling of the function α in (1.28), unless $\alpha = 0$ or $\alpha = \infty$. Indeed, by dividing by ϵ^2, we conclude that $\{\psi_j^\epsilon\}_{n\in\mathbb{N}} \subset \mathrm{dom}(-\Delta_{\epsilon^{-1}\alpha_\epsilon}^{\Omega_\epsilon})$.

After these prerequisites, verifying (1.31) is just the matter of a change of variables as above using (1.29). □

In the context of vibrational systems, a physical interpretation of Theorem 1.20 is that moving any membrane in space does not change the resonant frequences, while homothetically expanding (respectively, shrinking) a membrane with fixed or free edges by a parameter $\epsilon > 1$ (respectively, $\epsilon < 1$) will lower (respectively, raise) the frequences exactly by the factor ϵ^{-1}. The same change of resonant frequences in the case of Robin boundary conditions requires a simultaneous re-scaling of the boundary function α.

An analogous interpretation can be given in the context of bound-state energies of a quantum particle constrained to a nanostructure of shape Ω.

Chapter 2

Quasi-conical domains

In this chapter we are concerned with spectral properties of the Dirichlet Laplacian $-\Delta_D^\Omega$ in the situation where Ω is a quasi-conical domain. Recall (*cf* Definition 0.1) that Ω is called quasi-conical if it contains an arbitrarily large ball (see Figure 2.1 for an example). This class of domains contains the whole Euclidean space $\mathbb{R}^d$ as a particular example (in quantum mechanics, $-\Delta_D^{\mathbb{R}^d}$ represents the kinetic energy of a free particle). Another example is given by cones (or their exteriors).

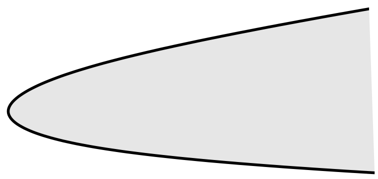


Figure 2.1: A quasi-conical planar domain.

2.1 Location of the spectrum

Let Ω be an arbitrary quasi-conical open set. By definition, there exist sequences of centres $\{x_j\}_{j\in\mathbb{N}} \subset \Omega$ and radii $\{R_j\}_{j\in\mathbb{N}} \subset (0,\infty)$ such that $B_{R_j}(x_j) \subset \Omega$ and $R_j \to \infty$ as $j \to \infty$. Here $B_R(x) := \{x \in \mathbb{R}^d : |x| < R\}$ denotes the open ball of centre x and radius R. Notice that Ω is necessarily unbounded.

2.1.1 The spectrum is non-negative

Let $\lambda \in \sigma(H)$. By our definition of the spectrum (*cf* Proposition 1.13), there exists a sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset \mathrm{dom}(-\Delta_D^\Omega)$ such that $\|\psi_n\| = 1$ for every $n \in \mathbb{N}$ and $-\Delta_D^\Omega \psi_n - \lambda\psi_n \to 0$ as $n \to \infty$. We have

$$\begin{aligned}
\lambda &= \lambda \|\psi_n\|^2 \\
&= \lim_{n\to\infty} \lambda \|\psi_n\|^2 \\
&= \lim_{n\to\infty} (\psi_n, \lambda\psi_n) \\
&= \lim_{n\to\infty} (\psi_n, -\Delta_D^\Omega \psi_n) \\
&= \lim_{n\to\infty} Q_D^\Omega(\psi_n, \psi_n) \\
&= \lim_{n\to\infty} \|\nabla\psi_n\|^2 \\
&\geq 0\,.
\end{aligned}$$

Hence, λ is not only real (as one would expect from a self-adjoint operator), but it is in fact non-negative. Notice that, in the proof, we have not used the geometric property of Ω being quasi-conical. So this result actually holds for any open set Ω.

Proposition 2.1. *Let $\Omega \subset \mathbb{R}^d$ be any open set. Then*

$$\sigma(-\Delta_D^\Omega) \subset [0, \infty) \, .$$

Remark 2.2. It is clear from the proof of Proposition (2.1) that the spectral property follows from the fact that the quadratic form of the Dirichlet Laplacian is non-negative. In fact, the proof remains true without any changes for the Neumann Laplacian, *i.e.*, $\sigma(-\Delta_N^\Omega) \subset [0, \infty)$ as well (for an arbitrary open set Ω). More generally, one has $\sigma(-\Delta_\alpha^\Omega) \subset [0, \infty)$ for every $\alpha \geq 0$ (at least for the open sets satisfying (1.24)).

On the other hand, there might be a negative spectrum for the Robin Laplacian $-\Delta_\alpha^\Omega$ with $\alpha < 0$. For instance, it is easy to verify that $-\alpha^2$ is a (unique) eigenvalue of $-\Delta_\alpha^{(0,\infty)}$ whenever $\alpha < 0$. Indeed, the corresponding eigenfunction (satisfying the differential equation $-\psi'' = -\alpha^2 \psi$ together with the Robin boundary condition $-\psi'(0) + \alpha \psi(0) = 0$) explicitly reads $\psi(x) := e^{\alpha x}$.

2.1.2 Looking for eigenvalues

Let us consider the eigenvalue problem $-\Delta_D^\Omega \psi = \lambda \psi$ with $\lambda \geq 0$. This is equivalent to looking for non-zero solutions of the Helmholtz equation

$$-\Delta \psi = \lambda \psi \quad \text{in} \quad \Omega \tag{2.1}$$

with $\lambda \geq 0$ such that $\psi \in W_0^{1,2}(\Omega)$ and $\Delta \psi \in L^2(\Omega)$. The differential equation (2.1) admits a classical solution (plane waves)

$$w_k(x) := e^{ik\cdot x} \qquad \text{with any} \quad k \in \mathbb{R}^d \quad \text{such that} \quad |k|^2 = \lambda \, . \tag{2.2}$$

This suggests that $\sigma_{\mathrm{p}}(-\Delta_D^\Omega) = [0, \infty)$. What is wrong?

Of course, the solutions (2.2) are not admissible, because $w_k \notin W_0^{1,2}(\Omega)$. Indeed, without mentioning the violation of Dirichlet boundary conditions, we have

$$\|w_k\|^2 = \int_\Omega 1 = |\Omega| = \infty$$

(because the volume of Ω is infinite for quasi-conical domains), so w_k does not even belong to the Hilbert space $L^2(\Omega)$. We do not get any eigenvalue of the Dirichlet Laplacian $-\Delta_D^\Omega$ by considering (2.2). Anyway, we can use these classical solutions of (2.1) to construct approximate eigenfunctions.

2.1.3 Construction of approximate eigenfunctions

The key observation is that the classical solutions (2.2) are *bounded*, so that an approximation of these plane-wave solutions by a sequence playing the role of the approximate eigenfunction of Definition 1.10 is possible.

Let φ be a function from $C_0^\infty(\mathbb{R}^d)$, normalised to 1 in $L^2(\mathbb{R}^d)$, *i.e.* $\|\varphi\|_{L^2(\mathbb{R}^d)} = 1$. For any $n \in \mathbb{N}^*$ and $\{a_n\}_{n\in\mathbb{N}^*} \subset \mathbb{R}^d$, we set

$$\varphi_n(x) := N_n \, \varphi\!\left(\frac{x - a_n}{n}\right) \qquad \text{with} \qquad N_n := n^{-d/2} \, .$$

The prefactor N_n is chosen in such a way that also each φ_n is normalised to 1 in $L^2(\mathbb{R}^d)$. Indeed, by an obvious change of variables, we have

$$\|\varphi_n\|_{L^2(\mathbb{R}^d)}^2 = |N_n|^2 \int_{\mathbb{R}^d} \left|\varphi\!\left(\frac{x - a_n}{n}\right)\right|^2 \mathrm{d}x = \int_{\mathbb{R}^d} |\varphi(y)|^2 \, \mathrm{d}y = \|\varphi\|_{L^2(\mathbb{R}^d)}^2 = 1 \, . \tag{2.3}$$

With respect to the support of φ, the support of φ_n is translated by the vector a_n and scaled by n (see Figure 2.2):

$$\operatorname{supp} \varphi_n = a_n + n \operatorname{supp} \varphi \, . \tag{2.4}$$

By the property of the set Ω being quasi-conical, for each $n \in \mathbb{N}^*$ there exists $j_n \in \mathbb{N}^*$ such that

$$\operatorname{supp} \varphi_n \subset B_{R_{j_n}}(x_{j_n}) \subset \Omega \qquad \text{with} \qquad a_n := x_{j_n} .$$

Hence, $\varphi_n \in \operatorname{dom}(-\Delta_D^\Omega)$. For any $n \in \mathbb{N}^*$, we define

$$\psi_n(x) := \varphi_n(x)\, e^{ik\cdot x} , \tag{2.5}$$

which also belongs to $\operatorname{dom}(-\Delta_D^\Omega)$. By (2.3), $\|\psi_n\| = 1$ for every $n \in \mathbb{N}^*$.

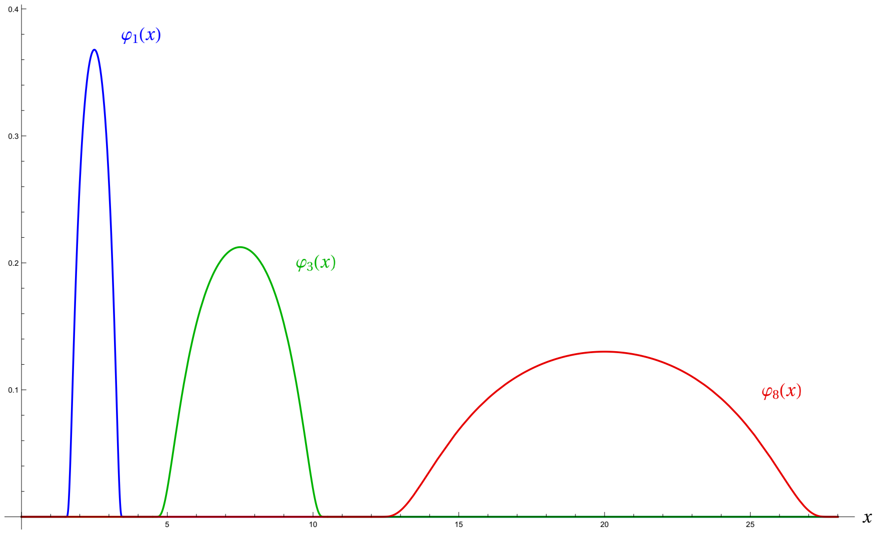


Figure 2.2: The sequence of functions φ_n for $d = 1$ smearing out and locating at $+\infty$ as $n \to \infty$.

In order to ensure that $\{\psi_n\}_{n\in\mathbb{N}^*}$ is the approximate eigenfunction corresponding to the approximate eigenvalue k^2, it remains to verify that $-\Delta_D^\Omega \psi_n - k^2\psi_n \to 0$ in $L^2(\Omega)$ as $n \to \infty$. Since $\psi_n \in C_0^\infty(\Omega)$, the action of $-\Delta_D^\Omega$ is that of the classical Laplacian. We compute

$$\begin{aligned}
\nabla\psi_n(x) &= [\nabla\varphi_n(x) + ik\,\varphi_n(x)]\, e^{ik\cdot x} ,\\
\Delta\psi_n(x) &= \nabla\cdot\nabla\psi_n(x) = \big[\Delta\varphi_n(x) + 2ik\cdot\nabla\varphi_n(x) - k^2\,\varphi_n(x)\big]\, e^{ik\cdot x} .
\end{aligned}$$

Consequently,

$$-\Delta_D^\Omega\psi_n - k^2\psi_n = [-\Delta\varphi_n(x) - 2ik\cdot\nabla\varphi_n(x)]\, e^{ik\cdot x} ,$$

and therefore

$$\| - \Delta_D^\Omega\psi_n - k^2\psi_n\| \leq \|\Delta\varphi_n\| + 2\,|k|\,\|\nabla\varphi_n\| .$$

The right-hand side vanishes as $n \to \infty$, indeed:

$$\begin{aligned}
\|\nabla\varphi_n\|^2 &= |N_n|^2 \int_{\mathbb{R}^d} \left|\frac{1}{n}\nabla\varphi\left(\frac{x-a_n}{n}\right)\right|^2 \mathrm{d}x = \frac{1}{n^2}\int_{\mathbb{R}^d} |\nabla\varphi(y)|^2\,\mathrm{d}y = \frac{1}{n^2}\|\nabla\varphi\|^2 ,\\
\|\Delta\varphi_n\|^2 &= |N_n|^2 \int_{\mathbb{R}^d} \left|\frac{1}{n^2}\Delta\varphi\left(\frac{x-a_n}{n}\right)\right|^2 \mathrm{d}x = \frac{1}{n^4}\int_{\mathbb{R}^d} |\Delta\varphi(y)|^2\,\mathrm{d}y = \frac{1}{n^4}\|\Delta\varphi\|^2 .
\end{aligned}$$

In summary, we have just proven the following theorem.

Theorem 2.3 (Spectrum of quasi-conical domains). *If Ω is a quasi-conical open set, then*

$$\sigma(-\Delta_D^\Omega) = [0,\infty) .$$

2.2 The whole Euclidean space

According to Theorem 2.3, the case of quasi-conical domains is boring, in the sense that the spectrum of the Dirichlet Laplacian $-\Delta_D^\Omega$ is independent of the geometry of Ω. Is there anything spectral-geometrically interesting? The answer is yes if one looks at finer spectral properties. Here we restrict ourselves to the case of the whole Euclidean space $\Omega = \mathbb{R}^d$ and investigate the role of the dimension.

2.2.1 Density properties

First of all, let us state useful properties of Sobolev spaces.

Recall that $W_0^{1,2}(\Omega)$ is the subspace of $W^{1,2}(\Omega)$ which is, roughly, characterised by that its elements vanish on the boundary $\partial\Omega$. Since the whole Euclidean space $\mathbb{R}^d$ has no boundary, the following result is not surprising.

Proposition 2.4. *For every $d \geq 1$,*

$$W_0^{1,2}(\mathbb{R}^d) = W^{1,2}(\mathbb{R}^d) .$$

Proof. The inclusion $\subset$ holds due to Proposition 1.5. Conversely, let us assume that $\psi \in W^{1,2}(\mathbb{R}^d)$. We have to show that there exists a sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset C_0^\infty(\mathbb{R}^d)$ such that $\psi_n \to \psi$ and $\nabla\psi_n \to \nabla\psi$ as $n \to \infty$.

Approximation by compactly supported functions. First of all, let us show that there exists a sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset W_c^{1,2}(\mathbb{R}^d)$ such that $\psi_n \to \psi$ and $\nabla\psi_n \to \nabla\psi$ as $n \to \infty$, where

$$W_c^{1,2}(\mathbb{R}^d) := \{\psi \in W^{1,2}(\mathbb{R}^d) : \ \operatorname{supp}\psi \text{ is compact}\} .$$

Let $\xi \in C_0^\infty(\mathbb{R}^d)$ be any function such that $0 \leq \xi \leq 1$ and $\xi(x) = 1$ for every $|x| \leq 1$. For every $n \in \mathbb{N}^*$, set $\xi_n(x) := \xi(x/n)$, so that $\xi_n \in C_0^\infty(\mathbb{R}^d)$, $0 \leq \xi_n \leq 1$ and $\xi_n(x) = 1$ for every $|x| \leq n$. Since $\xi_n \to 1$ pointwise as $n \to \infty$ (see Figure 2.3) and $|\xi_n\psi| \leq |\psi| \in L^2(\mathbb{R}^2)$, it follows that $\psi_n := \xi_n\psi \in L_0^2(\mathbb{R}^d)$ converges to ψ in $L^2(\mathbb{R}^d)$ as $n \to \infty$ by the dominated convergence theorem. At the same time,

$$\|\nabla\psi_n - \nabla\psi\| = \|(\xi_n - 1)\nabla\psi\| + \|(\nabla\xi_n)\psi\| \leq \|(\xi_n - 1)\nabla\psi\| + n^{-1}\|\nabla\xi\|_{L^\infty(\mathbb{R}^d)}\|\psi\| \xrightarrow[n\to\infty]{} 0 .$$

Here the first term on the right-hand side converges to zero as $n \to \infty$ by the previous argument.

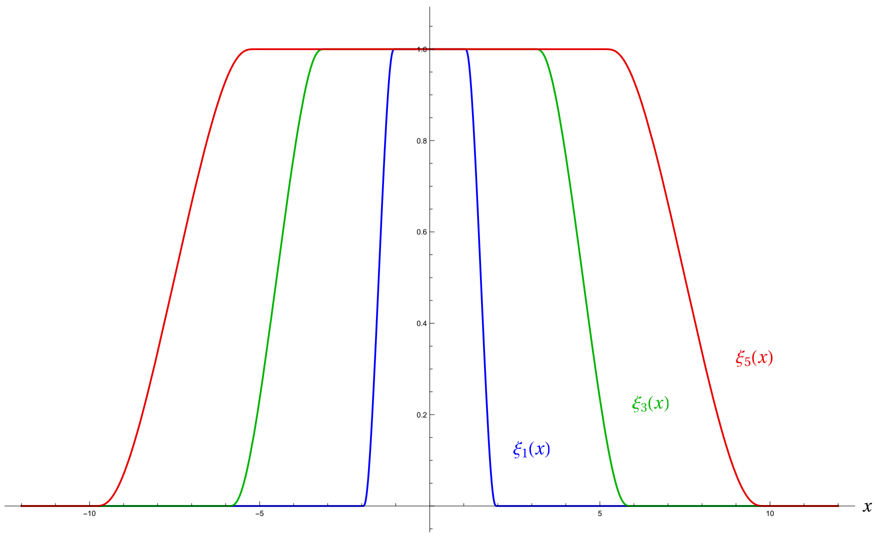


Figure 2.3: The sequence of cut-off functions ξ_n for $d = 1$ approximating 1 pointwise as $n \to \infty$.

Approximation by smooth functions. This is established by a standard mollification argument. Because of the previous step, we may assume that $\psi \in W_c^{1,2}(\mathbb{R}^d)$. Let $\rho \in C_0^\infty(\mathbb{R}^d)$ be any function such that

$$\rho(x) \begin{cases} = 0 & \Leftrightarrow \quad |x| \geq 1 , \\ \geq 0 & \Leftrightarrow \quad |x| < 1 , \end{cases} \qquad \text{and} \qquad \int_{\mathbb{R}^d} \rho(x)\,\mathrm{d}x = 1 .$$

For every $n \in \mathbb{N}^*$, define $\rho_n(x) := n^d\rho(nx)$, so that $\int_{\mathbb{R}^d}\rho_n(x)\,\mathrm{d}x = 1$. Note that $\rho_n \to \delta$ (*Dirac delta*) in the sense of distributions as $n \to \infty$ (see Figure 2.4). We define the approximation sequence by the convolution

$$\psi_n(x) := \int_{\mathbb{R}^d} \rho_n(x-y)\,\psi(y)\,\mathrm{d}y .$$

It is straightforward to verify that $\psi_n \in C_0^\infty(\mathbb{R}^d)$ for each $n \in \mathbb{N}^*$ and $\psi_n \to \psi$ in $W^{1,2}(\mathbb{R}^d)$ as $n \to \infty$ (see, *e.g.*, [23, Sec. 3.2] for more details). □

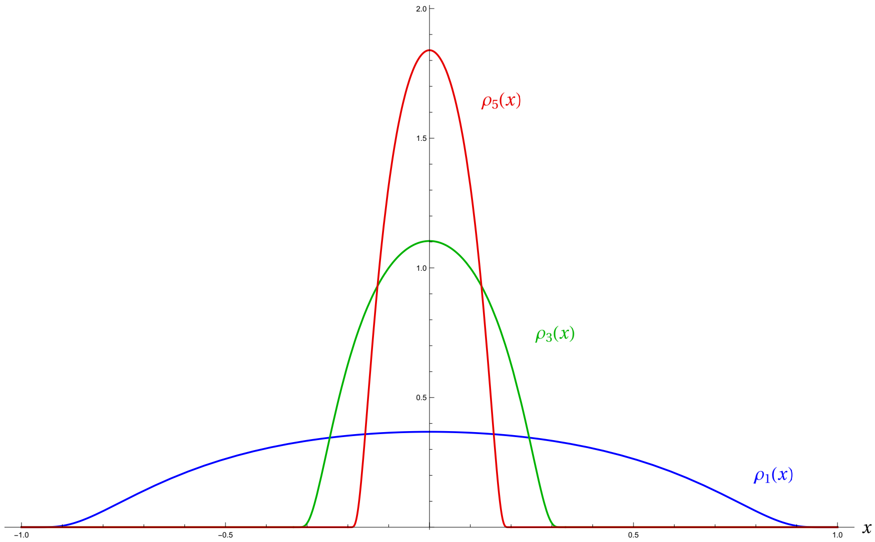


Figure 2.4: The sequence of functions ρ_n for $d = 1$ converging to the Dirac delta as $n \to \infty$.

Proposition 2.4 particularly implies that the Dirichlet Laplacian $-\Delta_D^{\mathbb{R}^d}$ and the Neumann Laplacian $-\Delta_N^{\mathbb{R}^d}$ in the whole Euclidean space $\mathbb{R}^d$ coincide. We simply write $-\Delta^{\mathbb{R}^d} := -\Delta_D^{\mathbb{R}^d} = -\Delta_N^{\mathbb{R}^d}$.

The second density result concerns the question which sets are "negligible" in the setting of Sobolev spaces. More specifically, the sets of measure zero are negligible in the setting of Lebesgue spaces in the following sense:

$$E \subset \Omega \text{ is a set of measure zero} \qquad \Longleftrightarrow \qquad L^2(\Omega \setminus E) = L^2(\Omega)\,.$$

What is an analogue of this result in the setting of Sobolev spaces? Functions in Sobolev spaces are more regular then Lebesgue functions, so it is expected that the class of sets of measure zero must be replaced by a more restrictive class of sets. It turns out that the correct notion is that of *capacity* (indeed the electrostatic capacity, *i.e.* the ability of sets to hold electrical charge). For our purposes, it will be enough to consider the special case of points. Any finite number of points is definitely a set of measure zero, so points, in any dimension, are negligible in the setting of Lebesgue spaces. For Sobolev spaces, however, points are negligible if, and only if, the dimension is at least two (points are able to hold an electrostatic charge in dimension one only).

Proposition 2.5. *One has*

$$d \geq 2 \qquad \Longleftrightarrow \qquad W_0^{1,2}(\mathbb{R}^d \setminus \{0\}) = W_0^{1,2}(\mathbb{R}^d)\,.$$

Proof. The proof of the main direction ($\Longrightarrow$) is somewhat easier in three and higher dimensions. In view of Proposition 2.4, it is enough to show that, given any function $\psi \in C_0^\infty(\mathbb{R}^d)$, there exists a sequence $\{\psi_n\}_{n\in\mathbb{N}} \in C_0^\infty(\mathbb{R}^d \setminus \{0\})$ such that $|||\psi_n - \psi||| \to 0$ as $n \to \infty$.

$\boxed{d \geq 3.}$ Let $\eta \in C^\infty([0,\infty))$ be such that

$$0 \leq \eta \leq 1 \qquad \text{and} \qquad \eta(r) = \begin{cases} 0 & \text{if} \quad r < 1\,, \\ 1 & \text{if} \quad r > 2\,. \end{cases}$$

Define $\eta_n(r) := \eta(nr)$ (see Figure 2.5) and set $\psi_n(x) := \eta_n(|x|)\psi(x)$ for all $n \in \mathbb{N}$. Then

$$\|\psi - \psi_n\|^2 = \int_{\mathbb{R}^d} \left|1 - \eta_n(|x|)\right|^2 |\psi(x)|^2 \, dx \xrightarrow[n\to\infty]{} 0$$

by the dominated convergence theorem. At the same time,

$$\|\nabla(\psi-\psi_n)\|^2 \le 2\int_{\mathbb{R}^d}\big|1-\eta_n(|x|)\big|^2\,|\nabla\psi(x)|^2\,\mathrm{d}x + 2\int_{\mathbb{R}^d}|\nabla\eta_n(|x|)|^2\,|\psi(x)|^2\,\mathrm{d}x\,.$$

Here the first integral vanishes as $n\to\infty$ by the dominated convergence theorem as before. For the second integral, a passage to spherical coordinates $x=r\sigma$ with $r:=|x|$ and $\sigma\in\mathbb{S}^{d-1}$ together with the formula $|\nabla\eta_n(|x|)| = n|\eta'(nr)|$ yields

$$\begin{aligned}\int_{\mathbb{R}^d}|\nabla\eta_n(|x|)|^2\,|\psi(x)|^2\,\mathrm{d}x &= n^2\int_{1/n}^{2/n}\int_{\mathbb{S}^{d-1}}|\eta'(nr)|^2\,|\psi(r\sigma)|^2\,\mathrm{d}\sigma\, r^{d-1}\,\mathrm{d}r\\ &\le n^2\,|\mathbb{S}^{d-1}|\,\|\psi\|^2_{L^\infty(\mathbb{R}^d)}\int_{1/n}^{2/n}|\eta'(nr)|^2\,r^{d-1}\,\mathrm{d}r\\ &= n^{2-d}\,|\mathbb{S}^{d-1}|\,\|\psi\|^2_{L^\infty(\mathbb{R}^d)}\int_1^2|\eta'(u)|^2\,u^{d-1}\,\mathrm{d}u\,.\end{aligned}$$

Here the right-hand side tends to zero as $n\to\infty$ whenever $d>2$, so the desired density result follows.

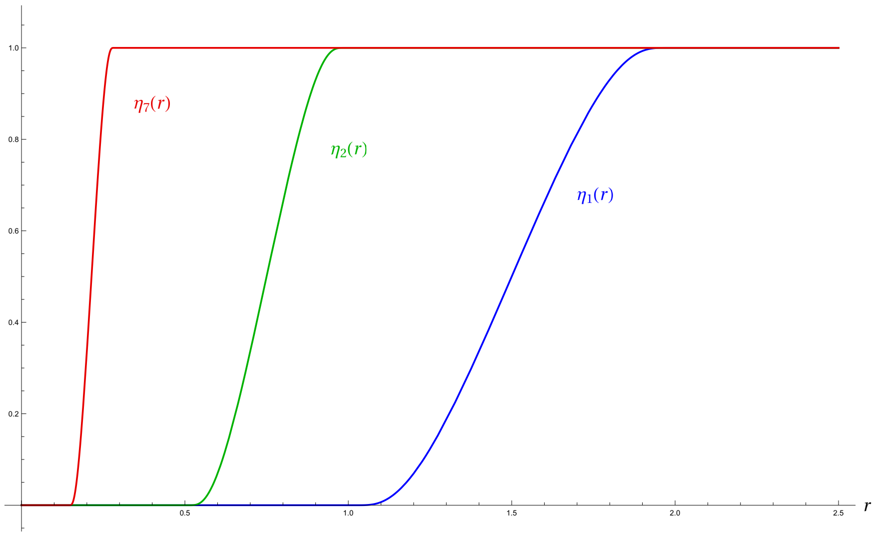


Figure 2.5: The sequence of functions η_n converging to 1 pointwise as $n\to\infty$.

$\boxed{d=2.}$ In the critical case we modify the argument above as follows. Let $\xi\in C^\infty([0,1])$ be such that $\xi=0$ in a right neighbourhood of 0 and $\xi=1$ in a left neighbourhood of 1. For every $n\in\mathbb{N}$ with $n\ge 2$, we define

$$\xi_n(x) := \begin{cases}\xi\left(\dfrac{\log(n^2|x|)}{\log n}\right) & \text{if} \quad 1/n^2\le|x|\le 1/n\,,\\ 0 & \text{if} \quad |x|\le 1/n^2\,,\\ 1 & \text{if} \quad |x|\ge 1/n\,,\end{cases}$$

and set $\psi_n:=\xi_n\psi$. As above (relying on the dominated convergence theorem), it is easy to see that $\|(\xi_n-1)\psi\|$ and $\|(\xi_n-1)\nabla\psi\|$ tend to zero as $n\to\infty$. Using in addition,

$$\begin{aligned}\int_{\mathbb{R}^d}|\nabla\xi_n(x)|^2\,|\psi(x)|^2\,\mathrm{d}x &= \frac{1}{\log^2 n}\int_{1/n^2}^{1/n}\int_{\mathbb{S}^1}\left|\xi'\left(\frac{\log(n^2r)}{\log n}\right)\right|^2\frac{1}{r^2}\,|\psi(r\sigma)|^2\,\mathrm{d}\sigma\, r\,\mathrm{d}r\\ &\le \frac{1}{\log^2 n}\,|\mathbb{S}^1|\,\|\xi'\|^2_{L^\infty([0,1])}\,\|\psi\|^2_{L^\infty(\mathbb{R}^d)}\int_{1/n^2}^{1/n}\frac{\mathrm{d}r}{r}\\ &= \frac{1}{\log n}\,|\mathbb{S}^1|\,\|\xi'\|^2_{L^\infty([0,1])}\,\|\psi\|^2_{L^\infty(\mathbb{R}^d)}\,,\end{aligned}$$

we therefore conclude with $|||\psi_n-\psi|||\to 0$ as $n\to\infty$.

$\boxed{d=1.}$ Since $W^{1,2}(\mathbb{R})$ is embedded in $C^0(\overline{\mathbb{R}})$ (*cf* (1.15)), the equality $W_0^{1,2}(\mathbb{R}\setminus\{0\}) = W_0^{1,2}(\mathbb{R})$ would imply that any function $\psi\in C_0^\infty(\mathbb{R})$ can be approximated by a sequence $\{\psi_n\}_{n\in\mathbb{N}}\in C_0^\infty(\mathbb{R}\setminus\{0\})$ in the uniform topology, *i.e.* $\|\psi - \psi_n\|_{L^\infty(\mathbb{R})} \to 0$ as $n \to \infty$. But this is impossible (take $\psi(0) = 1$ for which $\|\psi - \psi_n\|_{L^\infty(\mathbb{R})} \geq 1$). More specifically, without referring to the embedding,

$$|\psi(0)|^2 = |\psi(0) - \psi_n(0)|^2 = \int_{-\infty}^0 |\psi - \psi_n|^{2\prime} = \int_{-\infty}^0 2\Re(\bar{\psi} - \bar{\psi}_n)(\psi - \psi_n)' \leq 2\|\psi - \psi_n\|\|\psi' - \psi_n'\|\,,$$

where the right-hand side should tend to zero as $n \to \infty$, while the left-hand side is independent of n and can be chosen non-zero. □

2.2.2 Subcriticality of high dimensions

The following theorem is one of the most important results established in this course.

Theorem 2.6 (Hardy inequality)**.** *Let $d \geq 3$. Then*

$$\forall \psi \in W^{1,2}(\mathbb{R}^d)\,, \qquad \int_{\mathbb{R}^d} |\nabla\psi(x)|^2 \, dx \geq \frac{(d-2)^2}{4} \int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|^2} \, dx\,. \tag{2.6}$$

Proof. For any $\alpha \in \mathbb{R}$, we have

$$\begin{aligned} 0 \leq \int_{\mathbb{R}^d} \left|\nabla\psi(x) - \alpha \frac{x}{|x|^2}\,\psi(x)\right|^2 dx &= \int_{\mathbb{R}^d} |\nabla\psi(x)|^2 \, dx + \alpha^2 \int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|^2} \, dx - \alpha \int_{\mathbb{R}^d} \frac{x}{|x|^2} \cdot \nabla|\psi|^2(x) \, dx \\ &= \int_{\mathbb{R}^d} |\nabla\psi(x)|^2 \, dx + \alpha^2 \int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|^2} \, dx + \alpha \int_{\mathbb{R}^d} \operatorname{div}\left(\frac{x}{|x|^2}\right) |\psi(x)|^2 \, dx \\ &= \int_{\mathbb{R}^d} |\nabla\psi(x)|^2 \, dx + [\alpha^2 + \alpha(d-2)] \int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|^2} \, dx\,, \end{aligned}$$

where the second equality employs an integration by parts (or, more precisely, the divergence theorem). Consequently,

$$\int_{\mathbb{R}^d} |\nabla\psi(x)|^2 \, dx \geq -[\alpha^2 + \alpha(d-2)] \int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|^2} \, dx \tag{2.7}$$

for every $\alpha \in \mathbb{R}$. Optimising with respect to α (the parabola achieves its (positive) maximum for $\alpha = -(d-2)/2$, see Figure 2.6), we arrive at the desired inequality with the right constant.

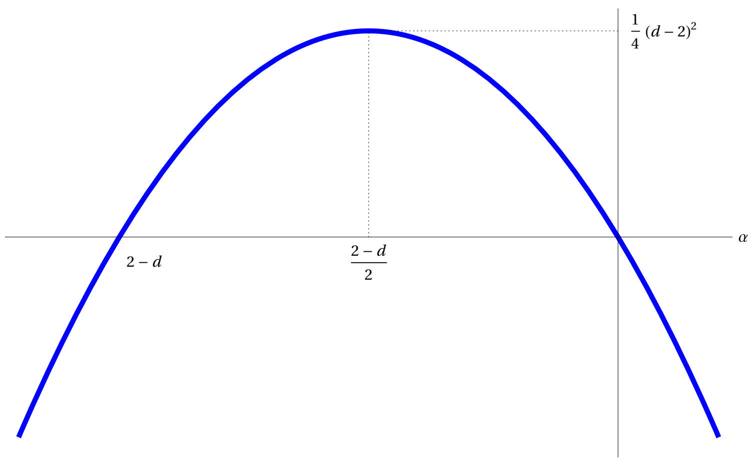


Figure 2.6: The maximum of the parabola corresponds to the best constant in (2.7).

Where did we use the requirement $d \geq 3$ in the proof? The inequality (2.6) is trivial if $d = 2$ (interpreting the right-hand side of (2.6) as being zero), so we should comment on the case $d = 1$. The point is that the vector field $x \mapsto x/|x|^2$ is too singular in dimension one, in order to justify the usage of the divergence theorem. More specifically, one customarily justifies the manipulations above by using functions $\psi \in C_0^\infty(\mathbb{R}^d \setminus \{0\})$ instead of $W^{1,2}(\mathbb{R}^d)$ and employs the density result of Proposition 2.5. However, this is possible if, and only if, $d \geq 1$. □

The Hardy inequality (2.6) is related to spectral properties of the Dirichlet Laplacian in the following way. The left-hand side of (2.6) is just the quadratic form of the Dirichlet (or Neumann) Laplacian in $\mathbb{R}^d$, indeed

$$(\psi, -\Delta_D^{\mathbb{R}^d}\psi) = (\psi, -\Delta\psi) = (\nabla\psi, \nabla\psi) = \|\nabla\psi\|^2$$

for every $\psi \in \operatorname{dom}(-\Delta_D^{\mathbb{R}^d})$, while the result makes sense for every $\psi \in W^{1,2}(\mathbb{R}^d)$. The right-hand side of (2.6) is the quadratic form of the operator of multiplication by the function

$$\rho(x) := \frac{(d-2)^2}{4}\frac{1}{|x|^2}\,. \tag{2.8}$$

Hence, we can write

$$-\Delta_D^{\mathbb{R}^d} \geq \rho \tag{2.9}$$

in the sense of quadratic forms in $L^2(\mathbb{R}^d)$. By Theorem 2.3, the spectrum of $-\Delta_D^{\Omega}$ starts by zero, so it is impossible that (2.9) holds with ρ being replaced by a positive constant. Anyway, if $d \geq 3$, inequality (2.9) with a positive function ρ vanishing at infinity is admissible. In summary, although the spectrum of the Dirichlet Laplacian $-\Delta_D^{\mathbb{R}^d}$ starts by zero, there is a “sort of repulsivity” at the zero energy if $d \geq 3$.

The notion of subcriticality can be generalised to abstract operators, at least if the Hilbert space is a function space.

First of all, let us recall that there is a natural order relation between operators by means of the corresponding quadratic forms. The following definition takes domains into account, which is necessary for unbounded operators.

Definition 2.7 (Operator inequality)**.** Let H_-, H_+ be two self-adjoint operators on $\mathcal{H}$ that are bounded from below, and let h_-, h_+ be the associated sesquilinear forms.

- $H_- \leq H_+ \quad :\Longleftrightarrow \quad \begin{array}{ll} \text{(i)} & \operatorname{dom} h_- \supset \operatorname{dom} h_+\,, \\ \text{(ii)} & \forall \psi \in \operatorname{dom} h_+, \quad h_-[\psi] \leq h_+[\psi]\,. \end{array}$

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

Let H be any non-negative self-adjoint operator in $L^2(\Omega)$ and let h be its associated sesquilinear form. Given any positive function $\rho \in L^1_{\mathrm{loc}}(\Omega)$, we denote by M_ρ the operator of multiplication in $L^2(\Omega)$ generated by ρ. With an abuse of notation, we often write ρ instead of M_ρ. The operator M_ρ is associated with the quadratic form

$$m_\rho[\psi] := \int_\Omega \rho(x)\,|\psi(x)|^2\,\mathrm{d}x\,, \qquad \operatorname{dom} m_\rho := \left\{\psi \in L^2(\Omega) : \int_\Omega \rho(x)\,|\psi(x)|^2\,\mathrm{d}x < \infty\right\}.$$

We say that H is *subcritical* if $H \geq \rho$. The inequality $H \geq \rho$ is called the *(generalised) Hardy inequality.*

If the spectrum of H starts by zero but there is no positive $\rho \in L^1_{\mathrm{loc}}(\Omega)$ such that $H \geq \rho$ (*i.e.* H is not subcritical), we say that H is *critical.* If the spectrum of H starts below zero, we say that H is *supercritical.*

Hence, if $d \geq 3$, the Dirichlet Laplacian $-\Delta_D^{\mathbb{R}^d}$ is subcritical and satisfies the Hardy inequality (2.6).

The Hardy inequality finds applications in many areas of mathematics and physics. Here we just mention its role in the quantum stability of matter.

2.2.3 Stability of matter

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

Now, the following classical paradox arises: According to the laws of classical electrodynamics, an accelerated charged particle emits electromagnetic radiation and loses in this way its total energy. Consequently, the electron particle would move on a spiral trajectory and finally collapse on the nucleus, *cf* Figure 2.7. The atoms should not be stable. (For instance, the lifetime of a hydrogen atom calculated according to the classical electrodynamics is less than 1 nanosecond!)

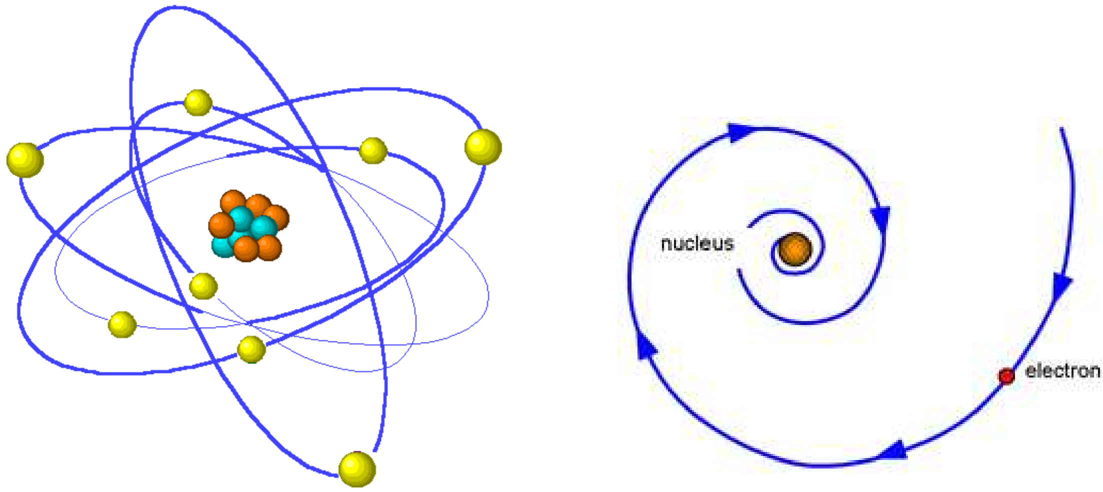


Figure 2.7: Rutherford's planetary model of the atom and its collapse due to classical physics.

Let us look at the simplest chemical element - hydrogen - and argue that it cannot be classically stable. In classical physics, the hydrogen atom is described by the Hamilton function

$$H(x,p) := \frac{|p|^2}{2m} - \frac{e^2}{|x|} \tag{2.10}$$

in the phase space $\mathbb{R}^3 \times \mathbb{R}^3 \ni (x,p)$. Here x and p is the position and momentum, respectively, m is the reduced mass of the electron-proton couple (*i.e.* $m^{-1} = m_e^{-1} + m_p^{-1}$) and $e \approx 1.6 \times 10^{-19}\,\mathrm{C}$ is the elementary charge. The first term represents the kinetic energy of the system, while the second term is the Coulomb electrostatic potential. The instability of the atom can be then mathematically understood through the unboundedness of the total energy from below, *i.e.*,

$$\inf_{(x,p)\in\mathbb{R}^3\times\mathbb{R}^3} H(x,p) = -\infty, \tag{2.11}$$

which is exactly caused by making the distance $|x|$ between the electron and the nucleus infinitesimal.

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

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

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

In quantum mechanics, the momentum p is represented by the differential operator

$$p := -i\hbar\nabla\,, \qquad \operatorname{dom} p := W^{1,2}(\mathbb{R}^3;\mathbb{C}^3)\,, \tag{2.12}$$

in the auxiliary Hilbert space $L^2(\mathbb{R}^3;\mathbb{C}^3)$, where $\hbar \approx 10^{-34}\,\mathrm{J\,s}$ is the reduced Planck constant. The position x is just an operator of multiplication. The square $|p|^2 := p^*p = -\hbar^2\Delta$ is therefore a multiple of the (Dirichlet) Laplacian in the scalar Hilbert space $L^2(\mathbb{R}^3)$. The hydrogen atom is consequently described by the Hamilton operator

$$H := -\frac{\hbar^2}{2m}\Delta - \frac{e^2}{|x|}$$

acting in the Hilbert space $L^2(\mathbb{R}^3)$. A quantum-mechanical analogue of the lowest energy of the classical system (2.11) is the variational quantity

$$E_1 := \inf_{\substack{\psi\in\mathrm{dom}(H)\\ \|\psi\|=1}} (\psi, H\psi)\,.$$

We claim that $E_1 > -\infty$, which implies the stability of the hydrogen atom in the quantum setting. Indeed, for every $\psi \in \mathrm{dom}(H)$ and any $R > 0$, one has

$$\begin{aligned}
(\psi, H\psi) &= \frac{\hbar^2}{2m}\int_{\mathbb{R}^3} |\nabla\psi(x)|^2\,\mathrm{d}x - e^2\int_{B_R(0)} \frac{|\psi(x)|^2}{|x|}\,\mathrm{d}x - e^2\int_{\mathbb{R}^3\setminus B_R(0)} \frac{|\psi(x)|^2}{|x|}\,\mathrm{d}x \\
&\geq \frac{\hbar^2}{2m}\int_{\mathbb{R}^3} |\nabla\psi(x)|^2\,\mathrm{d}x - e^2 R\int_{B_R(0)} \frac{|\psi(x)|^2}{|x|^2}\,\mathrm{d}x - \frac{e^2}{R}\int_{\mathbb{R}^3\setminus B_R(0)} |\psi(x)|^2\,\mathrm{d}x \\
&\geq \frac{\hbar^2}{2m}\int_{\mathbb{R}^3} |\nabla\psi(x)|^2\,\mathrm{d}x - e^2 R\int_{\mathbb{R}^3} \frac{|\psi(x)|^2}{|x|^2}\,\mathrm{d}x - \frac{e^2}{R}\int_{\mathbb{R}^3} |\psi(x)|^2\,\mathrm{d}x \\
&\geq \left(\frac{\hbar^2}{2m} - 4e^2 R\right)\int_{\mathbb{R}^3} |\nabla\psi(x)|^2\,\mathrm{d}x - \frac{e^2}{R}\int_{\mathbb{R}^3} |\psi(x)|^2\,\mathrm{d}x\,,
\end{aligned}$$

where the last estimate is the Hardy inequality (2.6) for $d = 3$. Choosing R in such a way that the round bracket vanishes, namely $R := \hbar^2/(8me^2)$, and assuming the normalisation $\|\psi\| = 1$, we therefore get the bound

$$E_1 \geq -8\,\frac{me^4}{\hbar^2} > -\infty\,.$$

It is remarkable that this estimate is not so far from the actual value

$$E_1 = -\frac{1}{2}\,\frac{me^4}{\hbar^2}\,,$$

which can be obtained by solving the spectral problem for the hydrogen atom explicitly in terms of special functions (see, *e.g.*, [39, Sec. 4.2]).

Remark 2.8 (Uncertainty principle)**.** Probably the deepest reason behind the stability of atoms in quantum mechanics is the non-commutative feature of the theory. It is reflected in the *Heisenberg uncertainty relations* implying an inevitable limitations for the preparation of states with sharper and sharper values of both position and momentum. From this point of view, the Hardy inequality of Theorem 2.6 can be interpreted as a sort of the *uncertainty principle*. Indeed, the boundedness from below of the hydrogen Hamiltonian H is its consequence and $E_1 > -\infty$ is equivalent to

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

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

2.2.4 Criticality of low dimensions

It turns out that the Dirichlet Laplacian $-\Delta_D^{\mathbb{R}^d}$ is critical in dimensions $d = 1, 2$. In other words, there is no Hardy inequality, that is, no inequality of the type (2.9) with a positive function ρ is admissible.

Theorem 2.9. *Let $d = 1, 2$. For any positive function $\rho \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$, one has*

$$\inf_{\substack{\psi\in C_0^\infty(\mathbb{R}^d)\\ \psi\neq 0}} \left(\int_{\mathbb{R}^d} |\nabla\psi(x)|^2\,\mathrm{d}x - \int_{\mathbb{R}^d} \rho(x)\,|\psi(x)|^2\,\mathrm{d}x\right) < 0\,. \tag{2.13}$$

Before proving the theorem, let us first comment on why the result (2.13) contradicts the validity of the Hardy inequality (2.9). The latter precisely means that if $\psi \in W^{1,2}(\mathbb{R}^d)$, then $\rho^{1/2}\psi \in L^2(\mathbb{R}^d)$ and the quadratic form

$$Q[\psi] := \int_{\mathbb{R}^d} |\nabla\psi(x)|^2 \, \mathrm{d}x - \int_{\mathbb{R}^d} \rho(x)\, |\psi(x)|^2 \, \mathrm{d}x \tag{2.14}$$

is non-negative. Since $C_0^\infty(\mathbb{R}^d) \subset W^{1,2}(\mathbb{R}^d)$, it follows that $Q[\psi] \geq 0$ for every $\psi \in C_0^\infty(\mathbb{R}^d)$. But this is an obvious contradiction with (2.13). So, indeed, no Hardy inequality (2.9) is available in dimensions $d = 1, 2$.

Proof. Clearly, to establish (2.13), it is enough to find a (so-called "trial") function $\psi \in C_0^\infty(\mathbb{R}^d)$ such that $Q[\psi] < 0$. Forgetting for a moment that 1 (*i.e.* the constant function everywhere equal to one) is not admissible and using the pointwise identity $\nabla 1 = 0$, we formally have

$$Q[1] = -\int_{\mathbb{R}^d} \rho(x) \, \mathrm{d}x < 0 \,. \qquad \text{(formally!)} \tag{2.15}$$

Hence, the idea is to use a trial function which approximates 1, but it is still an admissible element of $C_0^\infty(\mathbb{R}^d)$. We thus look for a sequence $\{\psi_n\}_{n=1}^\infty \subset C_0^\infty(\mathbb{R}^d)$ such that

(i) $\forall x \in \mathbb{R}^d, \quad \psi_n(x) \xrightarrow[n\to\infty]{} 1,$

(ii) $\|\nabla\psi_n\| \xrightarrow[n\to\infty]{} 0.$

Such a sequence exists only in dimensions $d = 1, 2$.

$\boxed{d = 1.}$ If $d = 1$, we pick a function $\varphi \in C_0^\infty(\mathbb{R})$ such that

$$0 \leq \varphi \leq 1\,, \qquad \varphi = 1 \quad \text{on} \quad [-1, 1]\,, \qquad \varphi = 0 \quad \text{outside} \quad [-2, 2]\,.$$

For every $n \in \mathbb{N}^*$, we then define (*cf* Figure 2.8)

$$\psi_n(x) := \varphi\left(\frac{x}{n}\right) .$$

Notice that $\psi_n = 1$ on $[-n, n]$ and $\psi_n = 0$ outside $[-2n, 2n]$, so it is certainly an admissible approximation of the constant function 1; in fact $\psi_n \to 1$ pointwise as $n \to \infty$. By an obvious change of variables, we have

$$\int_{\mathbb{R}} |\psi_n'(x)|^2 \, \mathrm{d}x = \int_{\mathbb{R}} \left|\frac{1}{n}\, \varphi'\left(\frac{x}{n}\right)\right|^2 \mathrm{d}x = \frac{1}{n} \int_{\mathbb{R}} |\varphi'(x)|^2 \, \mathrm{d}x \xrightarrow[n\to\infty]{} 0\,,$$

so the first term on the right-hand side of (2.14) vanishes as $n \to \infty$. For the second term, we have

$$\int_{\mathbb{R}^d} \rho(x)\, |\psi_n(x)|^2 \, \mathrm{d}x \xrightarrow[n\to\infty]{} \int_{\mathbb{R}^d} \rho(x) \, \mathrm{d}x$$

by the monotone convergence theorem (the limit can be infinite). In summary,

$$Q[\psi_n] \xrightarrow[n\to\infty]{} -\int_{\mathbb{R}^d} \rho(x) \, \mathrm{d}x\,,$$

so the formal result (2.15) is obtained in a limit sense. Since the right hand-side is negative (possibly $-\infty$), there obviously exists $n \in \mathbb{N}^*$ such that $Q[\psi_n] < 0$. This concludes the proof in the one-dimensional case.

$\boxed{d = 2.}$ If $d = 2$, we have to use a more refined approximation of 1. We start by picking a function $\eta \in C^\infty([0, 1])$ such that

$$0 \leq \eta \leq 1\,, \qquad \eta = 0 \quad \text{on} \quad [0, \tfrac{1}{4}]\,, \qquad \eta = 1 \quad \text{on} \quad [\tfrac{3}{4}, 1]\,.$$

For every $n \in \mathbb{N}$ with $n \geq 2$, we then define (*cf* Figure 2.8)

$$\psi_n(x) := \begin{cases} 1 & \text{if} \quad |x| \leq n\,, \\ \eta\left(\dfrac{\log n^2 - \log|x|}{\log n^2 - \log n}\right) & \text{if} \quad n < |x| < n^2, \\ 0 & \text{if} \quad |x| \geq n^2\,. \end{cases}$$

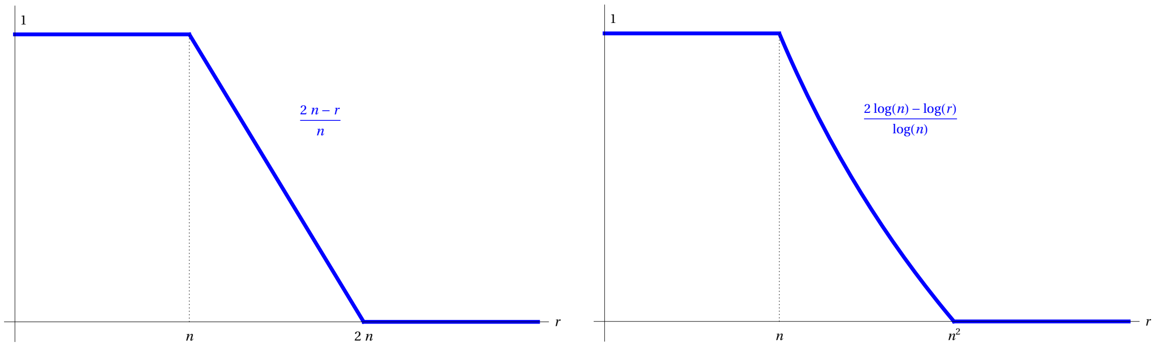


Figure 2.8: The radial profile of the functions ψ_n approximating 1 pointwise as $n \to \infty$ are smoothed version of the profiles on the left and right for $d = 1$ and $d = 2$, respectively.

Again $\psi_n \in C_0^\infty(\mathbb{R}^2)$ for every $n \geq 2$ and $\psi_n \to 1$ pointwise as $n \to \infty$. Passing to polar coordinates and making an obvious change of variables, we have

$$\begin{aligned}\int_{\mathbb{R}^2} |\nabla\psi_n(x)|^2 \, \mathrm{d}x &= 2\pi \int_n^{n^2} \left| \frac{-1}{r\,(\log n^2 - \log n)} \, \eta'\left(\frac{\log n^2 - \log r}{\log n^2 - \log n}\right) \right|^2 r \, \mathrm{d}r \\ &= \frac{2\pi}{\log n^2 - \log n} \int_0^1 |\eta'(s)|^2 \, \mathrm{d}s \xrightarrow[n\to\infty]{} 0 \,,\end{aligned}$$

so the first term on the right-hand side of (2.14) again vanishes as $n \to \infty$. The rest of the proof is the same as in the one-dimensional case. □

Let us summarise the dimensional features of the Euclidean space $\mathbb{R}^d$. Due to Theorem 2.3, the spectrum of the Dirichlet Laplacian in $\mathbb{R}^d$ is the same, namely it is equal to the interval $[0, \infty)$. However, there is a fundamental difference at the zero energy. There is a "sort of repulsivity" (respectively, "sort of attractivity") at the zero energy if $d \geq 3$ (respectively, $d = 1, 2$). We have quantified this by the respective existence or non-existence of Hardy inequalities. More specifically, Theorems 2.6 and 2.9 can be schematically summarise into the following equivalence:

$$-\Delta_D^{\mathbb{R}^d} \text{ satisfies a Hardy inequality} \qquad \Longleftrightarrow \qquad d \geq 3. \tag{2.16}$$

This observation has far reaching consequences in many areas of physics and mathematics. For instance, in stochastic analysis, it is related to the very different behaviour of the Brownian motion in $\mathbb{R}^d$ depending on whether $d = 1, 2$ or $d \geq 3$. Namely, the Brownian motion is *recurrent* on the real line and in the plane (meaning that the Brownian particle visits every region infinitely many times), while it is *transient* in $\mathbb{R}^d$ with $d \geq 3$ (meaning that it escapes from any bounded region after some time forever).

In this course, we have interpreted (2.16) through the stability of matter: $\mathbb{R}^3$ is the lowest dimensional Euclidean space for which the atoms and molecules are quantum-mechanically stable.

2.3 The half-line and the optimality of the Hardy inequality

. The Hardy inequality (Theorem 2.6) is so important that we dedicate this section to provide more insights into it. First of all, we give an alternative proof of it based on the following one-dimensional Hardy inequality.

Theorem 2.10 (One-dimensional Hardy inequality)**.** *One has*

$$\forall \psi \in W_0^{1,2}((0,\infty))\,, \qquad \int_0^\infty |\psi'(x)|^2 \, \mathrm{d}x \geq \frac{1}{4} \int_0^\infty \frac{|\psi(x)|^2}{|x|^2} \, \mathrm{d}x \,. \tag{2.17}$$

Obviously, the same inequality holds for $\psi \in W_0^{1,2}(\mathbb{R} \setminus \{0\})$ with the integrals over $\mathbb{R}$. Note carefully that, in any case, the function ψ is required to vanish at the origin. Without this requirement there is no one-dimensional Hardy inequality due to Theorem 2.9. In other words, while $-\Delta_D^{\mathbb{R}}$ is critical, both $-\Delta_D^{\mathbb{R}\setminus\{0\}}$

and $-\Delta_D^{(0,\infty)}$ are subcritical. Indeed, (2.17) is equivalent to the inequality

$$-\Delta_D^{(0,\infty)} \geq \rho$$

in the sense of quadratic forms in $L^2((0,\infty))$, where ρ is given by (2.8) with $d=1$.

Alternative proof of Theorem 2.6. By Proposition 2.5, it is enough to prove the Hardy inequality (2.6) of Theorem 2.6 for $\psi \in C_0^\infty(\mathbb{R}^d \setminus \{0\})$. Passing to spherical coordinates $(r,\theta) \in (0,\infty) \times \mathbb{S}^{d-1}$ and neglecting the angular-derivative term, we get the bound

$$\begin{aligned}\int_{\mathbb{R}^d} |\nabla\psi(x)|^2 \, \mathrm{d}x &= \int_{(0,\infty)\times\mathbb{S}^{d-1}} \left(|\partial_r \tilde{\psi}(r,\theta)|^2 + \frac{|\nabla_\theta \tilde{\psi}(r,\theta)|^2}{r^2} \right) r^{d-1} \, \mathrm{d}r \, \mathrm{d}\theta \\ &\geq \int_{(0,\infty)\times\mathbb{S}^{d-1}} |\partial_r \tilde{\psi}(r,\theta)|^2 \; r^{d-1} \, \mathrm{d}r \, \mathrm{d}\theta =: t[\tilde{\psi}] \,,\end{aligned}$$

where $\tilde{\psi}$ is the function ψ expressed in the spherical coordinates, $\mathrm{d}\theta$ is the surface element of the $(d-1)$-dimensional sphere $\mathbb{S}^{d-1}$ and ∇_θ denotes the spherical gradient. Making the change of test function

$$\phi(r,\theta) := \sqrt{r^{d-1}}\, \tilde{\psi}(r,\theta) \tag{2.18}$$

and integrating by parts, we arrive at the identity

$$t[\tilde{\psi}] = \int_{(0,\infty)\times\mathbb{S}^{d-1}} \left\{ |\partial_r \phi(r,\theta)|^2 + \left[\frac{(d-1)^2}{4} - \frac{d-1}{2} \right] \frac{|\phi(r,\theta)|^2}{r^2} \right\} \mathrm{d}r \, \mathrm{d}\theta \,.$$

For every $\theta \in \mathbb{S}^{d-1}$, the function $r \mapsto \phi(r,\theta)$ belongs to $C_0^\infty((0,\infty))$. Consequently, applying the one-dimensional Hardy inequality (2.17) of Theorem 2.10 with help of Fubini's theorem, we finally get

$$t[\tilde{\psi}] \geq \left[\frac{1}{4} + \frac{(d-1)^2}{4} - \frac{d-1}{2} \right] \int_{(0,\infty)\times\mathbb{S}^{d-1}} \frac{|\phi(r,\theta)|^2}{r^2} \, \mathrm{d}r \, \mathrm{d}\theta \,.$$

This estimate coincides with the desired inequality (2.6) after coming back to Cartesian coordinates.

Again we see that the proof does not give any non-trivial inequality in low dimensions $d = 1,2$. In $d = 2$, our proof holds but the outcome is trivial (the right-hand side of (2.6) vanishes). In $d = 1$, the technical reason for the breakdown of the proof is Proposition 2.5, which prevents us from restricting to functions supported outside the origin. We can still take $\psi \in C_0^\infty(\mathbb{R})$, which is a dense subspace of $W^{1,2}(\mathbb{R})$ (see Proposition 2.4), but then the test function ϕ would not vanish at the origin, so Theorem 2.10 does not apply. Indeed, in one dimension, the "spherical" coordinates are trivial, there is no Jacobian, so in fact $\phi = \tilde{\psi}$. □

The one-dimensional Hardy inequality of Theorem 2.10 can be established by the idea of the original proof of Theorem 2.6 given in Section 2.2.2. An alternative proof goes as follows.

Proof of Theorem 2.10. For every $\psi \in C_0^\infty((0,\infty))$,

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

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

Both Theorems 2.6 and 2.10 are optimal in various aspects [24]. Here we discuss the optimality of Theorem 2.10 only. The analogous claims for the multidimensional Theorem 2.6 can be obtained by means of spherical coordinates, using the optimising functions independent of the spherical variables.

2.3.1 Non-attainability

The Hardy inequality (2.17) is never achieved (by a non-trivial function), meaning that there is no (non-zero) function $\psi \in W_0^{1,2}((0,\infty))$ for which there is equality in (2.17). Indeed, for any $\psi \in C_0^\infty((0,\infty))$, it is easy to check that

$$a[\psi] := \int_0^\infty \left(|\psi'(x)|^2 - \frac{1}{4}\frac{|\psi(x)|^2}{x^2} \right) \mathrm{d}x = \int_0^\infty \left| \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\psi(x)}{\sqrt{x}}\right) \right|^2 x \, \mathrm{d}x \geq 0 \tag{2.19}$$

and by density the identity extends to all $\psi \in W_0^{1,2}((0,\infty))$. (This is yet another proof of Theorem 2.10.) Now, assume that there exists $\psi \in W_0^{1,2}((0,\infty))$ such that the Hardy inequality turns into equality. Then $a[\psi] = 0$. It follows from identity (2.19) that $\psi(x) = C\sqrt{x}$ for a.e. $x \in (0,\infty)$ with some constant $C \in \mathbb{C}$. But this is an admissible function from $W_0^{1,2}((0,\infty))$ only if $C = 0$.

2.3.2 Asymptotic attainability

The Hardy inequality (2.17) is achieved asymptotically, meaning that

$$\inf_{\substack{\psi \in W_0^{1,2}((0,\infty)) \\ \psi \neq 0}} \frac{a[\psi]}{\|\psi\|^2} = 0 \, .$$

Motivated by the result of the previous remark, we construct an optimising sequence by regularising the square-root function $x \mapsto \sqrt{x}$.

As in the proof of Proposition 2.5 for $d = 2$, let $\xi \in C^\infty([0,1])$ be such that $\xi = 0$ in a right neighbourhood of 0 and $\xi = 1$ in a left neighbourhood of 1. For every $n \in \mathbb{N}$ with $n \geq 2$, we define (see Figure 2.9)

$$\xi_n(x) := \begin{cases} 0 & \text{if} \quad x \in [0, 1/n^2) \, , \\ \xi\left(\dfrac{\log(n^2 x)}{\log n}\right) & \text{if} \quad x \in [1/n^2, 1/n) \, , \\ 1 & \text{if} \quad x \in [1/n, n) \, , \\ \xi\left(\dfrac{\log(n^2/x)}{\log n}\right) & \text{if} \quad x \in [n, n^2) \, , \\ 0 & \text{if} \quad x \in [n^2, \infty) \, . \end{cases}$$

Note that $\xi_n \in C_0^\infty((0,\infty))$ and $\xi_n(x) \to 1$ as $n \to \infty$ for every $x \in (0,\infty)$. We set $\psi_n(x) := \xi_n(x)\sqrt{x}$ for every $x > 0$. Then $\|\psi_n\| \to \infty$ as $n \to \infty$, while

$$\begin{aligned} a[\psi_n] &= \int_0^\infty |\xi_n'(x)|^2 \, x \, \mathrm{d}x \\ &= \frac{1}{\log^2 n} \int_{1/n^2}^{1/n} \left| \xi'\left(\frac{\log(n^2 x)}{\log n}\right) \right|^2 \frac{1}{x} \, \mathrm{d}x + \frac{1}{\log^2 n} \int_n^{n^2} \left| \xi'\left(\frac{\log(n^2/x)}{\log n}\right) \right|^2 \frac{1}{x} \, \mathrm{d}x \\ &\leq \frac{\|\xi'\|_\infty^2}{\log^2 n} \int_{1/n^2}^{1/n} \frac{1}{x} \, \mathrm{d}x + \frac{\|\xi'\|_\infty^2}{\log^2 n} \int_n^{n^2} \frac{1}{x} \, \mathrm{d}x \\ &= 2\, \frac{\|\xi'\|_\infty^2}{\log n} \xrightarrow[n \to \infty]{} 0 \, , \end{aligned}$$

where we have denoted $\|\xi'\|_\infty := \max |\xi'|$.

Optimality of the constant

The constant $\frac{1}{4}$ in (2.17) cannot be improved, meaning that

$$\inf_{\substack{\psi \in W_0^{1,2}((0,\infty)) \\ \psi \neq 0}} \frac{\displaystyle\int_0^\infty |\psi'(x)|^2 \, \mathrm{d}x}{\displaystyle\int_0^\infty \frac{|\psi(x)|^2}{x^2} \, \mathrm{d}x} = \frac{1}{4} \, .$$

Using the same sequence $\{\psi_n\}_{n=2}^\infty$ as above, one has

$$\int_0^\infty \frac{|\psi_n(x)|^2}{x^2} \, \mathrm{d}x \geq \int_{1/n}^n \frac{1}{x} \, \mathrm{d}x = 2 \log n \xrightarrow[n \to \infty]{} \infty \, .$$

Consequently,

$$\frac{\displaystyle\int_0^\infty |\psi_n'(x)|^2\,\mathrm{d}x}{\displaystyle\int_0^\infty \frac{|\psi_n(x)|^2}{x^2}\,\mathrm{d}x} = \frac{1}{4} + \frac{a[\psi_n]}{\displaystyle\int_0^\infty \frac{|\psi_n(x)|^2}{x^2}\,\mathrm{d}x} \xrightarrow[n\to\infty]{} \frac{1}{4}\,.$$

2.3.3 Optimality of the weight

The weight on the right-hand side of (2.17) cannot be improved, meaning that

$$\inf_{\substack{\psi\in W_0^{1,2}((0,\infty))\\ \psi\neq 0}} \frac{a[\psi]+v[\psi]}{\|\psi\|^2} < 0\,, \qquad \text{where} \qquad v[\psi] := \int_0^\infty V(x)\,|\psi(x)|^2\,\mathrm{d}x\,,$$

for any non-positive non-trivial function $V \in L^1_{\mathrm{loc}}((0,\infty))$. In other words, the shifted operator $-\Delta_D^{(0,\infty)} - \rho$ is critical. Obviously, this result is stronger than the optimality of the constant above. (In the terminology of [24], combining this result with the non-attainability above, the shifted operator $-\Delta_D^{(0,\infty)} - \rho$ is actually *null-critical.*)

It is enough to show that there exists a trial function $\psi \in W_0^{1,2}((0,\infty))$ such that $a[\psi]+v[\psi] < 0$. Using still the same sequence $\{\psi_n\}_{n=2}^\infty$ as above, one has

$$\lim_{n\to\infty} \left(a[\psi_n]+v[\psi_n]\right) = \lim_{n\to\infty} v[\psi_n] = \int_0^\infty V(x)\,x\,\mathrm{d}x < 0\,,$$

where the last equality follows by the monotone convergence theorem (the final integral can be $-\infty$). Consequently, there exists $n_0 \geq 2$ such that $a[\psi_n]+v[\psi_n] < 0$ for all $n \geq n_0$.

2.3.4 Optimality of the weight at infinity

The weight on the right-hand side of (2.17) is optimal also in the sense that it has the optimal decay at infinity, meaning that

$$\inf_{\substack{\psi\in W_0^{1,2}((0,\infty)\setminus K)\\ \psi\neq 0}} \frac{\displaystyle\int_0^\infty |\psi'(x)|^2\,\mathrm{d}x}{\displaystyle\int_0^\infty \frac{|\psi(x)|^2}{x^2}\,\mathrm{d}x} = \frac{1}{4}$$

for any compact set $K \in (0,\infty)$. To prove it, we modify the optimising sequence $\{\psi_n\}_{n=2}^\infty$ from above as follows. For every $n \in \mathbb{N}$ with $n \geq 2$, we now define (see Figure 2.9)

$$\tilde{\xi}_n(x) := \begin{cases} 0 & \text{if} \quad x \in [0,n)\,, \\ \xi\left(\dfrac{\log(x/n)}{\log n}\right) & \text{if} \quad x \in [n,n^2)\,, \\ 1 & \text{if} \quad x \in [n^2,2n^2)\,, \\ \xi\left(\dfrac{\log(2n^4/x)}{\log n^2}\right) & \text{if} \quad x \in [2n^2,2n^4)\,, \\ 0 & \text{if} \quad x \in [2n^4,\infty)\,. \end{cases}$$

Note that $\tilde{\xi}_n \in C_0^\infty((0,\infty))$ and $\inf\operatorname{supp}\tilde{\xi}_n \geq n \to \infty$ as $n \to \infty$. In particular, $K \cap \operatorname{supp}\tilde{\xi}_n = \varnothing$ for any compact set $K \in (0,\infty)$. We set $\tilde{\psi}_n(x) := \tilde{\xi}_n(x)\sqrt{x}$ for every $x > 0$. Then

$$\begin{aligned} a[\tilde{\psi}_n] &= \int_0^\infty |\tilde{\xi}_n'(x)|^2\,x\,\mathrm{d}x \\ &= \frac{1}{\log^2 n}\int_n^{n^2} \left|\xi'\left(\frac{\log(x/n)}{\log n}\right)\right|^2 \frac{1}{x}\,\mathrm{d}x + \frac{1}{\log^2 n^2}\int_{2n^2}^{2n^4} \left|\xi'\left(\frac{\log(2n^4/x)}{\log n^2}\right)\right|^2 \frac{1}{x}\,\mathrm{d}x \\ &\leq \frac{\|\xi'\|_\infty^2}{\log^2 n}\int_n^{n^2} \frac{1}{x}\,\mathrm{d}x + \frac{\|\xi'\|_\infty^2}{\log^2 n^2}\int_{2n^2}^{2n^4} \frac{1}{x}\,\mathrm{d}x \\ &= \frac{3}{2}\,\frac{\|\xi'\|_\infty^2}{\log n}\,, \end{aligned}$$

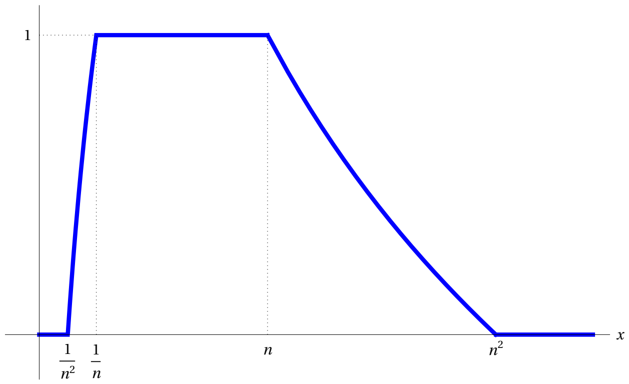


Figure 2.9: The regularising functions ξ_n and $\tilde{\xi}_n$ are smoothed versions of the profiles on the left and right, respectively.

while

$$\int_0^\infty \frac{|\tilde{\psi}_n(x)|^2}{x^2}\,\mathrm{d}x = \int_n^{2n^4} \frac{|\tilde{\xi}_n(x)|^2}{x}\,\mathrm{d}x \geq \int_{n^2}^{2n^2} \frac{1}{x}\,\mathrm{d}x = \log 2\,.$$

Consequently,

$$\frac{\displaystyle\int_0^\infty |\tilde{\psi}_n'(x)|^2\,\mathrm{d}x}{\displaystyle\int_0^\infty \frac{|\tilde{\psi}_n(x)|^2}{x^2}\,\mathrm{d}x} = \frac{1}{4} + \frac{a[\tilde{\psi}_n]}{\displaystyle\int_0^\infty \frac{|\tilde{\psi}_n(x)|^2}{x^2}\,\mathrm{d}x} \xrightarrow[n\to\infty]{} \frac{1}{4}\,.$$

2.3.5 A logarithmic Hardy inequality and a generic subcriticality

Let us conclude this section by the following one-dimensional Hardy-type inequality.

Lemma 2.11. *For any positive number x_0,*

$$\forall \psi \in W_0^{1,2}((x_0,\infty))\,, \qquad \int_{x_0}^\infty |\psi'(x)|^2\,x\,\mathrm{d}x \geq \frac{1}{4}\int_{x_0}^\infty \frac{|\psi(x)|^2}{x^2\log^2(x/x_0)}\,x\,\mathrm{d}x\,. \tag{2.20}$$

Proof. It is enough to prove the inequality for ψ from $C_0^\infty((x_0,\infty))$, a dense subspace of $W_0^{1,2}((x_0,\infty))$. For any real constant α, we employ the usual integration-by-parts trick:

$$\begin{aligned}\int_{x_0}^\infty \left|\psi'(x) - \frac{\alpha}{x\log(x/x_0)}\psi(x)\right|^2 x\,\mathrm{d}x &= \int_{x_0}^\infty |\psi'(x)|^2\,x\,\mathrm{d}x + \alpha^2\int_{r_0}^\infty \frac{|\psi(x)|^2}{x^2\log^2(x/x_0)}\,x\,\mathrm{d}x - \alpha\int_{x_0}^\infty \frac{(|\psi(x)|^2)'}{\log(x/x_0)}\,\mathrm{d}x\\ &= \int_{x_0}^\infty |\psi'(x)|^2\,x\,\mathrm{d}x + (\alpha^2-\alpha)\int_{x_0}^\infty \frac{|\psi(x)|^2}{x^2\log^2(x/x_0)}\,x\,\mathrm{d}x\,.\end{aligned}$$

Choosing $\alpha := 1/2$, we get (2.20). ∎

We note that the left-hand side of (2.20) is the radial component of the quadratic form of the two-dimensional Laplacian in the exterior of the ball of radius x_0. It follows that the Dirichlet Laplacian in this exterior is subcritical, a property which cannot be deduced from the classical Hardy inequalities of Theorems 2.6 and 2.10. What is more, we have the following robust result.

Theorem 2.12. *Let $\Omega \subset \mathbb{R}^d$ be an arbitrary open set satisfying*

$$\mathbb{R}^d \setminus \overline{\Omega} \neq \varnothing\,.$$

Then $-\Delta_D^\Omega$ is subcritical.

Proof. The proof is very similar to the alternative proof of the classical Hardy inequality presented in Section 2.3. Without loss of generality, we may assume that $0 \in \Omega^{\text{ext}} := \mathbb{R}^d \setminus \overline{\Omega}$. By hypothesis, there exists $\varepsilon > 0$ such that the ball $B_\varepsilon(0)$ is contained in Ω^{ext} (because it is a non-empty open set). Let $\psi \in C_0^\infty(\Omega)$ and extend it by zero to the whole $\mathbb{R}^d$.

$\boxed{d \neq 2}$ We can proceed exactly as in the alternative proof of Theorem 2.6: passing to spherical coordinates, neglecting the angular-derivative term and using the one-dimensional Hardy inequality (Theorem 2.10) after the change of trial function (2.18), we arrive at the inequality ($\mathbb{R}^d$ can be replaced by Ω)

$$\int_{\mathbb{R}^d} |\nabla\psi(x)|^2 \, \mathrm{d}x \geq \frac{(d-2)^2}{4} \int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|^2} \, \mathrm{d}x \,. \tag{2.21}$$

It looks like the classical Hardy inequality of Theorem 2.6, but the difference is that the present inequality holds in *all* dimensions (including $d = 1, 2$). This is due to the fact that the function

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

where $\tilde{\psi}$ is the function ψ expressed in the spherical coordinates, belongs (for every $\theta \in \mathbb{S}^{d-1}$) to $W_0^{1,2}((0,\infty))$ even if $d = 1, 2$, just because it is identically zero in a neighbourhood of $r = 0$ by the hypothesis. By density, (2.21) extends to all $\psi \in W_0^{1,2}(\Omega)$ and we may write

$$-\Delta_D^\Omega \geq \frac{(d-2)^2}{4} \frac{1}{|x|^2} \,,$$

in the sense of quadratic forms in $L^2(\Omega)$. The right hand side is a positive function whenever $d \neq 2$.

$\boxed{d = 2}$ If $d = 2$, inequality (2.21) still holds, but it is trivial. In the two-dimensional situation, we slightly modify the proof above. Passing to polar coordinates $(r, \theta) \in (0, \infty) \times \mathbb{S}^1$ and neglecting the angular-derivative term as above, but using Lemma 2.11 (instead of Theorem 2.6), we get the bound

$$\begin{aligned}
\int_\Omega |\nabla\psi(x)|^2 \, \mathrm{d}x &= \int_{(\varepsilon,\infty)\times\mathbb{S}^1} \left(|\partial_r \tilde{\psi}(r,\theta)|^2 + \frac{|\nabla_\theta \tilde{\psi}(r,\theta)|^2}{r^2} \right) r \, \mathrm{d}r \, \mathrm{d}\theta \\
&\geq \int_{(\varepsilon,\infty)\times\mathbb{S}^1} |\partial_r \tilde{\psi}(r,\theta)|^2 \; r \, \mathrm{d}r \, \mathrm{d}\theta \\
&\geq \frac{1}{4} \int_{(\varepsilon,\infty)\times\mathbb{S}^1} \frac{|\tilde{\psi}(r,\theta)|^2}{r^2 \log^2(r/\varepsilon)} \; r \, \mathrm{d}r \, \mathrm{d}\theta \\
&= \frac{1}{4} \int_\Omega \frac{|\psi(x)|^2}{|x|^2 \log^2(|x|/\varepsilon)} \, \mathrm{d}x \,.
\end{aligned}$$

By density, it extends to all $\psi \in W_0^{1,2}(\Omega)$ and we may write

$$-\Delta_D^\Omega \geq \frac{1}{4} \frac{1}{|x|^2 \log^2(|x|/\varepsilon)} \,,$$

in the sense of quadratic forms in $L^2(\Omega)$. $\square$

Remark 2.13. Let the boundary $\partial\Omega$ be sufficiently regular, say continuous. Then the boundary $\partial\Omega$ (if non-empty) is $(d-1)$-dimensional and the domain Ω cannot lie on both sides of any part of its boundary (*cf* [2, Sec. 3.21]). Then the exterior Ω^{ext} is always non-empty whenever $\Omega \neq \mathbb{R}^d$.

2.4 Absence of eigenvalues and the virial theorem

Apart from the criticality/subcriticality properties, there is another aspect which makes the quasi-conical domains spectrally interesting, despite the fact that the spectrum as a set is independent of the geometry (Theorem 2.3). Namely, what happens inside the interval $[0, \infty)$? In particular, are there eigenvalues? Since these eigenvalues are necessarily not isolated points in the spectrum, there are sometimes called *embedded* eigenvalues (in the "continuum" $[0, \infty)$). It turns out that that the existence/absence of embedded eigenvalues is a highly non-trivial question in spectral theory.

Already in 1943 Rellich [61] proved that there are no embedded eigenvalues for the Dirichlet Laplacian in the exterior of a compact set (such a domain is necessarily quasi-conical).

Theorem 2.14 (Rellich [61])**.** *Let $\Omega \subset \mathbb{R}^d$ be a domain for which there exists a positive number R such that $\Omega \setminus B_R = \mathbb{R}^d \setminus B_R$. Then*

$$\sigma_{\mathrm{p}}(-\Delta_D^\Omega) = \varnothing \,.$$

Other quasi-conical domains were considered by Jones [46]. Examples of quasi-conical domains for which there are embedded eigenvalues do not seem to exist in the literature. For disconnected open sets, however, it is easy to construct examples with embedded eigenvalues (*e.g.* a union of any bounded set and its exterior).

Instead of giving a full proof of Theorem 2.14, we establish it for the whole Euclidean space $\mathbb{R}^d$ only. Of course, the absence of eigenvalues in this special geometry can be established straightforwardly by Fourier transform. However, we use this occasion to present a more robust tool proving the absence of eigenvalues in spectral theory: the *virial theorem* (see [60, Sec. 13 & Notes] for a historical background).

Formal statement

Let H and A be self-adjoint operators in a Hilbert space $\mathcal{H}$. Assume that the commutator of A with H is *positive* in a sense. For instance, in a very restricitve sense, that there exists a positive number a such that (we do not care about operator domains for a moment)

$$i[H,A] \geq a\,I\,. \tag{2.22}$$

Now, let λ be an eigenvalue of H corresponding to an eigenvector ψ, normalised to 1 in $\mathcal{H}$. Then we get a contradiction

$$a \leq (\psi, i[H,A]\psi) = i(H\psi, A\psi) - i(A\psi, H\psi) = i(\lambda\psi, A\psi) - i(A\psi, \lambda\psi) = 0\,, \tag{2.23}$$

where the first and last equalities employ the self-adjointness of H and A. Hence, the positivity of the commutator prevents the existence of eigenvalues. This is the formal statement of the virial theorem. Schematically:

$$i[H,A] \geq a\,I \qquad \Longrightarrow \qquad \sigma_{\mathrm{p}}(H) = \varnothing\,.$$

Method of multipliers

The virial theorem is closely related with the *method of multipliers*, usually attributed to the original development of Morawetz [58] (the relationship has been recently pointed out in [17]).

As above, let H and A be arbitrary self-adjoint operators in a Hilbert space $\mathcal{H}$. Consider the eigenvalue equation $H\psi = \lambda\psi$, take an inner product of both sides with the vector $\phi := iA\psi$ (this is the multiplier of the method) and take twice the real part of the obtained identity:

$$(\psi, i[H,A]\psi) = (iA\psi, H) + (H, iA\psi) = 2\Re(\phi, H\psi)0 \overset{\downarrow}{=} \lambda\, 2\Re(\phi,\psi) = \lambda\left[(iA\psi,\psi) + (\psi, iA\psi)\right] = 0$$

(here the arrow points to the initial identity, the other equalities are manipulations). In this way we have arrived at the same identity as in (2.23) and the same contradiction under the positivity hypothesis (2.22).

Heuristic considerations

Why the positivity of the commutator is related to the (total) absence of eigenvalues? How to choose the auxiliary (so-called *conjugate*) operator A? It is useful to get a physical insight first.

Recall that, in quantum mechanics, a state of a physical system is described by a vector Ψ in a Hilbert space $\mathcal{H}$ which evolves according to the Schrödinger equation (1.2), where H is the self-adjoint operator representing the Hamiltonian (total energy operator) of the system.

Let A be another self-adjoint operator in $\mathcal{H}$, representing a physical observable in quantum mechanics. The expectation value of A for the system in the state Ψ is given by the inner product (we do not care about operator domains in these heuristic considerations)

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

Differentiating it with respect to time t and using (1.2), we (formally) get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle A \rangle &= \left(\frac{\mathrm{d}}{\mathrm{d}t}\Psi, A\Psi\right) + \left(\Psi, A\frac{\mathrm{d}}{\mathrm{d}t}\Psi\right) \\ &= \big(-iH\Psi, A\Psi\big) + \big(\Psi, A(-iH\Psi)\big) \\ &= i\big(\Psi, HA\Psi\big) - i\big(\Psi, AH\Psi\big) \\ &= \big(\Psi, i[H,A]\Psi\big) \\ &= \big\langle i[H,A]\big\rangle\,. \end{aligned} \tag{2.24}$$

Hence the evolution of the expectation value of A is given by the expectation value of the commutator with H multiplied by i (without this multiplication, the commutator $[H, A]$ is skew-adjoint).

It follows from (2.24) and (2.22) that the differential inequality

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A \rangle > a$$

holds (assuming $\|\Psi\| = 1$), which in turn implies

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

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

$$\lim_{t\to+\infty} \langle A \rangle(t) = +\infty\,. \tag{2.25}$$

Now, let A be the quantum counterpart of the radial momentum of a quantum particle (we take $\hbar = 1$)

$$A := \frac{x\cdot p + p\cdot x}{2} = -i\,x\cdot\nabla - i\,\frac{d}{2}\,, \tag{2.26}$$

where x and p are the position and momentum operators, respectively (recall (2.12)). Note that we had to take a symmetrized version of $x\cdot p$ (in order to make A self-adjoint, at least formally), since the observables x and p do not commute in quantum mechanics. Then (2.25) can be interpreted in physical terms as that the particle escapes to infinity of $\mathbb{R}^d$ for large times (for the radial derivative diverges). That is, the particle is not bound, it propagates. More specifically, the stationary solutions of the Schrödinger equation (1.2), corresponding to initial data being eigenfunctions, do not exist.

In summary, the positivity of the commutator naturally arises in evolution processes in quantum mechanics and the natural choice for the conjugate operator A is given by the radial derivative (2.26).

It remains to verify (2.22) in concrete models. In this section, we are primarily interested in the free Hamiltonian $H_0 := |p|^2 = -\Delta$ in $\mathbb{R}^d$. In this case, it is easily verified that, with the choice (2.26), we have (still formally)

$$i[H_0, A] = 2H_0\,.$$

Here the right-hand side is non-negative (because $(\phi, H_0\phi) = (\phi, -\Delta\phi) = \|\nabla\phi\|^2 \geq 0$ for every $\phi \in \operatorname{dom} H_0$), but it is not positive in the strict sense (2.22). Nonetheless, a contradiction in the spirit of (2.23) is still in order:

$$2\,\|\nabla\psi\|^2 = (\psi, 2H_0\psi) \stackrel{\downarrow}{=} (\psi, i[H_0, A]\psi) = 0\,, \tag{2.27}$$

whenever ψ is an eigenfunction of H_0. Indeed, from this identity we deduce that ψ is constant, which is not possible for a non-trivial function in $L^2(\mathbb{R}^d)$.

There is yet another support for the choice (2.26), at least if we deal with the Laplacian and its perturbations. In fact, the conjugate operator A by itself arises as a commutator with the Laplacian:

$$A = i\left[H_0, \frac{|x|^2}{4}\right].$$

Consequently,

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\left\langle \frac{|x|^2}{4} \right\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \langle i[H_0, A]\rangle \,,$$

so the positivity of the commutator $i[H_0, A]$ actually shows that the expectation value of the square of the magnitude of the position is a convex function in time: there is a *dispersion*.

Rigorous implementation for the free Hamiltonian

There are certainly a number of formal manipualtions in the arguments given above. Let us now show how to justify them.

Recalling Definition 1.4, we have rigorously introduced the free Hamiltonian H_0 as the Dirichlet Laplacian in $L^2(\mathbb{R}^d)$:

$$-\Delta_D^{\mathbb{R}^d}\psi = -\Delta\psi \,, \qquad \mathrm{dom}(-\Delta_D^{\mathbb{R}^d}) = \{\psi \in W^{1,2}(\mathbb{R}^d) : \ \Delta\psi \in L^2(\mathbb{R}^d)\} = W^{2,2}(\mathbb{R}^d) \,.$$

Here we employ Proposition 2.4 and (1.14). The latter can be established for $\mathbb{R}^d$ rather elementarily (for no boundary is present) by interior elliptic regularity, see (3.34) below. (These extra observations are not needed if we make an extra regularisation of the multiplier below with help of the difference quotient instead of the derivative, see [17, 16].)

The following is the justification of (2.27).

Lemma 2.15 (Virial theorem for the free Hamiltonian)**.** *If $\psi \in W^{2,2}(\mathbb{R}^d)$ is any solution of $-\Delta_D^{\mathbb{R}^d}\psi = \lambda\psi$ with $\lambda \in \mathbb{R}$, then*

$$\|\nabla\psi\| = 0 \,. \tag{2.28}$$

Proof. Recalling that $-\Delta_D^{\mathbb{R}^d}$ has been introduced as the operator associated with the quadratic form $Q_D^{\mathbb{R}^d}$, the equation $-\Delta_D^{\mathbb{R}^d}\psi = \lambda\psi$ precisely means that there exists a non-trivial function $\psi \in W^{2,2}(\mathbb{R}^d)$ such that

$$\forall\phi \in W^{1,2}(\mathbb{R}^d) \,, \qquad (\nabla\phi, \nabla\psi) = \lambda\,(\phi, \psi) \,. \tag{2.29}$$

This is sometimes called the weak formulation of the Helmholtz equation (4) in $\mathbb{R}^d$. (By Propisition 2.1, we may restrict to $\lambda \geq 0$.)

Following the arguments given above, our aim is to choose $iA\psi$ for the test function (the multiplier) ϕ, where the conjugate operator A is given by (2.26). However, it is not clear that $\psi \in \mathrm{dom}\,A$ (the domain of A has not been even discussed) and, even if so, that $\phi \in W^{1,2}(\mathbb{R}^d)$. Indeed, the problem is the unbounded position operator x in the definition of A. To proceed rigorously, we therefore choose the regularised multiplier

$$\phi := x \cdot \nabla\psi_n + \frac{d}{2}\psi_n \qquad \text{with} \qquad \psi_n := \xi_n\psi \,,$$

where ξ_n is the cut-off function from the first part of the proof of Proposition 2.4. To be more specific, for every $n \in \mathbb{N}^*$, we define $\xi_n(x) := \xi(x/n)$, where $\xi \in C_0^\infty(\mathbb{R}^d)$ is such that $0 \leq \xi \leq 1$, $\xi(x) = 1$ for every $|x| \leq 1$ and $\xi(x) = 0$ for every $|x| \geq 2$. Then $\phi \in W^{1,2}(\mathbb{R}^d)$ because $\psi \in W^{2,2}(\mathbb{R}^d)$ and the multiplication by x is bounded on the support of ψ_n. In fact,

$$\nabla\phi := x \cdot \nabla^2\psi_n + \left(1 + \frac{d}{2}\right)\nabla\psi_n \,.$$

$\boxed{\text{Right-hand side of (2.29).}}$ Writing $\psi = \psi_n + \psi - \psi_n$, one has

$$(\phi, \psi) = \underbrace{(x \cdot \nabla\psi_n, \psi_n)}_{R_1} + \underbrace{\frac{d}{2}\,\|\psi_n\|^2}_{R_2} + \underbrace{(x \cdot \nabla\psi_n, \psi - \psi_n)}_{R_3} + \underbrace{\frac{d}{2}\,(\nabla\psi_n, \psi - \psi_n)}_{R_4} \,.$$

As in the first part of the proof of Proposition 2.4, it is easy to see that

$$R_2 \xrightarrow[n\to\infty]{} \frac{d}{2}\,\|\psi\|^2 \qquad \text{and} \qquad R_4 \xrightarrow[n\to\infty]{} 0 \,.$$

The term R_1 is handled by an integration by parts as follows:

$$2\Re R_1 = \int_{\mathbb{R}^d} x \cdot \nabla |\psi_n|^2 \, \mathrm{d}x = -d \, \|\psi_n\|^2 \xrightarrow[n\to\infty]{} -d \, \|\psi\|^2 \,,$$

where we have used that $\operatorname{div} x = d$. To show that the real part of R_3 vanishes as $n \to \infty$, we first write

$$R_3 = \underbrace{\big(\psi \, x \cdot \nabla \xi_n, \psi - \psi_n\big)}_{R_3^{(1)}} + \underbrace{\big(\xi_n \, x \cdot \nabla \psi, \psi - \psi_n\big)}_{R_3^{(2)}} .$$

To handle both these terms, it is important to notice that $\operatorname{supp} \xi_n \subset B_{2n}$. Consequently, $|x| \leq 2n$ for every x in the domain of integration. This growth of $|x|$ can be controlled by any derivative of ξ_n because $\nabla \xi_n(x) = n^{-1} \nabla \xi(x/n)$. For instance,

$$\begin{aligned} |R_3^{(1)}| &\leq \|\psi \, |x| |\nabla \xi_n|\|_{L^2(B_{2n})} \, \|\psi - \psi_n\| \\ &\leq 2 \, \|\nabla \xi\|_\infty \, \|\psi\| \, \|\psi - \psi_n\| \\ &\xrightarrow[n\to\infty]{} 0 \,, \end{aligned}$$

where $\|\nabla \xi\|_\infty := \sup |\nabla \xi|$. An integration by parts is needed first to handle the other term:

$$\begin{aligned} 2\Re R_3^{(2)} &= \int_{B_{2n}} \xi_n (1 - \xi_n) \, x \cdot \nabla |\psi|^2 \, \mathrm{d}x \\ &= -d \int_{B_{2n}} \xi_n (1 - \xi_n) \, |\psi|^2 \, \mathrm{d}x - \int_{B_{2n}} x \cdot \nabla [\xi_n (1 - \xi_n)] \, |\psi|^2 \\ &\xrightarrow[n\to\infty]{} 0 \,. \end{aligned}$$

Indeed, the first term on the second line converges to zero by the dominated convergence theorem, while the other can be handled similarly as $R_3^{(1)}$. In summary,

$$\Re \left[\lambda \, (\phi, \psi) \right] = \lambda \, \Re(\phi, \psi) = 0 \,.$$

$\boxed{\text{Left-hand side of (2.29).}}$ Now we have

$$(\nabla \phi, \nabla \psi) = \underbrace{\big(x \cdot \nabla^2 \psi_n, \nabla \psi_n\big)}_{L_1} + \underbrace{\left(1 + \frac{d}{2}\right) \|\nabla \psi_n\|^2}_{L_2} + \underbrace{\big(x \cdot \nabla^2 \psi_n, \nabla(\psi - \psi_n)\big)}_{L_3} + \underbrace{\left(1 + \frac{d}{2}\right) \big(\nabla \psi_n, \nabla(\psi - \psi_n)\big)}_{L_4} .$$

It is easy to see that

$$L_2 \xrightarrow[n\to\infty]{} \left(1 + \frac{d}{2}\right) \|\nabla \psi\|^2 \qquad \text{and} \qquad L_4 \xrightarrow[n\to\infty]{} 0 \,.$$

The term L_1 is handled by an integration by parts as follows:

$$2\Re L_1 = \int_{\mathbb{R}^d} x \cdot \nabla |\nabla \psi_n|^2 \, \mathrm{d}x = -d \, \|\nabla \psi_n\|^2 \xrightarrow[n\to\infty]{} -d \, \|\nabla \psi\|^2 \,.$$

The integral L_3 can be handled similarly to R_3 above. Differentiating ψ_n and $\psi - \psi_n$, we observe that the terms containing any derivative of ξ_n vanish as $n \to \infty$ (similarly to the term $R_3^{(1)}$). On the other hand, for the term without any derivative of ξ_n, we employ an integration by parts first:

$$\begin{aligned} 2\Re\big(\xi_n \, x \cdot \nabla^2 \psi, (1 - \xi_n) \, \nabla \psi\big) &= \int_{B_{2n}} \xi_n (1 - \xi_n) \, x \cdot \nabla |\nabla \psi|^2 \, \mathrm{d}x \\ &= -d \int_{B_{2n}} \xi_n (1 - \xi_n) \, |\nabla \psi|^2 \, \mathrm{d}x - \int_{B_{2n}} x \cdot \nabla [\xi_n (1 - \xi_n)] \, |\nabla \psi|^2 \\ &\xrightarrow[n\to\infty]{} 0 \,. \end{aligned}$$

In summary,

$$\Re(\nabla \phi, \nabla \psi) = \|\nabla \psi\|^2 \,.$$

This concludes the proof of the lemma. □

As a direct consequence of Lemma 2.15, we get Theorem 2.14 in the very special case of the whole Euclidean space $\mathbb{R}^d$. Indeed, from (2.28) it follows that $\nabla \psi = 0$ almost everywhere in $\mathbb{R}^d$, therefore ψ is a constant function in $L^2(\mathbb{R}^d)$, which is not possible unless the constant is zero, a contradiction.

Chapter 3

Quasi-bounded domains

Now we shall focus on quasi-bounded domains, *i.e.* those which are neither quasi-conical nor quasi-cylindrical. Bounded domains are a special case of quasi-bounded domains, but the latter class is much wider. In addition to bounded domains, it contains unbounded domains which are "narrow at infinity", or more precisely

$$\text{unbounded } \Omega \text{ is quasi-bounded} \qquad \Longleftrightarrow \qquad \lim_{\substack{|x|\to\infty \\ x\in\Omega}} \operatorname{dist}(x,\partial\Omega) = 0\,. \tag{3.1}$$

Figure 3.1 represents a highly irregular unbounded quasi-bounded domain (with empty exterior).

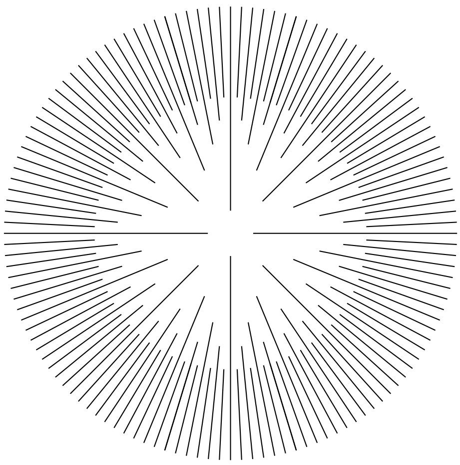


Figure 3.1: *Spiny urchin* as an example of a highly irregular unbounded quasi-bounded domain:
$$\Omega := \mathbb{R}^2 \setminus \bigcup_{m=1}^{\infty} \Big\{ (r\cos\vartheta, r\sin\vartheta) : \quad r \geq m \quad \wedge \quad \vartheta = n\pi/2^m \quad \text{for} \quad n = 1,2,\dots,2^{m+1} \Big\}$$

Recall that the spectrum of the Dirichlet Laplacian $-\Delta_D^\Omega$ is non-negative for any domain $\Omega \subset \mathbb{R}^d$ (*cf* Proposition 2.1). For quasi-conical domains, we have seen that the whole interval $[0,\infty)$ constitutes the spectrum (*cf* Theorem 2.3). The quasi-bounded domains Ω are the other extreme case: the spectrum of $-\Delta_D^\Omega$ is typically composed of isolated pointes only (at least under some regularity assumptions).

Because our life time is finite (unfortunately for this lecture, but fortunately for other respects of our life), in this chapter we shall mainly (but not exclusively) consider quasi-bounded domains which are **bounded**. Then we have a classical interpretation of the spectrum of the Dirichlet Laplacian in a bounded domain Ω: it is composed of squares of resonant frequences of an elastic membrane of shape Ω with fixed edges. Musically talented students will support our expectation that there is just a countable set of such frequences. Let us confirm this intuition by a mathematical analysis.

3.1 Discrete and essential spectra

First of all, let us make precise the distinction between spectra composed of non-degenerate intervals and isolated points.

In Section 1.3, we decomposed the spectrum to the disjoint union of the point and continuous spectra (the former are the eigenvalues, while the latter is the rest). An alternative decomposition is as follows.

Definition 3.1. Let H be an operator in a Hilbert space $\mathcal{H}$. The *essential spectrum* of H is defined by:

$$\sigma_{\text{ess}}(H) := \Big\{\lambda \in \mathbb{C} : \ \exists \text{ non-compact } \underset{\|\psi_n\|=1}{\{\psi_n\}_{n\in\mathbb{N}}} \subset \operatorname{dom} H, \quad \|H\psi_n - \lambda\psi_n\| \xrightarrow[n\to\infty]{} 0\Big\}.$$

The *discrete spectrum* is the rest:

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

Any corresponding sequence $\{\psi_n\}_{n\in\mathbb{N}}$ is called the *singular sequence* of H corresponding to the approximate eigenvalue λ.

By definition,

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

and the union is again disjoint.

Notice that contrary to Proposition 1.13, where a general characterisation of points in the spectrum is provided, the definition of the essential spectrum requires that the sequence playing the role of the approximate eigenfunction is *non-compact*. By this we mean that the sequence contains no converging subsequence in $\mathcal{H}$.

An operator H in a Hilbert space is said to be *continuous* if for every $\psi \in \operatorname{dom} H$ and $\{\psi_n\}_{n\in\mathbb{N}} \subset \operatorname{dom} H$,

$$\operatorname{dom} H \ni \psi_n \xrightarrow[n\to\infty]{\mathcal{H}} \psi \in \operatorname{dom} H \quad \Longrightarrow \quad H(\psi_n - \psi) \xrightarrow[n\to\infty]{\mathcal{H}} 0.$$

If $\mathcal{H}$ were finite-dimensional, then every operator is continuous (easily verified by using the representation through matrices). More generally, any operator H in an arbitrary Hilbert space is continuous if, and only if, it is *bounded* (*i.e.* there exists a non-negative number M such that $\|H\psi\| \leq M\|\psi\|$ for all $\psi \in \operatorname{dom} H$).

The continuity of bounded operators is so useful that we need to have a replacement for it in the general situation. This is provided by the notion of closedness: H is said to be *closed* if, for every $\psi, \phi \in \mathcal{H}$ and $\{\psi_n\}_{n\in\mathbb{N}} \subset \operatorname{dom} H$,

$$\left.\begin{aligned} \operatorname{dom} H \ni \psi_n &\xrightarrow[n\to\infty]{\mathcal{H}} \psi \in \mathcal{H} \\ H\psi_n &\xrightarrow[n\to\infty]{\mathcal{H}} \phi \in \mathcal{H} \end{aligned}\right\} \quad \Longrightarrow \quad \begin{cases} \psi \in \operatorname{dom} H \\ H\psi = \phi \end{cases}.$$

Here the logical connective between the vertical statements is *and* (logical conjuction). Self-adjoint operators are closed (just because the adjoint of any densely defined operator is closed). (So, in particular, the Dirichlet Laplacian $-\Delta_D^\Omega$ is closed for any domain Ω, *cf* Section 1.2.) For closed operators, we have the following inclusion for the discrete spectrum.

Proposition 3.2. *If H is a closed operator, then*

$$\sigma_{\text{disc}}(H) \subset \big\{\lambda \in \sigma_{\text{p}}(H) : \ m_g(\lambda) < \infty\big\}.$$

Proof. If λ belongs to the discrete spectrum of H, then there exists a *compact* sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset \operatorname{dom} H$ satisfying $\|\psi_n\| = 1$ for every $n \in \mathbb{N}$ and $H\psi_n - \lambda\psi_n \to 0$ in $\mathcal{H}$ as $n \to \infty$. The compactness implies that there exists a subsequence $\{\psi_{n_j}\}_{j\in\mathbb{N}}$ and an element $\psi \in \mathcal{H}$ such that $\psi_{n_j} \to \psi$ in $\mathcal{H}$ as $j \to \infty$. Consequently, $H\psi_{n_j} \to \lambda\psi$ in $\mathcal{H}$ as $j \to \infty$ and $\|\psi\| = 1$. The closedness implies that $\psi \in \operatorname{dom} H$ and $H\psi = \lambda\psi$. Hence, λ is an eigenvalue of H with eigenfunction ψ. If the multiplicity of λ were infinite, then there would be a non-compact sequence $\{\phi_k\}_{k\in\mathbb{N}} \subset \ker(H - \lambda I)$, a contradiction. □

For self-adjoint operators, we have the complete characterisation

$$\sigma_{\mathrm{disc}}(H) = \big\{\lambda \in \sigma_{\mathrm{p}}(H) : \ \lambda \text{ is isolated} \quad \wedge \quad m_g(\lambda) < \infty\big\}\,, \tag{3.2}$$

but we shall not prove this equality, avoiding the usage of the spectral theorem at this point. Then the essential spectrum contains either accumulation points of $\sigma(H)$ or isolated eigenvalues of infinite multiplicity. Notice that the discrete spectrum is precisely the property of the spectrum in finite-dimensional vector spaces. All the ugly "rarities" due to the infinite dimension are then included in the essential spectrum.

In quantum mechanics, the discrete spectrum typically corresponds to *bound states*, *i.e.* stationary solutions of the Schrödinger equation. On the other hand, the essential spectrum typically corresponds to *propagating* or *scattering states*, with the lowest value having the meaning of the *ionisation energy.* This terminology comes from atomic physics, where the energy of the highest possible orbital corresponds to the maximal allowed energy under which the electron is still bound to the nucleus; exceeding this energy, the electron is emitted as a free electron (see Figure 3.2). Of course, the "typicality" is very rough, because the essential spectrum may in principle contain also bound-state energies (non-isolated eigenvalues or eigevalues of infinite multiplicity) and other unwanted components of the continuous spectrum (namely, the so-called *singular continuous spectrum*). One of the main goals of scattering theory is precisely to establish the typicality, *i.e.* the absence of eigenvalues embedded in the essential spectrum and the absence of singular continuous spectrum.

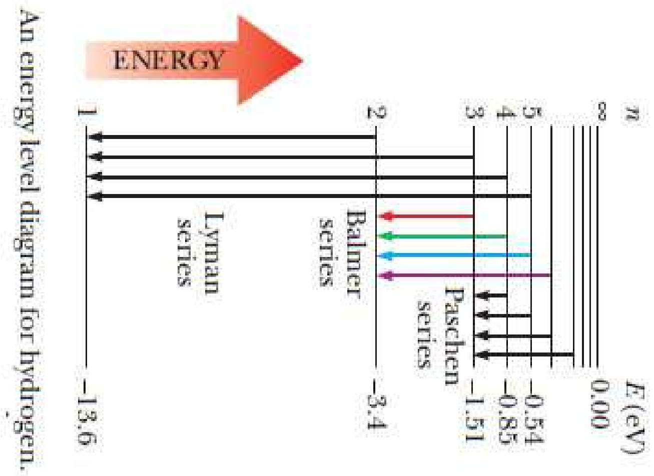


Figure 3.2: Schematic picture of discrete energy levels and the ionisation energy (corresponding the level 0 in the picture) for the hydrogen atom.

If the essential (respectively, discrete) spectrum is empty, we say that the spectrum is *purely discrete* (respectively, *purely essential*).

Due to Theorem 2.3, the spectrum of the Dirichlet Laplacian in quasi-conical domains is purely essential. Our goal is to show that the situation in bounded domains is quite opposite, namely the spectrum is purely discrete, so that the spectrum of the Dirichlet Laplacian in bounded domains looks precisely as the spectrum of operators in finite-dimensional vector spaces.

Let us conclude this technical section by the following equivalent characterisation of the essential spectrum. Recall that a sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset \mathcal{H}$ is said to be *weakly* converging to $\psi \in \mathcal{H}$ if

$$\forall \phi \in \mathcal{H}\,, \qquad (\phi, \psi_n) \xrightarrow[n\to\infty]{} (\phi, \psi)\,.$$

We then write $\psi_n \xrightarrow{w} \psi$ as $n \to \infty$.

Proposition 3.3. *For any operator H in a Hilbert space $\mathcal{H}$, one has:*

$$\sigma_{\mathrm{ess}}(H) = \Big\{\lambda \in \mathbb{C} : \ \exists \underset{\|\psi_n\|=1}{\{\psi_n\}_{n\in\mathbb{N}}} \subset \operatorname{dom} H, \quad \psi_n \xrightarrow[n\to\infty]{w} 0 \quad \wedge \quad \|H\psi_n - \lambda\psi_n\| \xrightarrow[n\to\infty]{} 0\Big\}. \tag{3.3}$$

Proof. As usual, we prove the equality of the sets as the validity of two inclusions.

$\boxed{\subset}$ If $\lambda \in \sigma_{\mathrm{ess}}(H)$, then there exists a singular sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset \operatorname{dom} H$ satisfying $\|\psi_n\| = 1$ for every $n \in \mathbb{N}$ and $H\psi_n - \lambda\psi_n \to 0$ as $n \to \infty$. The normalisation condition implies that $\{\psi_n\}_{n\in\mathbb{N}}$ is a *bounded* sequence in $\mathcal{H}$. It follows that $\{\psi_n\}_{n\in\mathbb{N}}$ is *weakly compact* (see Exercise 4) meaning that there exists a subsequence $\{\psi_{n_j}\}_{j\in\mathbb{N}}$ converging weakly to a limit $\psi \in \mathcal{H}$. (This is a generalisation of the well-known fact (Bolzano–Weierstrass theorem) that any bounded sequence of points in the Euclidean space contains a converging subsequence; in infinite-dimensional Hilbert spaces we get just the weak convergence.) Since $\{\psi_n\}_{n\in\mathbb{N}}$ is non-compact, there exists a positive δ such that $\|\psi_{n_j} - \psi_{n_k}\| \geq \delta$ for every $j, k \in \mathbb{N}$. Then the sequence $\{\phi_j\}_{j\in\mathbb{N}} \subset \operatorname{dom} H$ defined by

$$\phi_j := \frac{\psi_{n_{j+1}} - \psi_{n_j}}{\|\psi_{n_{j+1}} - \psi_{n_j}\|}$$

satisfies all the required conditions: $\|\phi_j\| = 1$ for every $j \in \mathbb{N}$, $\phi_j \xrightarrow{w} 0$ and $H\phi_j - \lambda\phi_j \to 0$ in $\mathcal{H}$ as $j \to \infty$.

$\boxed{\supset}$ Conversely, if a sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset \operatorname{dom} H$ satisfies the requirements on the right-hand side of (3.3), it cannot contain a convergent subsequence without contradicting the two requirements $\|\psi_n\| = 1$ and $\psi_n \xrightarrow{w} 0$ as $n \to \infty$. Hence, $\{\psi_n\}_{n\in\mathbb{N}}$ is a singular sequence of H corresponding to λ. Therefore $\lambda \in \sigma_{\mathrm{ess}}(H)$. □

3.2 Rectangular boxes

Let us now determine the spectrum of simplest bounded domains: straight segments and their Cartesian products. The case of the whole space $\mathbb{R}^d$ (which can be considered as a Cartesian product of real lines) was considered in the previous chapter. Here we consider the other extreme situation: a Cartesian product of bounded intervals. Given positive numbers $a_1, \dots, a_d$, let

$$\mathcal{R}_{a_1,\dots,a_d} := (-a_1, a_1) \times \cdots \times (-a_d, a_d) \tag{3.4}$$

denote a *rectangular box* of half-sides $a_1, \dots, a_d$.

$\boxed{d = 1}$

Let us start with the one-dimensional situation of an interval $\mathcal{R}_a = (-a, a)$ with $a > 0$. The point spectrum of the Dirichlet Laplacian $-\Delta_D^{(-a,a)}$ is determined by non-trivial solutions of the boundary-value problem

$$\begin{cases} -\psi'' = \lambda\psi & \text{in} \quad (-a, a)\,, \\ \quad \psi = 0 & \text{at} \quad \pm\, a\,. \end{cases} \tag{3.5}$$

By virtue of Proposition 1.7, we require that the solution ψ belongs to $W^{2,2}((-a, a)) \supset \operatorname{dom}(-\Delta_D^{(-a,a)})$. By the Sobolev embedding (*cf* [2, Thm. 4.12.(6)]) $W^{2,2}((-a, a)) \hookrightarrow C^1([-a, a])$, the boundary values are well defined in a classical sense. Moreover, by elliptic regularity theory (see, *e.g.*, [26, Thm. 6.3.6]), any solution of (3.5) belongs to $C^\infty([-a, a])$, so we are actually dealing with a classical boundary-value problem. However, we shall not need these advanced facts, the characterisation (1.13) due to Proposition 1.7 will be enough for our purposes.

Since $-\Delta_D^{(-a,a)}$ is a non-negative operator (*cf* Proposition 2.1), we know that $\lambda \geq 0$. Then the general solution of the differential equation of (3.5) reads (the special case $\lambda = 0$, when the fundamental solutions are given by linear functions, are covered by this formula)

$$\psi(x) = A\sin(\sqrt{\lambda}x) + B\cos(\sqrt{\lambda}x)\,, \tag{3.6}$$

where $A, B \in \mathbb{C}$ are constants to be determined by the boundary conditions of (3.5). The letter leads to two equations for three unknowns (A, B and λ) which we conveniently write in the matrix form

$$M_\lambda \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad \text{with} \qquad M_\lambda := \begin{pmatrix} \sin(\sqrt{\lambda}a) & \cos(\sqrt{\lambda}a) \\ -\sin(\sqrt{\lambda}a) & \cos(\sqrt{\lambda}a) \end{pmatrix}. \tag{3.7}$$

Since we are looking for solutions with A, B not being simultaneously equal to zero (the eigenfunction cannot be identically equal to zero), it is necessary to require

$$0 \overset{\downarrow}{=} \det(M_\lambda) = 2\sin(\sqrt{\lambda}\,a)\cos(\sqrt{\lambda}\,a) = 2\sin(2\sqrt{\lambda}\,a) \tag{3.8}$$

(here the arrow points to the requirement, the other equalities are manipulations). This is an equation that the eigenvalues $\lambda \geq 0$ of $-\Delta_D^{(-a,a)}$ must necessarily satisfy. Consequently,

$$\sigma_{\mathrm{p}}\big(-\Delta_D^{(-a,a)}\big) \subset \left\{ \left(\frac{k\pi}{2a}\right)^2 \right\}_{k=0}^{\infty}.$$

Note that we carefully write just an inclusion here. Indeed, while (3.8) is also sufficient to get a non-trivial solution of (3.7) (*i.e.*, A, B are not simultaneously equal to zero), it is still possible that this non-trivial pair (A, B) will lead to the function (3.6) being identically equal to zero. It is easy to see that this is precisely what happens if, and only if, $k = 0$ (*i.e.*, $\lambda = 0$). For $k > 0$ we get non-trivial functions (3.6): cosines (respectively, sines) if k is odd (respectively, even).

In summary, the point spectrum is given by

$$\sigma_{\mathrm{p}}\big(-\Delta_D^{(-a,a)}\big) = \left\{ \left(\frac{k\pi}{2a}\right)^2 \right\}_{k=1}^{\infty} \tag{3.9}$$

and the eigenfunctions corresponding to the eigenvalues of $-\Delta_D^{(-a,a)}$, ordered as in (3.9), are given by

$$\psi_k^D(x) := \begin{cases} \sqrt{\dfrac{1}{a}}\cos\left(\dfrac{k\pi}{2a}x\right) & \text{if} \quad k \text{ is odd}, \\ \sqrt{\dfrac{1}{a}}\sin\left(\dfrac{k\pi}{2a}x\right) & \text{if} \quad k \text{ is even}. \end{cases} \tag{3.10}$$

The constants before the sine and cosine functions are chosen in such a way that the eigenfunctions are normalised to 1 in $L^2((-a, a))$.

It is a standard result of Fourier analysis (see Exercise 5) that $\{\psi_k^D\}_{k\in\mathbb{N}^*}$ is a *complete* orthonormal set in $L^2((-a, a))$. The orthonormality has the same meaning as in finite-dimensional spaces, while the completeness means that if $(\psi_k^D, \psi) = 0$ for every $k \in \mathbb{N}^*$ with an arbitrary $\psi \in L^2((-a, a))$, then necessarily $\psi = 0$. Consequently, one has the orthogonal-basis decomposition

$$\forall \psi \in L^2((-a, a)), \qquad \psi = \sum_{k=1}^{\infty} c_k\, \psi_k^D \qquad \text{with} \qquad c_k := (\psi_k^D, \psi).$$

Here the equality should be interpreted in the usual L^2-sense, *i.e.*,

$$\lim_{N\to\infty} \left\| \psi - \sum_{k=1}^{N} c_k\, \psi_k^D(x) \right\| = 0.$$

Interpreting the eigenvalues as squares of resonant frequencies of a vibrating string with fixed ends, we get the intuitive result that enlarging the string leads to lower tones. At the same time, the result tells us that enlarging a box to which a quantum particle is constrained diminishes its bound-state energies.

$\boxed{d \geq 1}$

The multidimensional situation of a rectangular box can be then solved by a separation of variables. More specifically, the point spectrum of the Dirichlet Laplacian in $\mathcal{R}_{a_1,\dots,a_d}$ satisfies

$$\sigma_{\mathrm{p}}\big(-\Delta_D^{\mathcal{R}_{a_1,\dots,a_d}}\big) = \left\{\left(\frac{k_1\pi}{2a_1}\right)^2 + \dots + \left(\frac{k_d\pi}{2a_d}\right)^2\right\}_{k_1,\dots,k_d=1}^{\infty} . \tag{3.11}$$

The corresponding eigenfunctions are given by

$$\psi_{k_1,\dots,k_d}^D(x) := \psi_{k_1}^D(x_1)\dots\psi_{k_d}^D(x_d)$$

and they again form a complete orthonormal set in $L^2(\mathcal{R}_{a_1,\dots,a_d})$. That is,

$$\forall\psi \in L^2(\mathcal{R}_{a_1,\dots,a_d}), \qquad \psi = \sum_{k_1,\dots,k_d=1}^{\infty} c_{k_1,\dots,k_d}\,\psi_{k_1,\dots,k_d}^D \qquad \text{with} \qquad c_{k_1,\dots,k_d} := (\psi_{k_1,\dots,k_d}^D,\psi) . \tag{3.12}$$

Note that all the eigenvalues of $-\Delta_D^{\mathcal{R}_{a_1,\dots,a_d}}$ are isolated and of finite multiplicity. The lowest eigenvalue is simple and the corresponding eigenfunction is nowhere zero (in fact, it is positive for our normalisation). As usual in spectral theory, we arrange the eigenvalues into a non-decreasing sequence

$$\sigma_{\mathrm{p}}\big(-\Delta_D^{\mathcal{R}_{a_1,\dots,a_d}}\big) = \{\lambda_k^D\}_{k=1}^{\infty} = \{\lambda_1^D < \lambda_2^D \leq \lambda_3^D \leq \dots\} ,$$

where each eigenvalue is repeated according to its multiplicity (so the sequence is *not strictly* increasing if there are degeneracies). The corresponding set of eigenfunctions will be denoted by $\{\psi_k^D\}_{k\in\mathbb{N}^*}$. It is not completely trivial to obtain the non-decreasing sequence of eigenvalues for higher-dimensional rectangular boxes and analyse the degeneracies (see Exercise 6 for the special case of square).

The availability of the eigenfunctions forming the orthonormal basis enables one to deduce that the spectrum is purely discrete.

Proposition 3.4. $\sigma_{\mathrm{ess}}\big(-\Delta_D^{\mathcal{R}_{a_1,\dots,a_d}}\big) = \varnothing$.

Proof. First of all, notice that the point spectrum (3.11) consists of isolated eigenvalues of finite multiplicities and that the set admits no finite accumulation points. Then the claim follows from (3.2) provided that we show that there is no continuous spectrum. We shall prove the absence of the essential spectrum directly, without using (3.2).

Let us abbreviate $\mathcal{R} := \mathcal{R}_{a_1,\dots,a_d}$. By contradiction, let us assume that there exists $\lambda \in \sigma_{\mathrm{ess}}(-\Delta_D^{\mathcal{R}})$. Then, by Proposition 3.3, there exists a singular sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset \mathrm{dom}(-\Delta_D^{\mathcal{R}})$ satisfying $\|\psi_n\| = 1$ for every $n \in \mathbb{N}$, $\psi_n \xrightarrow{w} 0$ and $-\Delta_D^{\mathcal{R}}\psi_n - \lambda\psi_n \to 0$ in $L^2(\mathcal{R})$ as $n \to \infty$. We complete the proof by considering two alternatives separately.

$\boxed{\lambda \notin \sigma_{\mathrm{p}}(-\Delta_D^{\mathcal{R}})}$ In this case, using (3.12), we have

$$\|-\Delta_D^{\mathcal{R}}\psi_n - \lambda\psi_n\|^2 = \left\|\sum_{k=1}^{\infty}(\psi_k^D,-\Delta\psi_n)\,\psi_k^D - \lambda\sum_{k=1}^{\infty}(\psi_k^D,\psi_n)\,\psi_k^D\right\|^2 .$$

Integrating by parts, $(\psi_k^D,-\Delta\psi_n) = (-\Delta\psi_k^D,\psi_n) = \lambda_k^D(\psi_k^D,\psi_n)$, and therefore

$$\begin{aligned}
\|-\Delta_D^{\mathcal{R}}\psi_n - \lambda\psi_n\|^2 &= \left\|\sum_{k=1}^{\infty}(\lambda_k^D - \lambda)\,(\psi_k^D,\psi_n)\,\psi_k^D\right\|^2 \\
&= \sum_{k=1}^{\infty}|\lambda_k^D - \lambda|^2\,|(\psi_k^D,\psi_n)|^2 \\
&\geq \mathrm{dist}\big(\lambda,\sigma_{\mathrm{p}}(-\Delta_D^{\mathcal{R}})\big)^2\sum_{k=1}^{\infty}|(\psi_k^D,\psi_n)|^2 \\
&= \mathrm{dist}\big(\lambda,\sigma_{\mathrm{p}}(-\Delta_D^{\mathcal{R}})\big)^2\,\|\psi_n\|^2 = \mathrm{dist}\big(\lambda,\sigma_{\mathrm{p}}(-\Delta_D^{\mathcal{R}})\big)^2 .
\end{aligned}$$

Here the second and third equalities are just the Parseval equality. Since the left-hand side converges to zero as $n \to \infty$, while the right-hand side is positive (because the set (3.11) admits no finite accumulation points) and independent of n, we get a contradiction.

$\boxed{\lambda \in \sigma_{\mathrm{p}}(-\Delta_D^{\mathcal{R}})}$ In this case, there exists a natural number $k_0 \in \mathbb{N}^*$ such that $\lambda = \lambda_k$ if, and only if, $k \in \{k_0, k_0+1, \dots, k_0+m_g(\lambda)-1\} =: J$, where J is a finite set (because the eigenvalues from the set (3.11) have finite multiplicities). By the same procedure as above, we have

$$\begin{aligned} \| -\Delta_D^{\mathcal{R}}\psi_n - \lambda\psi_n\|^2 &= \sum_{k\notin J} |\lambda_k^D - \lambda|^2 \, |(\psi_k^D, \psi_n)|^2 \\ &\geq \operatorname{dist}\big(\lambda, \sigma_{\mathrm{p}}(-\Delta_D^{\mathcal{R}} \setminus \{\lambda\})\big)^2 \sum_{k\notin J} |(\psi_k^D, \psi_n)|^2 \,. \end{aligned}$$

It follows that

$$\sum_{k\notin J} |(\psi_k^D, \psi_n)|^2 \xrightarrow[n\to\infty]{} 0 \,.$$

At the same time, since $\{\psi_n\}_{n\in\mathbb{N}}$ is weakly converging to zero (see Exercise 4b), one has

$$\forall k \in \mathbb{N}^* \,, \qquad (\psi_k^D, \psi_n) \xrightarrow[n\to\infty]{} 0 \,.$$

Altogether, we therefore get

$$1 = \|\psi_n\|^2 = \sum_{k=1}^{\infty} |(\psi_k^D, \psi_n)|^2 \xrightarrow[n\to\infty]{} 0 \,,$$

a contradiction. □

In summarry, for any rectangular box $\mathcal{R}_{a_1,\dots,a_d}$, we have established the desired result

$$\sigma\big(-\Delta_D^{\mathcal{R}_{a_1,\dots,a_d}}\big) = \sigma_{\mathrm{disc}}\big(-\Delta_D^{\mathcal{R}_{a_1,\dots,a_d}}\big) \,.$$

In particular, this property holds for (hyper)cubes

$$Q_a := \mathcal{R}_{a,\dots,a} \,.$$

As a preparation for the following section, let us prove the following result.

Recall that an operator H in a Hilbert space $\mathcal{H}$ is called *compact* if every bounded sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset \operatorname{dom} H$ contains a subsequence $\{\psi_{n_j}\}_{j\in\mathbb{N}}$ for which $\{H\psi_{n_j}\}_{j\in\mathbb{N}}$ is convergent. This property is equivalent to the fact that there exists a sequence of operators $\{H_N\}_{N\in\mathbb{N}}$ of *finite rank* (*i.e.*, $\dim \operatorname{ran} H_N < \infty$) which converge in norm to H (see Exercise 7e).

Proposition 3.5. *The resolvent* $\big(-\Delta_D^{\mathcal{R}_{a_1,\dots,a_d}} + I\big)^{-1}$ *and* $\big(-\Delta_D^{\mathcal{R}_{a_1,\dots,a_d}} + I\big)^{-1/2}$ *are compact operators.*

Proof. The first part of the argument mimicks the proof of [23, Lem. 4.4.1]. First of all, it is easy to verify the decomposition formula for the resolvent

$$\big(-\Delta_D^{\mathcal{R}} + I\big)^{-1} = \sum_{k=1}^{\infty} (\lambda_k + 1)^{-1} \psi_k^D (\psi_k^D, \cdot) \,.$$

For every $N \in \mathbb{N}^*$, define the finite-rank operators

$$R_N := \sum_{k=1}^{N} (\lambda_k + 1)^{-1} \psi_k^D (\psi_k^D, \cdot) \,.$$

From the formula

$$\big(-\Delta_D^{\mathcal{R}} + I\big)^{-1} - R_N = \sum_{k=N+1}^{\infty} (\lambda_k + 1)^{-1} \psi_k^D (\psi_k^D, \cdot)$$

and the Bessel inequality, we deduce that, for every $\psi \in L^2(\mathcal{R})$,

$$\big\| \big[\big(-\Delta_D^{\mathcal{R}} + I \big)^{-1} - R_N \big] \psi \big\| \leq (\lambda_N + 1)^{-1} \|\psi\|^2 .$$

Since $\lambda_N \to \infty$ as $N \to \infty$, we see that R_N converges in norm to $\big(-\Delta_D^{\mathcal{R}} + I \big)^{-1}$ as $N \to \infty$.

The compactness of the square root follows by standard arguments (see Exercise 7f): $(-\Delta_D^{\mathcal{R}} + I)^{-1} = (-\Delta_D^{\mathcal{R}} + I)^{-1/2} (-\Delta_D^{\mathcal{R}} + I)^{-1/2}$ is compact if, and only if, $(-\Delta_D^{\mathcal{R}} + I)^{-1/2}$ is compact. □

Remark 3.6 (Neumann boundary conditions)**.** The spectral problem for the Laplacian in the rectangular box $\mathcal{R}_{a_1,\dots,a_d}$, subject to *Neumann* boundary conditions, can be solved in the same way. In the one-dimensional case, one finds

$$\sigma_{\mathrm{p}}\big(-\Delta_N^{(-a,a)} \big) = \left\{ \left(\frac{k\pi}{2a} \right)^2 \right\}_{k=0}^{\infty} , \tag{3.13}$$

so the only difference with respect to the Dirichlet boundary conditions is that the zero energy is allowed. Indeed, now non-zero constant functions are admissible as eigenfunctions. More specifically, the corresponding eigenfunctions read

$$\psi_k^N(x) := \begin{cases} \sqrt{\dfrac{1}{2a}} & \text{if} \quad k = 0 , \\ \sqrt{\dfrac{1}{a}} \cos\left(\dfrac{k\pi}{2a} x \right) & \text{if} \quad k \geq 1 \text{ is even} , \\ \sqrt{\dfrac{1}{a}} \sin\left(\dfrac{k\pi}{2a} x \right) & \text{if} \quad k \geq 1 \text{ is odd} . \end{cases} \tag{3.14}$$

Again, $\{\psi_k^N\}_{k\in\mathbb{N}}$ is a complete orthonormal set in $L^2((-a,a))$.

As in the Dirichlet case, the result (3.13) confirms the intuition that enlarging the length of a vibrating string with free ends leads to lower tones. It also explains why the *piccolo* produces higher tones than the *flute*: both can be modelled by a tube with open ends but the piccolo is half of the length of the flute's.

The multidimensional situation of the Neumann Laplacian in a rectangular box can be again solved by a separation of variables:

$$\sigma_{\mathrm{p}}\big(-\Delta_N^{\mathcal{R}_{a_1,\dots,a_d}} \big) = \left\{ \left(\frac{k_1\pi}{2a_1} \right)^2 + \dots + \left(\frac{k_d\pi}{2a_d} \right)^2 \right\}_{k_1,\dots,k_d=0}^{\infty} .$$

The corresponding eigenfunctions are given by

$$\psi_{k_1,\dots,k_d}^N(x) := \psi_{k_1}^N(x_1) \dots \psi_{k_d}^N(x_d)$$

and form a complete orthonormal set in $L^2(\mathcal{R}_{a_1,\dots,a_d})$.

Remark 3.7 (Combined boundary conditions)**.** Finally, let us consider the one-dimensional operator $-\Delta_{DN}^{(-a,a)}$ that acts as the Laplacian in the interval $(-a,a)$, subject to a Dirichlet (respectively, Neumann) boundary condition at $-a$ (respectively, a). Proceeding as above, we obtain that the spectrum is purely discrete and equal to the set

$$\sigma_{\mathrm{p}}\big(-\Delta_{DN}^{(-a,a)} \big) = \left\{ \left(\frac{(2k-1)\pi}{4a} \right)^2 \right\}_{k=1}^{\infty} . \tag{3.15}$$

The corresponding eigenfunctions are given by

$$\psi_k^{DN}(x) := \sqrt{\frac{1}{a}} \sin\left(\frac{(2k-1)\pi}{4a} \, x \right) \tag{3.16}$$

and they form a complete orthonormal set in $L^2((-a,a))$.

The operator $-\Delta_{DN}^{(-a,a)}$ is a classical model for resonant vibrations of a string with one end fixed and the other free. It also models standing waves in a *clarinet*, *i.e.* a tube with one open end and one closed end (at the reed). On the other hand, $-\Delta_N^{(-a,a)}$ models the situation of a *flute*, *i.e.* a tube with both ends open. Considering the hypothetical situation of a clarinet and a flute of the same length, we see by comparing (3.15) with (3.13) that the clarinet tones are lower than the tones of the flute (the zero mode is not counted).

3.3 Bounded domains

The main message of this chapter is that the spectrum of the Dirichlet Laplacian is purely discrete for *any* bounded domain. We shall establish this result by using the property for cubes (already proved) and the trivial extension of Dirichlet eigenfunctions in Ω to the whole Euclidean space $\mathbb{R}^d$. More specifically, assume, by contradiction, that $\lambda \in \sigma_{\text{ess}}(-\Delta_D^\Omega)$, where Ω is a bounded domain contained in a large cube Q_a. Then we construct from a singular sequence $\{\psi_n\}_{n\in\mathbb{N}}$ of $-\Delta_D^\Omega$ corresponding to λ a singular sequence $\{\tilde\psi_n\}_{n\in\mathbb{N}}$ of $-\Delta_D^{Q_a}$ simply by extending the elements of the former by zero ($\tilde\psi_n$ is called the *trivial extension* of ψ_n):

$$\tilde\psi_n(x) := \begin{cases} \psi_n(x) & \text{if} \quad x \in \Omega\,, \\ 0 & \text{if} \quad x \notin \Omega\,, \end{cases} \tag{3.17}$$

thus achieving a contradiction. Although $\tilde\psi_n \in W_0^{1,2}(Q_a)$ (the form domain of $-\Delta_D^{Q_a}$), it does not belong to the operator domain of $-\Delta_D^{Q_a}$. Hence, a necessary technical adaptation of the strategy must be developed, but the main idea of the proof of the following theorem is just that as described above.

Theorem 3.8. *Let $\Omega \subset \mathbb{R}^d$ be any bounded open set. Then*

$$\sigma_{\text{ess}}(-\Delta_D^\Omega) = \varnothing\,.$$

Proof. By contradiction, let us assume that there exists $\lambda \in \sigma_{\text{ess}}(-\Delta_D^\Omega)$. Then there exists a singular sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset \operatorname{dom}(-\Delta_D^\Omega) \subset W_0^{1,2}(\Omega)$ satisfying $\|\psi_n\|_{L^2(\Omega)} = 1$ for every $n \in \mathbb{N}$, $\psi_n \xrightarrow{w} 0$ and $-\Delta_D^\Omega\psi_n - \lambda\psi_n \to 0$ in $L^2(\Omega)$ as $n \to \infty$. The normalisation and the last limit imply that also

$$(\psi_n, -\Delta_D^\Omega\psi_n - \lambda\psi_n)_{L^2(\Omega)} = (\psi_n, -\Delta\psi_n)_{L^2(\Omega)} - \lambda\,\|\psi_n\|^2_{L^2(\Omega)} = \|\nabla\psi_n\|^2_{L^2(\Omega)} - \lambda$$

tends to zero as $n \to \infty$ (indeed $|(\psi_n, -\Delta_D^\Omega\psi_n - \lambda\psi_n)_{L^2(\Omega)}| \leq \|\psi_n\|_{L^2(\Omega)}\|-\Delta_D^\Omega\psi_n - \lambda\psi_n\|_{L^2(\Omega)}$ by the Schwarz inequality). Consequently,

$$\|\nabla\psi_n\|^2 \xrightarrow[n\to\infty]{} \lambda\,. \tag{3.18}$$

Since Ω is bounded, there exists a cube Q_a such that $\Omega \subset Q_a$. We define the sequence $\{\tilde\psi_n\}_{n\in\mathbb{N}} \subset W_0^{1,2}(Q_a)$ by employing the trivial extension (3.17). Finally, let us introduce the sequence $\{\phi_n\}_{n\in\mathbb{N}} \subset L^2(Q_a)$ defined by

$$\phi_n := (-\Delta_D^{Q_a} + I)^{-1/2}\,\tilde\psi_n\,.$$

This sequence satisfies the following two properties:

$\boxed{(1)\ \lim_{n\to\infty} \|\phi_n\|_{L^2(Q_a)} = 0}$ Since $\{\psi_n\}_{n\in\mathbb{N}}$ is weakly converging to zero in $L^2(\Omega)$, we have

$$\forall\varphi \in L^2(Q_a)\,, \qquad (\varphi, \tilde\psi_n)_{L^2(Q_a)} = (\varphi, \psi_n)_{L^2(\Omega)} \xrightarrow[n\to\infty]{} 0\,.$$

Hence, $\{\tilde\psi_n\}_{n\in\mathbb{N}}$ is weakly converging to zero in $L^2(Q_a)$. Since $(-\Delta_D^{Q_a} + I)^{-1/2}$ is a compact operator (*cf* Proposition 3.5) and compact operators maps weakly converging sequences to strongly converging sequences (see Exercise 7a) it follows that the sequence $\{\phi_n\}_{n\in\mathbb{N}}$ is (strongly) converging to zero in $L^2(Q_a)$.

$\boxed{(2)\ \liminf_{n\to\infty} \|\phi_n\|_{L^2(Q_a)} > 0}$ On the other hand, we have

$$
\begin{aligned}
\|\phi_n\|_{L^2(Q_a)} &= \big\|(-\Delta_D^{Q_a} + I)^{-1/2}\tilde{\psi}_n\big\|_{L^2(Q_a)} \\
&= \sup_{\substack{\varphi\in L^2(Q_a)\\ \varphi\neq 0}} \frac{\big|\big(\varphi, (-\Delta_D^{Q_a}+I)^{-1/2}\tilde{\psi}_n\big)_{L^2(Q_a)}\big|}{\|\varphi\|_{L^2(Q_a)}} \\
&= \sup_{\substack{\varphi\in L^2(Q_a)\\ \varphi\neq 0}} \frac{\big|\big((-\Delta_D^{Q_a}+I)^{-1/2}\varphi, \tilde{\psi}_n\big)_{L^2(Q_a)}\big|}{\|\varphi\|_{L^2(Q_a)}} \\
&= \sup_{\substack{u\in W_0^{1,2}(Q_a)\\ u\neq 0}} \frac{|(u,\tilde{\psi}_n)_{L^2(Q_a)}|}{\|u\|_{W^{1,2}(Q_a)}} \\
&\geq \frac{\|\tilde{\psi}_n\|^2_{L^2(Q_a)}}{\|\tilde{\psi}_n\|_{W^{1,2}(Q_a)}} = \frac{\|\psi_n\|^2_{L^2(\Omega)}}{\|\psi_n\|_{W^{1,2}(\Omega)}} = \frac{1}{\|\psi_n\|_{W^{1,2}(\Omega)}} \,.
\end{aligned}
$$

Here the fourth equality employs the facts that $(-\Delta_D^{Q_a}+I)^{-1/2} : L^2(Q_a) \to W_0^{1,2}(Q_a)$ is an isomorphism and $\|(-\Delta_D^{Q_a}+I)^{-1/2}u\|_{L^2(Q_a)} = \|u\|_{W^{1,2}(Q_a)}$. However, using (3.18), we have the limit

$$
\|\psi_n\|^2_{W^{1,2}(\Omega)} = \|\nabla\psi_n\|^2_{L^2(\Omega)} + \|\psi_n\|^2_{L^2(\Omega)} = \|\nabla\psi_n\|^2_{L^2(\Omega)} + 1 \xrightarrow[n\to\infty]{} \lambda + 1 \,.
$$

Consequently,

$$
\|\phi_n\|_{L^2(Q_a)} \geq \frac{1}{\sqrt{\lambda+1}} \,,
$$

which proves the desired property.

Comparing the properties (1) and (2), we arrive at an obvious contradiction. ☐

3.4 The spectral theorem

Our given proof of the discreteness of the spectrum of the Dirichlet Laplacian in arbitrary bounded domains has one flaw, namely it does not show that there is *an* eigenvalue. The non-emptiness of the (discrete) spectrum holds, and there are actually infinitely many eigenvalues, but to prove this, we need an extra tool.

This tool (in fact, *supertool*) is the **spectral theorem**, which is one of the most fundamental theorems of functional analysis.

From a basic course in linear algebra, you certainly know its finite-dimensional version.

Theorem 3.9 (Spectral theorem, finite dimensions)**.** *Let H be a self-adjoint operator in a Hilbert space $\mathcal{H}$ with $0 < \dim\mathcal{H} < \infty$. Then*

the eigenvectors of H form an orthonormal basis in $\mathcal{H}$.

In other words, any self-adjoint operator can be diagonalised, in the sense that its matrix with respect to the basis formed by the eigenvectors is diagonal. At the same time, H possesses exactly $\dim\mathcal{H}$ eigenvalues, provided that these are counted together with their multiplicities. You also know that this theorem fails for operators which are not self-adjoint (or at least *normal*, *i.e.* $HH^* = H^*H$) in general (for then there might be Jordan blocks).

The good news is that the spectral theorem (after suitable modifications) remains true in infinite-dimensional spaces. We present a version (without proof) suitable for operators with purely discrete spectrum.

Theorem 3.10 (Spectral theorem, purely discrete spectrum)**.** *Let H be a self-adjoint operator in any Hilbert space $\mathcal{H}$ and assume $\sigma_{\mathrm{ess}}(H) = \varnothing$. Then*

$$\text{the eigenvectors of } H \text{ form an orthonormal basis in } \mathcal{H}\,.$$

The proof of the theorem is rather involved and it requires the self-adjointness (a non-self-adjoint operator in an infinite-dimensional Hilbert space can have empty spectrum). Note that the orthogonality of eigenvectors corresponding to distinct eigenvalues is proved in the same way as in finite-dimensional spaces; it is the completeness of the set of eigenvectors which is non-trivial.

The absence of the essential spectrum is just a sufficient condition in Theorem 3.10 to have the conclusion about the orthonormal basis formed by the eigenvectors. Indeed, the same conclusion holds for compact operators, for which zero is always in the essential spectrum if $\mathcal{H}$ is infinite-dimensional.

Combining Theorem 3.10 with the absence of the essential spectrum in bounded domains (Theorem 3.8), it follows that the Dirichlet Laplacian in any bounded domain indeed possesses an infinite number of discrete eigenvalues.

3.5 The minimax principle

Let us now prove a highly important consequence of the spectral theorem (Theorem 3.10).

Recall that an operator H is *bounded from below* if there exists a constant $c \in \mathbb{R}$ such that $(\psi, H\psi) \geq c\|\psi\|^2$ for every $\psi \in \operatorname{dom} H$.

Theorem 3.11 (Minimax principle, purely discrete spectrum)**.** *Let H be a self-adjoint operator in $\mathcal{H}$ of dimension $N := \dim \mathcal{H} \in \mathbb{N}^* \cup \{\infty\}$, which is bounded from below and whose spectrum is purely discrete. Let us arrange its eigenvalues into a non-decreasing sequence $\sigma(H) = \{\lambda_k\}_{k=1}^N = \{\lambda_1 \leq \lambda_2 \leq \dots\}$, where each eigenvalue is repeated according to its multiplicity. Then, for every $k \in \{1, \dots, N\}$,*

$$\lambda_k = \inf_{\substack{\mathcal{L}_k \subset \operatorname{dom} H \\ \dim \mathcal{L}_k = k}} \sup_{\substack{\psi \in \mathcal{L}_k \\ \psi \neq 0}} \frac{(\psi, H\psi)}{\|\psi\|^2}\,. \tag{3.19}$$

Proof. Let us denote the right-hand side of (3.19) by $\tilde{\lambda}_k$. Our aim is to show that $\tilde{\lambda}_k = \lambda_k$ for every $k \in \{1, \dots, N\}$. We follow the proof of [23, Thm. 4.5.1].

$\boxed{\tilde{\lambda}_k \leq \lambda_k}$ Let $\{\psi_k\}_{k=1}^N$ denote the eigenvectors of H corresponding to $\{\lambda_k\}_{k=1}^N$. By Theorem 3.10, they can be normalised in such a way that $\{\psi_k\}_{k=1}^N$ is a complete orthonormal set in $\mathcal{H}$. For every $\psi \in \mathcal{M}_k := \operatorname{span}\{\psi_1, \dots, \psi_k\}$, one has

$$(\psi, H\psi) = \sum_{j=1}^k \lambda_j \, |(\psi_j, \psi)|^2 \leq \lambda_k \sum_{j=1}^k |(\psi_j, \psi)|^2 = \lambda_k \|\psi\|^2\,.$$

Consequently, choosing $\mathcal{L}_k := \mathcal{M}_k$ in (3.19), one gets $\tilde{\lambda}_k \leq \lambda_k$ for every $k \in \{1, \dots, N\}$.

$\boxed{\tilde{\lambda}_k \geq \lambda_k}$ If $k = 1$, the formula (3.19) reduces to

$$\tilde{\lambda}_1 = \inf_{\substack{\psi \in \operatorname{dom} H \\ \psi \neq 0}} \frac{(\psi, H\psi)}{\|\psi\|^2}\,.$$

Using that $\{\psi_k\}_{k=1}^N$ is a complete orthonormal set, one has, for every $\psi \in \operatorname{dom} H$,

$$(\psi, H\psi) = \sum_{j=1}^{N} \lambda_j \, |(\psi_j, \psi)|^2 \geq \lambda_1 \sum_{j=1}^{N} |(\psi_j, \psi)|^2 = \lambda_1 \|\psi\|^2 \,.$$

Consequently, $\tilde{\lambda}_1 \geq \lambda_1$.

If $k \in \{2, \dots, N\}$, we introduce the operator

$$P := \sum_{j=1}^{k-1} \psi_j (\psi_j, \cdot) \,, \qquad \operatorname{dom} P := \mathcal{H} \,.$$

It is an orthogonal projection on $\mathcal{H}$ (*i.e.*, $P^2 = P$ and $P^* = P$) with range $\mathcal{M}_{k-1}$. Clearly, $\dim \operatorname{ran} P = k-1$. Let $\mathcal{L}_k$ be any k-dimensional subspace of $\operatorname{dom} H$. Since $\dim \operatorname{ran} P_{\mathcal{L}_k} < \dim \mathcal{L}_k$, there must exist a non-zero vector $\phi \in \mathcal{L}_k$ such that $P\psi = 0$. We then have $(\psi_j, \phi) = 0$ for all $j \leq k-1$. It follows that

$$(\phi, H\phi) = \sum_{j=k}^{\infty} \lambda_j \, |(\psi_j, \phi)|^2 \geq \lambda_k \sum_{j=k}^{\infty} |(\psi_j, \phi)|^2 = \lambda_k \|\phi\|^2 \,.$$

We conclude that

$$\sup_{\substack{\psi \in \mathcal{L}_k \\ \psi \neq 0}} \frac{(\psi, H\psi)}{\|\psi\|^2} \geq \frac{(\phi, H\phi)}{\|\phi\|^2} \geq \lambda_k, .$$

Consequently, $\tilde{\lambda}_k \geq \lambda_k$ for every $k \in \{1, \dots, N\}$. □

Remark 3.12. Let H be as in Theorem 3.11 and let h be the associated sesquilinear form. Since $\operatorname{dom} H$ is a *core* of h (*i.e.*, $\operatorname{dom} H$ is dense in $\operatorname{dom} h$ with respect to the topology induced by the form h, namely by the norm $|||\psi||| := \sqrt{h[\psi] + \|\psi\|^2}$), it can be shown (see [23, Thm. 4.5.3]) that the formula (3.19) can be replaced by

$$\lambda_k = \inf_{\substack{\mathcal{L}_k \subset \operatorname{dom} h \\ \dim \mathcal{L}_k = k}} \sup_{\substack{\psi \in \mathcal{L}_k \\ \psi \neq 0}} \frac{h[\psi]}{\|\psi\|^2} \,. \tag{3.20}$$

Since the spectral theorem is not restricted to self-adjoint operators with purely discrete spectrum, there exists a version of Theorem 3.11 even for operators whose essential spectrum is not empty (see [23, Thm. 4.5.2]).

Theorem 3.13 (Minimax principle, with essential spectrum)**.** *Let H be a self-adjoint operator in an infinite-dimensional Hilbert space $\mathcal{H}$, which is bounded from below. Let h be the associated sesquilinear form. Let $\{\lambda_k\}_{k=1}^\infty$ be a non-decreasing sequence of numbers defined by*

$$\lambda_k := \inf_{\substack{\mathcal{L}_k \subset \operatorname{dom} H \\ \dim \mathcal{L}_k = k}} \sup_{\substack{\psi \in \mathcal{L}_k \\ \psi \neq 0}} \frac{(\psi, H\psi)}{\|\psi\|^2} = \inf_{\substack{\mathcal{L}_k \subset \operatorname{dom} h \\ \dim \mathcal{L}_k = k}} \sup_{\substack{\psi \in \mathcal{L}_k \\ \psi \neq 0}} \frac{h[\psi]}{\|\psi\|^2} \,, \tag{3.21}$$

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

1. $\lambda_\infty := \lim_{k \to \infty} \lambda_k = \inf \sigma_{\mathrm{ess}}(H) \,,$

   with the convention that $\sigma_{\mathrm{ess}}(H) = \varnothing$ if $\lambda_\infty = +\infty$;

2. $\{\lambda_k\}_{k=1}^\infty \cap (-\infty, \lambda_\infty) = \sigma_{\mathrm{disc}}(H) \cap (-\infty, \lambda_\infty) \,,$

   each $\lambda_k \in (-\infty, \lambda_\infty)$ being an eigenvalue of H repeated a number of times equal to its multiplicity.

In summary, the numbers as *defined* by (3.21) coincide with discrete eigenvalues of H *below the essential spectrum.* Hence, we have a complete variational characterisation for such eigenvalues. Regardless of whether the essential spectrum of H is empty or not, the bottom of the spectrum of H always coincides with λ_1:

$$\inf \sigma(H) = \lambda_1 = \inf_{\substack{\psi \in \operatorname{dom} H \\ \psi \neq 0}} \frac{(\psi, H\psi)}{\|\psi\|^2} = \inf_{\substack{\psi \in \operatorname{dom} h \\ \psi \neq 0}} \frac{h[\psi]}{\|\psi\|^2}. \tag{3.22}$$

At the same time, the bottom of the essential spectrum is always characterised by the limit

$$\inf \sigma_{\mathrm{ess}}(H) = \lim_{k \to \infty} \lambda_k \tag{3.23}$$

(with the convention that $\sigma_{\mathrm{ess}}(H) = \varnothing$ if the limit is $+\infty$). In particular, if H is a self-adjoint operator with purely discrete spectrum, its eigenvalues can accumulate at $+\infty$ only.

Theorems 3.11 and 3.23 enable one to compute the spectrum of self-adjoint semi-bounded operators variationally (it is thus interesting even in finite-dimensional vector spaces). Therefore they represent an extremely useful tool (in fact, *supertool* or *wonder weapon* (*Wunderwaffe*)) in practical problems in quantum mechanics (*e.g.*, for computation of eigenvalues of many-body Hamiltonians in quantum chemistry). In these lectures, however, we shall merely use the minimax principle to establish upper bounds to the eigenvalues of the Dirichlet Laplacian.

The minimax principle can be also used to compare the spectra of different operators. Recall Definition 2.7 introducing the order relation between (possibly unbounded) operators and let us write $\lambda_k(H)$ if we want to point out the dependence of the numbers (3.21) on the operator H.

Corollary 3.14. *If H_-, H_+ are two self-adjoint operators in $\mathcal{H}$ that are bounded from below. Then*

$$H_- \leq H_+ \qquad \Longrightarrow \qquad \forall k \in \mathbb{N}^*, \quad \lambda_k(H_-) \leq \lambda_k(H_+).$$

Let us conclude this overview of the minimax principle by the following useful observation, which is rarely made explicit in the literature. We stress that eigenvalues at the bottom of the essential spectrum are included in this proposition, too.

Proposition 3.15. *If* (3.21) *is achieved,* i.e. *there exists a non-trivial $\psi \in \operatorname{dom} h$ such that*

$$\lambda_k = \frac{h[\psi]}{\|\psi\|^2} \tag{3.24}$$

*and ψ is orthogonal to all the eigenvectors corresponding to $\lambda_1, \dots, \lambda_{k-1} < \lambda_\infty$ (*i.e. *no orthogonality condition if $k = 1$ or if there are no eigenvalues below the essential spectrum, while $\lambda_k = \lambda_\infty$ is permitted), then λ_k is an eigenvalue of H and ψ is a corresponding eigenvector.*

Proof. In the first part of the proof, we are inspired by [25, proof of Lem. XI 1.1]. Let $\psi_1, \dots, \psi_{k-1}$ denote the orthonormal eigenvectors of H corresponding to $\lambda_1, \dots, \lambda_{k-1}$. Denoting $\mathcal{G} := \operatorname{span}\{\psi_1, \dots, \psi_{k-1}\}$, we have the orthogonal sum decomposition $\mathcal{H} = \mathcal{G} \oplus \mathcal{G}^\perp$. Let H_1 and H_2 be the restrictions of H to $\mathcal{G}$ and $\mathcal{G}^\perp$, respectively. Clearly, H_1 and H_2 are self-adjoint operators in $\mathcal{G}$ and $\mathcal{G}^\perp$, respectively, and $H = H_1 \oplus H_2$. It is easy to verify that $\sigma(H_2) = \sigma(H) \setminus \{\lambda_1, \dots, \lambda_{k-1}\}$. By (3.22), it thus follows that

$$\lambda_k = \inf_{\substack{\psi \in \mathcal{G}^\perp \cap \operatorname{dom} h \\ \psi \neq 0}} \frac{h[\psi]}{\|\psi\|^2}.$$

Now, let us assume that this infimum is achieved. That is, there exists a non-trivial vector $\psi \in \mathcal{G}^\perp \cap \operatorname{dom} h$ such that (3.24) holds. In particular, ψ is the critical point of the functional

$$J[\psi] := \frac{h[\psi]}{\|\psi\|^2}.$$

Consequently, the first variation

$$\begin{aligned}\lim_{\varepsilon\to 0}\frac{J[\psi+\varepsilon\phi]-J[\psi]}{\varepsilon} &= \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\left(\frac{h[\psi]+2\varepsilon\Re h(\phi,\psi)+\varepsilon^2 h[\phi]}{\|\psi\|^2+2\varepsilon\Re(\phi,\psi)+\varepsilon^2\|\phi\|^2}-\frac{h[\psi]}{\|\psi\|^2}\right)\\ &= 2\Re h(\phi,\psi)-2\lambda_k\Re(\phi,\psi)\\ &= 2\Re\left[h(\phi,\psi)-\lambda_k(\phi,\psi)\right]\end{aligned}$$

must vanish, where $\phi\in\mathcal{G}^\perp\cap\operatorname{dom}h$ is arbitrary. Using the arbitrariness of ϕ, we conclude that

$$\forall\phi\in\mathcal{G}^\perp\cap\operatorname{dom}h\,,\qquad h(\phi,\psi)=\lambda_k(\phi,\psi)\,.$$

By the representation theorem (*cf* (1.11)), it follows that $\psi\in\operatorname{dom}H$ and $H\psi=\lambda_k\psi$. □

3.6 Monotonicity of eigenvalues

As above, for any bounded domain $\Omega\subset\mathbb{R}^d$, we arrange the eigenvalues of the Dirichlet Laplacian in $L^2(\Omega)$ into a non-decreasing sequence

$$\sigma(-\Delta_D^\Omega)=\left\{\lambda_1^D(\Omega)\leq\lambda_2^D(\Omega)\leq\lambda_3^D(\Omega)\leq\dots\right\},$$

where each eigenvalue is repeated according to its multiplicity. Here we emphasise the dependence on the domain Ω by the argument and the Dirichlet boundary conditions by the superscript.

The reason why Dirichlet boundary conditions are the easiest to treat in many respects is the existence of the trivial extension of functions from the form domain $W_0^{1,2}(\Omega)$ to the whole space $\mathbb{R}^d$, while preserving the Sobolev-space-type properties, *cf* (3.17). More generally, we have the natural conti nuous embedding

$$\Omega_1\subset\Omega_2\qquad\Longrightarrow\qquad W_0^{1,2}(\Omega_1)\hookrightarrow W_0^{1,2}(\Omega_2)\,, \tag{3.25}$$

just by extending the functions in $W_0^{1,2}(\Omega_1)$ by zero outside Ω_1 (as in (3.17)). Using (3.20), we therefore get, for every $k\in\mathbb{N}^*$,

$$\lambda_k^D(\Omega_2)=\inf_{\substack{\mathcal{L}_k\subset W_0^{1,2}(\Omega_2)\\ \dim\mathcal{L}_k=k}}\ \sup_{\substack{\psi\in\mathcal{L}_k\\ \psi\neq 0}}\frac{\|\nabla\psi\|^2_{L^2(\Omega_2)}}{\|\psi\|^2_{L^2(\Omega_2)}}\leq\inf_{\substack{\mathcal{L}_k\subset W_0^{1,2}(\Omega_1)\\ \dim\mathcal{L}_k=k}}\ \sup_{\substack{\psi\in\mathcal{L}_k\\ \psi\neq 0}}\frac{\|\nabla\psi\|^2_{L^2(\Omega_1)}}{\|\psi\|^2_{L^2(\Omega_1)}}=\lambda_k^D(\Omega_1)\,.$$

Let us formulate this crucial monotonicity property into the following important theorem.

Theorem 3.16 (Monotonicity of Dirichlet eigenvalues)**.** *Let $\Omega_1,\Omega_2\subset\mathbb{R}^d$ be bounded domains. Then*

$$\Omega_1\subset\Omega_2\qquad\Longrightarrow\qquad\forall k\in\mathbb{N}^*\,,\quad\lambda_k^D(\Omega_1)\geq\lambda_k^D(\Omega_2)\,.$$

Note that the larger membrane produces a lower fundamental tone (or a quantum particle in a larger cavity has a lower ground-state energy), which is in agreement with a physical intuition.

Remark 3.17 (General domains)**.** We have formulated Proposition 3.16 for *bounded* domains only, but the monotonicity actually holds for *any* domains, provided that the numbers λ_k's are interpreted through the formula (3.20). In particular, the monotonicity holds for (discrete) eigenvalues below the essential spectrum.

Proposition 3.16 enables one to obtain bounds for unknown Dirichlet eigenvalues in a complicated domain in terms of known geometric quantities. Indeed, for every $k\in\mathbb{N}^*$,

$$\mathcal{R}_{a_1,\dots,a_d}\subset\Omega\subset\mathcal{R}_{a_1',\dots,a_d'}\qquad\Longrightarrow\qquad\lambda_k^D(\mathcal{R}_{a_1,\dots,a_d})\geq\lambda_k^D(\Omega)\geq\lambda_k^D(\mathcal{R}_{a_1',\dots,a_d'})\,,$$

where the eigenvalues in the rectangular boxes are known explicitly, see Section 3.2.

3.7 General criteria for the absence of the essential spectrum

From our proof of the absence of the essential spectrum in bounded domains (Theorem 3.8), it is clear that the property is strongly related to *compactness*. To get an insight into this relationship, let us establish the following abstract criteria.

Theorem 3.18. *Let H be a non-negative self-adjoint operator in an infinite-dimensional $\mathcal{H}$. Let h be its associated sesquilinear form. Then the following conditions are equivalent:*

(1) $\sigma_{\mathrm{ess}}(H) = \varnothing$;

(2) $(H+I)^{-1}$ *is compact;*

(3) $(H+I)^{-1/2}$ *is compact;*

(4) $\operatorname{dom} H \hookrightarrow \mathcal{H}$ *is compact;*

(5) $\operatorname{dom} h \hookrightarrow \mathcal{H}$ *is compact;*

(6) $\lambda_\infty(H) = +\infty$.

Proof. We prove the equivalences as a chain of the following implications.

$\boxed{(1) \Leftrightarrow (6)}$ This is clear from Theorem 3.13.

$\boxed{(2) \Leftrightarrow (4)}$ The embedding $\operatorname{dom} H \hookrightarrow \mathcal{H}$ is realised by the inclusion map $\iota : \operatorname{dom} H \to \mathcal{H} : \{\psi \mapsto \psi\}$. Let us write

$$\iota : \underbrace{(H+I)^{-1}}_{\mathcal{H}\to\mathcal{H}} \underbrace{(H+I)}_{\operatorname{dom} H\to\mathcal{H}} : \operatorname{dom} H \to \mathcal{H} .$$

If $(H+I)^{-1}$ is compact in $\mathcal{H}$, then ι is a composition of the bounded isomorphism $H+I : \operatorname{dom} H \to \mathcal{H}$ and the compact operator $(H+I)^{-1} : \mathcal{H} \to \mathcal{H}$, therefore ι is compact by itself. Vice versa, if ι is compact, then the decomposition

$$(H+I)^{-1} = \underbrace{\iota}_{\operatorname{dom} H\to\mathcal{H}} \underbrace{(H+I)^{-1}}_{\mathcal{H}\to\operatorname{dom} H} : \mathcal{H} \to \mathcal{H} ,$$

where $(H+I)^{-1} : \mathcal{H} \to \operatorname{dom} H$ is a bounded isomorphism, shows that $(H+I)^{-1}$ is a compact operator in $\mathcal{H}$.

$\boxed{(3) \Leftrightarrow (5)}$ This equivalence can be established analogously to the precedent one. The embedding $\operatorname{dom} h \hookrightarrow \mathcal{H}$ is realised by the inclusion map $\iota : \operatorname{dom} h \to \mathcal{H} : \{\psi \mapsto \psi\}$. Writing

$$\iota : \underbrace{(H+I)^{-1/2}}_{\mathcal{H}\to\mathcal{H}} \underbrace{(H+I)^{1/2}}_{\operatorname{dom} h\to\mathcal{H}} : \operatorname{dom} h \to \mathcal{H} ,$$

we see that ι is compact if $(H+I)^{-1/2}$ is compact in $\mathcal{H}$, Vice versa, if ι is compact, then

$$(H+I)^{-1/2} = \underbrace{\iota}_{\operatorname{dom} h\to\mathcal{H}} \underbrace{(H+I)^{-1/2}}_{\mathcal{H}\to\operatorname{dom} H} : \mathcal{H} \to \mathcal{H} ,$$

is compact.

$\boxed{(2) \Leftrightarrow (3)}$ Write $(H+I)^{-1} = (H+I)^{-1/2}(H+I)^{-1/2}$ and observe that $(H+I)^{-1}$ is compact, if and only if, $(H+I)^{-1/2}$ is compact (see Exercise 7f).

$\boxed{(2) \Leftarrow (6)}$ We may proceed as in the proof of of Proposition 3.5. By Theorem 3.13, the spectrum of H is purely discrete. Let $\{\lambda_k\}_{k\in\mathbb{N}^*}$ denote the non-decreasing sequence of eigenvalues of H, where each eigenvalue is repeated according to its multiplicity. Let $\{\psi_k\}_{k\in\mathbb{N}^*}$ be the corresponding set of eigenvectors, which can be chosen as an orthonormal basis in $\mathcal{H}$ due to Theorem 3.10. First of all, it is easy to verify the decomposition formula for the resolvent

$$(H+I)^{-1} = \sum_{k=1}^{\infty} (\lambda_k+1)^{-1} \psi_k (\psi_k, \cdot) .$$

For every $N \in \mathbb{N}^*$, define the finite-rank operators

$$R_N := \sum_{k=1}^{N} (\lambda_k + 1)^{-1} \psi_k (\psi_k, \cdot) .$$

From the formula

$$(H+I)^{-1} - R_N = \sum_{k=N+1}^{\infty} (\lambda_k + 1)^{-1} \psi_k (\psi_k, \cdot)$$

and the Bessel inequality, we deduce that, for every $\psi \in \mathcal{H}$,

$$\big\| \big[(H+I)^{-1} - H_N \big] \psi \big\| \leq (\lambda_N + 1)^{-1} \|\psi\|^2 .$$

Since $\lambda_N \to \infty$ as $N \to \infty$, we see that H_N converges in norm to $(H+I)^{-1}$ as $N \to \infty$. It remains to recall that the limit of finite-rank operators is a compact operator (see Exercise 7e).

$\boxed{(2) \Rightarrow (6)}$ By contradiction, let us assume that $(H+I)^{-1}$ is compact, while $\lambda_\infty(H) < 0$. The latter implies that $\sigma_{\mathrm{ess}}(H) \neq \varnothing$ due to the previously established equivalence (1) $\Leftrightarrow$ (6). Consequently, by our Definition 3.1, there exists $\lambda \geq 0$ and a non-compact sequence $\{\psi_n\}_{n \in \mathbb{N}} \subset \operatorname{dom} H$ such that $\|\psi_n\| = 1$ for all $n \in \mathbb{N}$ and $\|H\psi_n - \lambda\psi_n\| \to 0$ as $n \to \infty$. From the identity

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

valid on $\operatorname{dom} H$, it follows that $(\lambda+1)^{-1} \in \sigma_{\mathrm{ess}}((H+I)^{-1})$. However, this is impossible, because the spectrum of any compact operator is purely discrete, except perhaps for the value 0 (which is always in the essential spectrum in infinite-dimensional spaces). □

In the last part of the proof, we have used the fact that the spectrum of compact operators shares many similarities with the spectrum of matrices (or operators in finite-dimensional spaces). Assuming the validity of the *spectral-mapping theorem* (see [25, Thm. IX.2.3])

$$\lambda \in \sigma(H) \qquad \Longleftrightarrow \qquad (\lambda+1)^{-1} \in \sigma\big((H+I)^{-1}\big) ,$$

together with analogous equivalences for discrete and essential components of the spectrum, the equivalence (1) $\Leftrightarrow$ (2) in Theorem 3.18 is therefore the very expected one.

An operator H for which $(H+I)^{-1}$ is called an *operator with compact resolvent*. By Theorem 3.18, any such operator has a purely discrete spectrum.

Let us use the criteria of Theorem 3.18 to provide alternative proofs of Theorem 3.8 about the absence of essential spectrum in bounded domains.

Alternative proof of Theorem 3.8: monotonicity of eigenvalues. Since Ω is bounded, there exists a cube Q such that $\Omega \subset Q$. By the monotonicity of Dirichlet eigenvalues (Theorem 3.16), one has

$$\forall k \in \mathbb{N}^* , \qquad \lambda_k(-\Delta_D^\Omega) \geq \lambda_k(-\Delta_D^Q) .$$

Since the spectrum of $-\Delta_D^Q$ is purely discrete (Proposition 3.4), it follows from Theorem 3.18 (implication (1) $\Rightarrow$ (6)) that $\lambda_k(-\Delta_D^Q) \to +\infty$ as $k \to \infty$. Consequently, we also have $\lambda_k(-\Delta_D^\Omega) \to +\infty$ as $k \to \infty$, so the desired claim about the absence of the essential spectrum follows from Theorem 3.18 (implication (1) $\Leftarrow$ (6)). □

Alternative proof of Theorem 3.8: extension property. Since Ω is bounded, there exists a cube Q such that $\Omega \subset Q$. We have the following bounded maps:

$$W_0^{1,2}(\Omega) \xrightarrow{E} W_0^{1,2}(Q) \xrightarrow{\iota} L^2(Q) \xrightarrow{R} L^2(\Omega) ,$$

where E is the trivial extension (3.17), ι is the embedding and R is just the restriction. By the absence of the essential spectrum in rectangular boxes (Proposition 3.4), the embedding ι is compact, thefore the composed map $E \circ \iota \circ R$ is compact too. It follows that the embedding $W_0^{1,2}(\Omega) \hookrightarrow L^2(\Omega)$ is compact, so the desired claim about the absence of the essential spectrum follows from Theorem 3.18 (implication (1) $\Leftarrow$ (5)). □

3.8 Counterexamples for Neumann boundary conditions

Neumann (and Robin) boundary conditions are much more delicate. In this section, we demonstrate that neither the emptiness of the essential spectrum for bounded domains nor the monotonicity of eigenvalues hold if we impose Neumann instead of Dirichlet boundary conditions.

3.8.1 Bounded domains with an essential spectrum

As in the Dirichlet case, it is also true that the spectrum of the Neumann Laplacian in any rectangular box $\mathcal{R}_{a_1,\dots,a_d}$ is purely discrete (recall Remark 3.6). However, this is no longer true for the Neumann Laplacian in an *arbitrary* bounded domain Ω: the **emptiness of the essential spectrum in bounded domains does not hold for Neumann**!

As a counterexample, here we present a construction which is originally due to Fraenkel [29], but we rather follow a presentation given in [25, Sec. V.4.9]. The example consists of a planar domain Ω referred to as "rooms and passages" and made up of an infinite sequence of square boxes ("rooms") of decreasing sizes joined together by thin pipes ("passages"), see Figure 3.3.

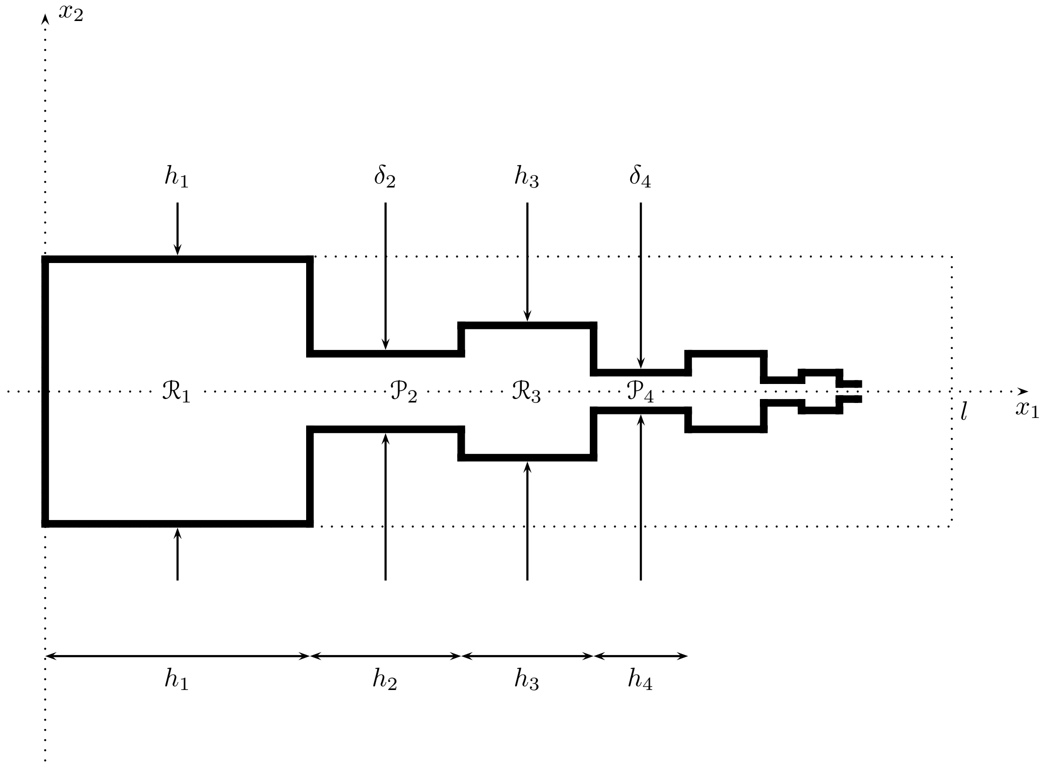


Figure 3.3: *Rooms and passages* as an example of a bounded domain for which the Neumann Laplacian has an essential spectrum.

Proposition 3.19 (Rooms and passages)**.** *If Ω is the (bounded) domain of Figure 3.3 with $h_j := j^{-3/2}$ and $\delta_j := j^{-6}$ for every $j \in \mathbb{N}^*$, then*

$$\sigma_{\text{ess}}(-\Delta_N^\Omega) \neq \varnothing\,.$$

Proof. More specifically, defining $h_0 := 0$, $h_j := j^{-3/2}$ and $\delta_j := j^{-6}$ for every $j \in \mathbb{N}^*$, we introduce an n^{th} room

$$\mathcal{R}_n := \big(h_0 + h_1 + \dots + h_{n-1}, h_0 + h_1 + \dots + h_{n-1} + h_n\big) \times \left(-\frac{h_n}{2}, \frac{h_n}{2}\right)$$

and an n^{th} passage

$$\mathcal{P}_n := [h_0 + h_1 + \dots + h_{n-1}, h_0 + h_1 + \dots + h_{n-1} + h_n] \times \left(-\frac{\delta_n}{2}, \frac{\delta_n}{2}\right)$$

and join together the odd rooms with even passages by setting

$$\Omega := \bigcup_{\substack{n\in\mathbb{N}^* \\ n \text{ odd}}} \mathcal{R}_n \cup \bigcup_{\substack{n\in\mathbb{N}^* \\ n \text{ even}}} \mathcal{P}_n \,.$$

Note that Ω is bounded because

$$\sum_{j=1}^{\infty} h_j = \zeta(3/2) =: l < \infty \,,$$

where ζ denotes the Riemann zeta function; in fact, $\Omega \subset [0,l] \times [-1/2, 1/2]$. However, the boundary $\partial\Omega$ is not of class C^0 because of the troublesome point $(l,0) \in \partial\Omega$.

We claim that

$$0 \in \sigma_{\mathrm{ess}}(-\Delta_N^\Omega) \,. \tag{3.26}$$

For each odd $n \in \mathbb{N}^*$, define a function $u_n \in W^{1,2}(\Omega)$ by requiring

$$u_n(x) := \begin{cases} h_n^{-1} & \text{if} \quad x \in \mathcal{R}_n \,, \\ 0 & \text{if} \quad x \in \Omega \setminus (\mathcal{P}_{n-1} \cup \mathcal{R}_n \cup \mathcal{P}_{n+1}) \,, \end{cases} \qquad \nabla u_n(x) := \pm\big((h_n h_{n\mp1})^{-1}, 0\big) \quad \text{if} \quad x \in \mathcal{P}_{n\mp1} \,.$$

We have

$$\begin{aligned} \|u_n\|^2 &= 1 + \tfrac{1}{3} h_n^{-2} (h_{n-1}\delta_{n-1} + h_{n+1}\delta_{n+1}) \geq 1 \,, \\ \|\nabla u_n\|^2 &= (h_n h_{n-1})^{-2} h_{n-1}\delta_{n-1} + (h_n h_{n+1})^{-2} h_{n+1}\delta_{n+1} \xrightarrow[n\to\infty]{} 0 \,. \end{aligned}$$

Consequently,

$$\frac{\|\nabla u_n\|^2}{\|u_n\|^2} \xrightarrow[n\to\infty]{} 0 \,,$$

which implies that $0 \in \sigma(-\Delta_N^\Omega)$ by the minimax principle, because the functions u_n span an infinite-dimensional subspace of $W^{1,2}(\Omega)$ (as the elements of the subsequence $\{u_{4n+1}\}_{n\in\mathbb{N}}$ have mutually disjoint supports). □

It follows from Proposition 3.19 and Theorem 3.18 that the embedding

$$W^{1,2}(\Omega) \hookrightarrow L^2(\Omega) \tag{3.27}$$

can be non-compact even if the domain Ω is bounded. The feature of the example of Proposition 3.19 is the irregular point $(l,0) \in \partial\Omega$, which is intimately related to the absence of the extension property for functions from the Sobolev space $W^{1,2}(\Omega)$. In general, a certain regularity of the boundary $\partial\Omega$ is needed in order to ensure the compactness of the embedding (3.27), and thus the emptiness of the essential spectrum for the Neumann Laplacian in bounded domains. The required regularity can be characterised in terms of the following extension property.

Definition 3.20. An open set $\Omega \subset \mathbb{R}^d$ is said to satisfy the *extension property* if there exists a bounded (linear) operator $E : W^{1,2}(\Omega) \to W^{1,2}(\mathbb{R}^d)$ satisfying $(E\psi)(x) = \psi(x)$ for all $\psi \in W^{1,2}(\Omega)$ and all $x \in \Omega$.

Note that an analogous definition for Dirichlet boundary conditions is trivial, just because of the availability of the trivial extension of $W_0^{1,2}(\Omega)$ to $W_0^{1,2}(\mathbb{R}^d) = W^{1,2}(\mathbb{R}^d)$ for an arbitrary domain Ω. This is the main reason behind the robust result of Theorem 3.8 about the emptiness of the essential spectrum of the Dirichlet Laplacian for *any* bounded domain. Now we are in a position to establish the same result under the extra hypothesis of Definition 3.20 (by Proposition 3.19, a restriction is necessary).

Theorem 3.21. *Let $\Omega \subset \mathbb{R}^d$ be any bounded open set with the extension property. Then*

$$\sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = \varnothing \,.$$

Proof. Since Ω is bounded, there exists a cube Q such that $\Omega \subset Q$. We have the following bounded maps:

$$W^{1,2}(\Omega) \xrightarrow{E} W^{1,2}(\mathbb{R}^d) \xrightarrow{R_1} W^{1,2}(Q) \xrightarrow{\iota} L^2(Q) \xrightarrow{R_2} L^2(\Omega)\,,$$

where E is the extension of Definition 3.20, ι is the embedding and R_1, R_2 are elementary restrictions. By the absence of the essential spectrum in rectangular boxes (*cf* Remark 3.6), the embedding ι is compact (recall Theorem 3.18), thefore the composed map $E\circ R_1\circ\iota\circ R_2$ is compact too. It follows that the embedding $W_0^{1,2}(\Omega) \hookrightarrow L^2(\Omega)$ is compact, so the desired claim about the absence of the essential spectrum follows from Theorem 3.18. ☐

The family of all open sets with the extension property is a wide one (see [25, Sec. V.4.4]). It includes the so-called open sets with *minimally smooth boundary*, which cover all bounded open sets with boundary of class $C^{0,1}$ (*i.e.* Lipschitz regularity). However, to have (3.27) (and thus the conclusion of Theorem 3.21), it is enough to assume that the boundary of Ω is merely continuous (see [25, Sec. V.4.17]).

3.8.2 Non-monotonicity of the eigenvalues

Recall that the availability of the trivial extension for the Sobolev space $W^{1,2}(\Omega)$ is behind the monotocity of Dirichlet eigenvalues (Theorem 3.16). The **monotonicity result does not hold for Neumann** (or more generally Robin) eigenvalues!

Example 3.22. A classical counterexample is given in Figure 3.4: an inscribed thin rectangle along the diagobal of a circumscribed rectangle. Of course, there is no contradiction for the lowest eigenvalue, because $\lambda_1^N(\Omega_1) = 0 = \lambda_1^N(\Omega_1)$ due to the availability of the constant eigenfunction. However, we get a contradiction already for the second eigenvalue. Let the lengths of the sides of the circumscribed (respectively inscribed) rectangle be $a_2 \geq b_2$ (respectively $a_1 \geq b_1$). Then

$$\begin{aligned}
\lambda_2^N(\Omega_1) &= \min\left\{(\pi/a_1)^2 + 0, 0 + (\pi/b_1)^2\right\} = (\pi/a_1)^2\,,\\
\lambda_2^N(\Omega_2) &= \min\left\{(\pi/a_2)^2 + 0, 0 + (\pi/b_2)^2 + 0\right\} = (\pi/a_2)^2\,.
\end{aligned}$$

It remains to notice that $a_1 = \sqrt{a_2^2+b_2^2} - b_1 a_2/b_2$ with $b_1 \leq b_2\sqrt{a_2^2+b_2^2}/(a_2+b_2)$, so that $a_1 > a_2$ for all sufficiently small b_1 (the result intuitively clear from the picture). Consequently,

$$\lambda_2^N(\Omega_2) > \lambda_2^N(\Omega_1)$$

for all sufficiently small b_1. (On the other hand, it is clear that there are scenarios of $\Omega_1 \subset \Omega_2$ with $a_1 \leq a_2$ and $b_1 \leq b_2$ for which we have the reverse (expected) inequality $\lambda_2^N(\Omega_2) < \lambda_2^N(\Omega_1)$.) ♢

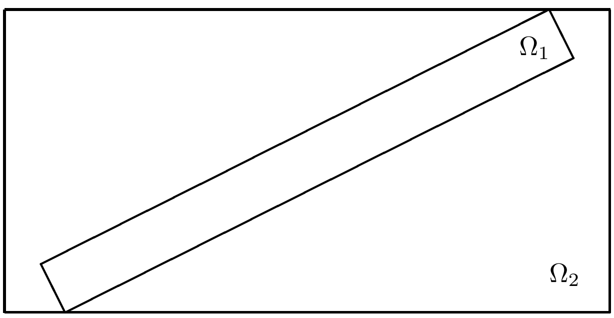


Figure 3.4: A classical counterexample to the monotonicity of Neumann eigenvalues.

Example 3.23. Yet another example to the monotonicity of Neumann eigenvalues is presented in Figure 3.5. If the radius of the circumscribed disk Ω_2 is R and the lengths of the sides of the inscribed rectangle are

$a \geq b$, then $R^2 = (a/2)^2 + (b/2)^2$, so that the second Neumann eigenvalues satisfy

$$\lambda_2^N(\Omega_2) = (j'_{1,1}/R)^2 > (\pi/a)^2 = \lambda_2^N(\Omega_1)$$

for all sufficiently small b, where $j'_{1,1}$ denotes the first root of $J'_1(x) = 0$. Indeed, $j'_{1,1} \approx 1.84$, while $\pi/2 \approx 1.57$. (On the other hand, if the disk Ω_2 is inscribed in the rectangle Ω_1, the inequality $\lambda_2^N(\Omega_2) < \lambda_2^N(\Omega_1)$ remains valid for all $a, b \geq 2R$.) ♢

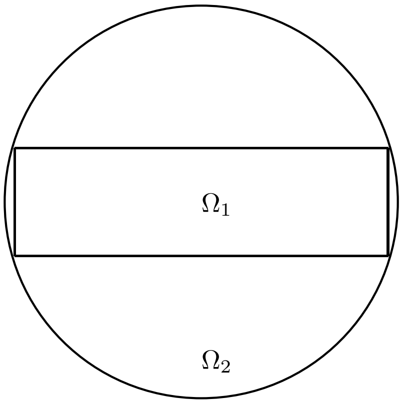


Figure 3.5: Another counterexample to the monotonicity of Neumann eigenvalues.

3.8.3 Zero is always in the spectrum

Finally, let us mention another peculiarity of Neumann boundary conditions. If Ω is bounded, then 0 is never in the spectrum of the Dirichlet Laplacian, for the spectrum is purely discrete and the only solution of (recall Proposition 3.15)

$$0 = \frac{\|\nabla\psi\|^2}{\|\psi\|^2}$$

is $\psi = 0$ (because ψ must be a constant function and the Dirichlet boundary conditions force the constant to be zero). On the other hand, non-zero constant functions are admissible eigenfunctions of the Neumann Laplacian in bounded domains (more generally in domains of finite volume), so 0 is always in the spectrum of the Neumann Laplacian in such domains. What is more, the property that 0 is in the spectrum of the Neumann Laplacian actually holds in the full generality of arbitrary domains. (Since the Neumann Laplacian is non-negative, the result says that the bottom of the spectrum starts by zero.)

Theorem 3.24. *Let $\Omega \subset \mathbb{R}^d$ be an arbitrary open set. Then*

$$0 \in \sigma(-\Delta_N^\Omega)\,.$$

Proof. The bound $\inf \sigma(-\Delta_N^\Omega) \geq 0$ follows by the non-negativity of the Neumann Laplacian. To prove the opposite inequality, we recall the minimax principle (*cf* (3.22)),

$$\inf \sigma(-\Delta_N^\Omega) = \inf_{\substack{\psi \in W^{1,2}(\Omega)\\ \psi \neq 0}} \frac{\|\nabla\psi\|^2}{\|\psi\|^2} \leq \frac{\|\nabla\psi\|^2}{\|\psi\|^2}\,,$$

where the inequality holds for any non-zero $\psi \in W^{1,2}(\Omega)$. For every $n \in \mathbb{N}^*$, we define $\psi_n(x) := \varphi_n(|x|)$, where $\varphi_n \in C_0^\infty([0,\infty))$ is such that $0 \leq \varphi_n \leq 1$ and $|\varphi'_n| \leq C$ for all $n \in \mathbb{N}^*$ with some constant C independent of n and

$$\varphi_n(r) := \begin{cases} 1 & \text{if} \quad r < n\,, \\ 0 & \text{if} \quad r > n+1\,. \end{cases}$$

Clearly, for every $n \in \mathbb{N}^*$, the restriction of ψ_n to Ω (that we again denote by ψ_n) belongs to $W^{1,2}(\Omega)$. Let us take n sufficiently large so that $\Omega \cap B_n \neq \varnothing$. Since $|\nabla\psi_n(x)| = |\varphi_n'(|x|)| = |\varphi_n'(|x|)|\chi_{B_{n+1}\setminus B_n}(x)$ and $\psi_n(x) \geq \chi_{B_n}(x)$ for all $x \in \mathbb{R}^d$, we have

$$\|\nabla\psi_n\|^2 \leq C^2\,|\Omega \cap (B_{n+1} \setminus B_n)|\,, \qquad \|\psi_n\|^2 \geq |\Omega \cap B_n|\,.$$

From the variational characterisation, we therefore get the bound

$$\inf\sigma(-\Delta_N^\Omega) \leq C^2\,\frac{|\Omega \cap (B_{n+1} \setminus B_n)|}{|\Omega \cap B_n|} = C^2\,\frac{|\Omega \cap B_{n+1}| - |\Omega \cap B_n|}{|\Omega \cap B_n|}\,. \tag{3.28}$$

If the right-hand side equals to zero for some n (which is the case of bounded domains) or in the limit as $n \to \infty$ (which is the case of the whole space $\mathbb{R}^d$), we deduce $\inf\sigma(-\Delta_N^\Omega) \leq 0$. In fact, it is enough to assume that one achieves the zero limit for a subsequence. By contradiction, let us assume

$$\exists c > 0,\ n_0 > 0, \quad \forall n \geq n_0, \qquad \frac{\omega_{n+1} - \omega_n}{\omega_n} \geq c\,.$$

That is, $\omega_{n+1} \geq (1+c)\,\omega_n$. By recurrence,

$$\forall k \in \mathbb{N}\,, \qquad \omega_{n+k} \geq (1+c)^k\,\omega_n\,.$$

Estimating the left-hand side by the volume of the whole ball B_{n+k}, we obtain

$$\forall k \in \mathbb{N}\,, \qquad (n+k)^d\,|B_1| = |B_{n+k}| \geq (1+c)^k\,\omega_n\,.$$

Since the right hand-side is exponentially growing with k, while the left-hand has a polynomial growth as a function of k, we arrive at a contradiction for all sufficiently large k. That is, the right-hand side of (3.28) tends to zero as $n \to \infty$ and the theorem is proved. □

Remark 3.25. The statement of Theorem 3.24 in a greater generality of Riemannian manifolds can be found in [22, Thm. 5.2.10]. Our proof is partially inspired by the proof of [19, Thm. 2.12]. We are grateful to Markus Holzmann for letting us know about the idea.

3.9 Unbounded domains

The situation becomes more difficult, even for the Dirichlet Laplacian, if Ω is an unbounded domain. It is still true that the spectrum of the Dirichlet Laplacian is purely discrete if Ω has finite volume. Another example of sufficient condition is the following result due to Berger and Schechter [8] (see [25, Thm. V.5.17] for a more general statement):

Theorem 3.26 (Berger–Schechter's criterion)**.** *One has*

$$\limsup_{\substack{|x|\to\infty \\ x\in\Omega}} \big|\Omega \cap B_1(x)\big| = 0 \qquad \Longrightarrow \qquad \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = \varnothing\,.$$

It is interesting to compare the sufficient condition of Theorem 3.26 with the characterisation (3.1): While quasi-bounded domains are just "narrow at infinity", the sufficient condition of Theorem 3.26 requires that the narrowness must be "inessential in an integral sense" to have a purely discrete spectrum.

The example of *spiny urchin* of Figure 3.1 (originally due to Clark [15]) shows that Theorem 3.26 represents just a sufficient condition. Indeed, since Ω is built by removing from $\mathbb{R}^2$ just sets of measure zero (semi-infinite lines), it follows that $|\Omega \cap B_1(x)| = |B_1(x)|$ for every $x \in \Omega$. On the other hand, the following proposition shows that the spectrum is still purely discrete.

Proposition 3.27 (Spiny urchin)**.** *If Ω is the (unbounded) domain of Figure 3.1, then*

$$\sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = \varnothing\,.$$

Proof. By the definition given in Figure 3.1, the domain Ω is obtained by deleting from the plane a union of infinite rays:

$$\Omega = \mathbb{R}^2 \setminus \bigcup_{m=1}^{\infty} S_m \,, \tag{3.29}$$

where the sets S_m are specified in polar coordinates $(r,\vartheta) \in [0,\infty) \times [0,2\pi)$ by

$$S_m := \left\{(r\cos\vartheta, r\sin\vartheta) : \quad r \geq m \quad \wedge \quad \vartheta = n\pi/2^m \quad \text{for} \quad n = 1,2,\dots,2^{m+1}\right\} .$$

Note that this domain, though quasi-bounded, is simply connected and has empty exterior.

To prove that the spectrum of the Dirichlet Laplacian in Ω is purely discrete, let us impose an extra Neumann condition on the circle $\Sigma_m := \partial B_m$. More specifically, for every $m \in \mathbb{N}^*$, we employ the decomposition

$$\Omega = \underbrace{(\Omega \cap B_m)}_{\Omega_m^{\text{int}}} \cap \underbrace{(\Omega \cap \partial B_m)}_{\Sigma_m} \cap \underbrace{(\Omega \setminus \overline{B}_m)}_{\Omega_m^{\text{ext}}} ,$$

which leads to the direct-sum decomposition of the Hilbert space

$$L^2(\Omega) = L^2(\Omega_m^{\text{int}}) \oplus L^2(\Omega_m^{\text{ext}}) \,. \tag{3.30}$$

Recall that the Dirichlet Laplacian $H := -\Delta_D^\Omega$ is the operator in $L^2(\Omega)$ associated with the form

$$h[\psi] := \int_\Omega |\nabla\psi|^2 \,, \qquad \operatorname{dom} h := W_0^{1,2}(\Omega) \,.$$

The same operator with the extra Neumann condition on Σ_m is introduced as the operator H_m^N in $L^2(\Omega)$ associated with the form

$$h_m^N[\psi] := \int_\Omega |\nabla\psi|^2 \,, \qquad \operatorname{dom} h_m^N := \left[W_0^{1,2}(\Omega) \restriction \Omega_m^{\text{int}}\right] \oplus \left[W_0^{1,2}(\Omega) \restriction \Omega_m^{\text{ext}}\right] ,$$

where $W_0^{1,2}(\Omega) \restriction \Omega_m^{\text{int}}$ means the set of restrictions $\psi \restriction \Omega_m^{\text{int}}$ with $\psi \in W_0^{1,2}(\Omega)$, and similarly for $W_0^{1,2}(\Omega) \restriction \Omega_m^{\text{ext}}$. Note that h_m^N acts in the same way as h, while the form domain of the former is larger (*cf* Figure 3.6). Consequently,

$$H \geq H_m^N = H_m^{\text{int},N} \oplus H_m^{\text{ext},N} \,, \tag{3.31}$$

where $H_m^{\text{int},N}$ is the operator in $L^2(\Omega_m^{\text{int}})$ associated with the form

$$h_m^{\text{int},N}[\psi] := \int_{\Omega_m^{\text{int}}} |\nabla\psi|^2 \,, \qquad \operatorname{dom} h_m^{\text{int},N} := W_0^{1,2}(\Omega) \restriction \Omega_m^{\text{int}} \,,$$

and $H_m^{\text{ext},N}$ in $L^2(\Omega_m^{\text{ext}})$ is defined analogously.

As a consequence of (3.31), we get (*cf* Corollary 3.14)

$$\forall k \in \mathbb{N}^* \,, \qquad \lambda_k(H) \geq \lambda_k(H_m^N) \,,$$

and therefore (taking the limit $k \to \infty$)

$$\begin{aligned} \inf \sigma_{\text{ess}}(H) &\geq \inf \sigma_{\text{ess}}(H_m^N) \\ &= \min\left\{\inf \sigma_{\text{ess}}(H_m^{\text{int},N}), \inf \sigma_{\text{ess}}(H_m^{\text{ext},N})\right\} \\ &= \inf \sigma_{\text{ess}}(H_m^{\text{ext},N}) \\ &\geq \inf \sigma(H_m^{\text{ext},N}) \\ &= \inf_{\substack{\psi \in \operatorname{dom} h_m^{\text{ext},N} \\ \psi \neq 0}} \frac{h_m^{\text{ext},N}[\psi]}{\|\psi\|^2_{L^2(\Omega_m^{\text{ext}})}} \,. \end{aligned} \tag{3.32}$$

Here the second equality follows from the fact that the spectrum of $H_m^{\text{int},N}$ is purely discrete (the extension of $\operatorname{dom} h_m^{\text{int},N}$ to $W^{1,2}(B_m)$ is trivial and the spectrum of the Neumann Laplacian in any disk is purely discrete, see Theorem 3.21). In summary, we have obtained a lower estimate to the threshold of the essential spectrum of H through the spectrum of the "exterior" operator $H_m^{\text{ext},N}$, for any m. It remains to analyse the spectral threshold of $H_m^{\text{ext},N}$.

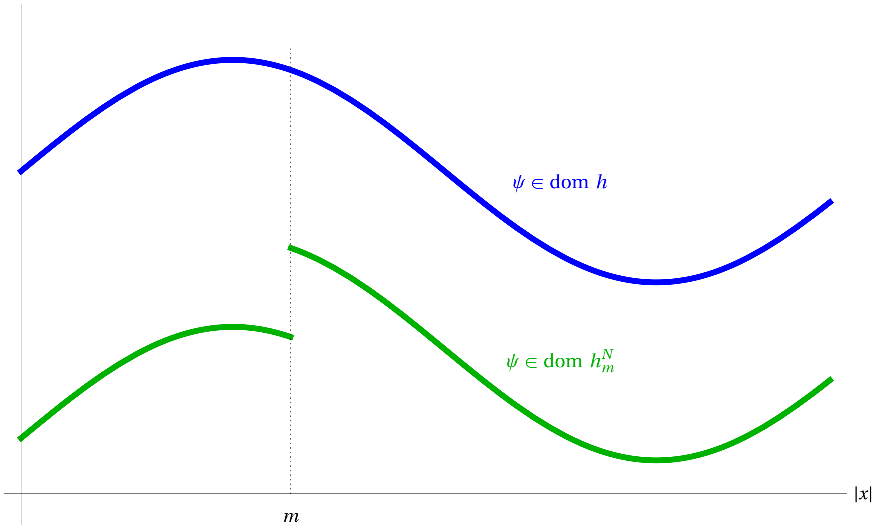


Figure 3.6: Schematical visualisation of the effect of introducing the Neumann boundary condition.

Figure 3.7: The angular distance between two closest rays of the spiny urchin.

Let $\psi \in C_0^\infty(\Omega) \upharpoonright \Omega_m^{\mathrm{ext}}$, a core of $h_m^{\mathrm{ext},N}$. Passing to polar coordinates and neglecting the radial component, we have

$$
\begin{aligned}
h_m^{\mathrm{ext},N}[\psi] &= \int_{(m,\infty)\times S^1} \left[|\partial_r\psi|^2 + \frac{|\partial_\vartheta\psi|^2}{r^2} \right] r\,\mathrm{d}r\,\mathrm{d}\vartheta \\
&\geq \sum_{j=0}^{\infty} \int_{(m+j,m+j+1)\times S^1} \frac{|\partial_\vartheta\psi|^2}{r^2}\, r\,\mathrm{d}r\,\mathrm{d}\vartheta \\
&\geq \sum_{j=0}^{\infty} \int_{(m+j,m+j+1)\times S^1} \left(\frac{\pi}{\pi/2^{m+j}}\right)^2 \frac{|\psi|^2}{r^2}\, r\,\mathrm{d}r\,\mathrm{d}\vartheta \\
&\geq \sum_{j=0}^{\infty} \int_{(m+j,m+j+1)\times S^1} \left(\frac{2^{m+j}}{m+j+1}\right)^2 |\psi|^2\, r\,\mathrm{d}r\,\mathrm{d}\vartheta \\
&\geq \left(\frac{2^m}{m+1}\right)^2 \int_{(m,\infty)\times S^1} |\psi|^2\, r\,\mathrm{d}r\,\mathrm{d}\vartheta \\
&= \left(\frac{2^m}{m+1}\right)^2 \|\psi\|^2_{L^2(\Omega_m^{\mathrm{ext}})}\,.
\end{aligned}
\tag{3.33}
$$

Here the second inequality follows from the one-dimensional spectral bound

$$
-\Delta_D^{(a,b)} \geq \left(\frac{\pi}{b-a}\right)^2
$$

for any real numbers $a<b$ (*cf* (3.9) and (3.22)), with help of Fubini's theorem, by noticing that the angular distance on the circle Σ_m between two closest rays of the urchin is $\pi/2^m$ (*cf* Figure 3.7).

In summary, from (3.32) and (3.33) we deduce

$$
\inf \sigma_{\mathrm{ess}}(H) \geq \left(\frac{2^m}{m+1}\right)^2 .
$$

Since the right-hand side tends to $+\infty$ as $m\to\infty$, while the left-hand side is independent of m, we obtain $\inf\sigma_{\mathrm{ess}}(H)=+\infty$. That is, $\sigma_{\mathrm{ess}}(H)=\varnothing$ by the minimax principle (Theorem 3.13). $\square$

In fact, it turns out that the property that the spectrum of the Dirichlet Laplacian in Ω is purely discrete depends in an essential way on the dimension of $\partial\Omega$. Any quasi-bounded domain whose boundary consists of reasonably regular $(d-1)$-dimensional hypersurfaces has no essential spectrum.

Remark 3.28 (Spiny urchin with sparse spines)**.** If we replace the lines in (3.29) by "dots accumulating at infinity", *i.e.*, we define $\dot\Omega$ as the domain in $\mathbb{R}^2$ obtained by deleting from the plane the union of the sets

$$
\dot S_m := \left\{ (r\cos\vartheta, r\sin\vartheta) : \quad r = m+\sqrt{j} \quad \text{for} \quad j\in\mathbb{N} \quad \wedge \quad \vartheta = n\pi/2^m \quad \text{for} \quad n=1,2,\dots,2^{m+1} \right\},
$$

then exactly the same proof as that of Theorem 2.3 for quasi-conical domains implies

$$
\sigma(-\Delta_D^{\dot\Omega}) = \sigma_{\mathrm{ess}}(-\Delta_D^{\dot\Omega}) = [0,\infty)\,.
$$

This is obvious since a finite number of points in an open planar set (*e.g.*, an arbitrarily large disc) form a *polar set* (*cf* Proposition 2.5), so that $W_0^{1,2}(\dot\Omega\cap B_R) = W_0^{1,2}(B_R)$ for any $R>0$.

More generally, one has the following result.

Theorem 3.29 ([1, Thm. 1])**.** *Let $d\geq 2$. If $\partial\Omega$ consists only of isolated points with no finite accumulation point, then*

$$
\sigma_{\mathrm{ess}}(-\Delta_D^{\Omega}) \neq \varnothing\,.
$$

Finally, let us remark that in $d=1$ one knows that quasi-boundedness is necessary and sufficient for an arbitrary (not necessary connected) open subset $\Omega\subset\mathbb{R}$ to have a purely discrete spectrum. In higher dimensions, the necessary and sufficient conditions can be obtained in terms of capacity (see [25, Thm. VIII.3.1]).

3.10 Properties of eigenfunctions

Up to now, we were exclusively interested in qualitative and quantitative properties of the spectrum. Let us now look at properties of the eigenfunctions. To ensure the existence of eigenvalues, we shall typically assume that the domain is bounded, but some of the results hold in a greater generality.

3.10.1 Regularity

Let Ω be an arbitrary open set. Recall that the Dirichlet Laplacian $-\Delta_D^\Omega$ acts as the weak Laplacian in Ω and its domain satisfy

$$\operatorname{dom}(-\Delta_D^\Omega) = \left\{\psi \in W_0^{1,2}(\Omega) : \ \Delta\psi \in L^2(\Omega)\right\} .$$

Elliptic regularity theory ensures that

$$\Delta\psi \in L^2(\Omega) \qquad \Longrightarrow \qquad \nabla^2\psi \in L^2_{\mathrm{loc}}(\Omega) \,. \tag{3.34}$$

What is more, if Ω is nice (*e.g.*, bounded with C^2-smooth boundary), the hypothesis $\Delta\psi \in L^2(\Omega)$ implies the global extra regularity $\nabla^2\psi \in L^2(\Omega)$; in that special case, $\operatorname{dom}(-\Delta_D^\Omega) = W_0^{1,2}(\Omega) \cap W^{2,2}(\Omega)$. The gain of regularity (3.34) is indeed remarkable: not only that the sum of second derivatives is square integrable, but each mixed second derivatives separately, at least locally. Heuristically, (3.34) can be understood by a formal(!) integration by parts:

$$\begin{aligned}
\|\Delta\psi\|^2 = \int_\Omega |\Delta\psi|^2 &= \sum_{j,k=1}^d \int_\Omega \partial_j\partial_j\bar\psi \ \partial_k\partial_k\psi \\
&= -\sum_{j,k=1}^d \int_\Omega \partial_j\bar\psi \ \partial_j\partial_k\partial_k\psi \\
&= -\sum_{j,k=1}^d \int_\Omega \partial_k\partial_j\bar\psi \ \partial_j\partial_k\psi = \int_\Omega |\nabla^2\psi|^2 = \|\nabla^2\psi\|^2 \,.
\end{aligned}$$

Of course, this formal computation suffers from at least the following defects:

1. the boundary terms are disregarded,
2. the third derivatives $\partial_j\partial_k\partial_k\psi$ are not defined,
3. the mixed derivatives $\partial_j\partial_k\psi$ for $j \neq k$ are not defined.

The tricks of elliptic regularity theory are precisely about overcoming these problems. First, the contact with the boundary $\partial\Omega$ is solved by multiplying ψ by a cut-off function; that is why only the local regularity is obtained in the full generality of arbitrary domains Ω. The other problems are solved by replacing the customary partial derivative $\partial_k\psi$ by the *difference quotient*

$$\partial_k^\delta\psi(x) := \frac{\psi(x_1,\dots,x_k+\delta,\dots,x_d)-\psi(x)}{\delta}$$

and taking the limit $\delta \to 0$ only after the manipulations in the spirit of the integration by parts above. We refer to [26, Sec. 6.3] for more details.

Now, let ψ be an eigenfunction of $-\Delta_D^\Omega$ corresponding to an eigenvalue λ. We know that $\psi \in W_0^{1,2}(\Omega) \cap W^{2,2}_{\mathrm{loc}}(\Omega)$. The validity of the equation

$$-\Delta\psi = \lambda\psi \qquad \text{in} \qquad \Omega \tag{3.35}$$

(in a weak sense, as usual) imply that $\Delta\psi \in W^{2,2}_{\mathrm{loc}}(\Omega)$. We can thus differentiate (3.35), apply (3.34) and conclude with $\psi \in W^{3,2}_{\mathrm{loc}}(\Omega)$. Repeating this procedure, we know that $\psi \in W^{k,2}_{\mathrm{loc}}(\Omega)$ for every $k \in \mathbb{N}$. However, the functions in the Sobolev space $W^{k,2}_{\mathrm{loc}}(\Omega)$ are more and more regular with the growing exponent k. More specifically, one has the Sobolev embedding (see [2, Thm. 4.12])

$$W^{k,2}(U) \hookrightarrow C^{k-[\frac{d}{2}]-1}(\overline{U}) \,, \tag{3.36}$$

where U is any bounded Lipschitz set and $k > d/2$. To see the idea, why integrability of derivatives ensure smoothness, let us establish the following result.

Proposition 3.30. *One has*
$$W^{d,2}(\mathbb{R}^d) \hookrightarrow C^0(\overline{\mathbb{R}^d})\,.$$

Proof. Let $\psi \in C_0^\infty(\mathbb{R}^d)$. Given any point $o \in \mathbb{R}^d$ and a positive number a, let $\eta \in C_0^\infty(Q_{2a}(o))$ be any (cut-off) function such that $\eta = 1$ in $Q_a(o)$. Then, for every $x \in Q_a(o)$,

$$\begin{aligned}
\psi(x) = (\eta\psi)(x) &= \int_{o_1-2a}^{x_1} \partial_1(\eta\psi)(\xi_1, x_2, x_3, \dots, x_d)\,\mathrm{d}\xi_1 \\
&= \int_{o_1-2a}^{x_1}\int_{o_2-2a}^{x_2} \partial_2\partial_1(\eta\psi)(\xi_1, \xi_2, x_3, \dots, x_d)\,\mathrm{d}\xi_2\,\mathrm{d}\xi_1 \\
&= \dots \\
&= \int_{o_1-2a}^{x_1} \cdots \int_{o_d-2a}^{x_d} \partial_d \dots \partial_1(\eta\psi)(\xi)\,\mathrm{d}\xi\,.
\end{aligned}$$

Consequently, differentiating the product $\eta\psi$ and using the Schwarz inequality together with elementary estimates, there exists a positive constant C_1 depending on d, a and $\|\eta\|_{C^d(\overline{Q_{2a}(o)})}$ such that

$$\|\psi\|_{L^\infty(Q_a(o))} \le C_1\,\|\psi\|_{W^{d,2}(Q_{2a}(o))} \le C_1\,\|\psi\|_{W^{d,2}(\mathbb{R}^d)}\,. \tag{3.37}$$

Since the choice of the point o is arbitrary and the constant C_1 does not depend on this choice, we conclude that

$$\|\psi\|_{L^\infty(\mathbb{R}^d)} \le C_1\,\|\psi\|_{W^{d,2}(\mathbb{R}^d)}\,.$$

Using the density of $C_0^\infty(\mathbb{R}^d)$ in $W^{d,2}(\mathbb{R}^d)$, this inequality extends to all $\psi \in W^{d,2}(\mathbb{R}^d)$. Hence, any function $\psi \in W^{d,2}(\mathbb{R}^d)$ is necessarily bounded, so we have the embedding

$$W^{d,2}(\mathbb{R}^d) \hookrightarrow L^\infty(\mathbb{R}^d)\,.$$

What is more, by proceeding similarly as above, for every $x, y \in Q_a(o)$, we have

$$\begin{aligned}
\psi(x) - \psi(y) &= \psi(x_1, x_2, x_3, x_4, \dots, x_{d-1}, x_d) - \psi(y_1, y_2, y_3, y_4, \dots, y_{d-1}, y_d) \\
&= \psi(x_1, x_2, x_3, x_4, \dots, x_{d-1}, x_d) - \psi(y_1, x_2, x_3, x_4, \dots, x_{d-1}, x_d) \\
&\quad + \psi(y_1, x_2, x_3, x_4, \dots, x_{d-1}, x_d) - \psi(y_1, y_2, x_3, x_4, \dots, x_{d-1}, x_d) \\
&\quad + \psi(y_1, y_2, x_3, x_4, \dots, x_{d-1}, x_d) - \psi(y_1, y_2, y_3, x_4, \dots, x_{d-1}, x_d) \\
&\quad \vdots \\
&\quad + \psi(y_1, y_2, y_3, y_4, \dots, x_{d-1}, x_d) - \psi(y_1, y_2, y_3, y_4, \dots, y_{d-1}, x_d) \\
&\quad + \psi(y_1, y_2, y_3, y_4, \dots, y_{d-1}, x_d) - \psi(y_1, y_2, y_3, y_4, \dots, y_{d-1}, y_d) \\
&= \int_{y_1}^{x_1} \partial_1(\eta\psi)(\xi_1, x_2, x_3, x_4, \dots, x_{d-1}, x_d)\, \mathrm{d}\xi_1 \\
&\quad + \int_{y_2}^{x_2} \partial_2(\eta\psi)(y_1, \xi_2, x_3, x_4, \dots, x_{d-1}, x_d)\, \mathrm{d}\xi_2 \\
&\quad + \int_{y_3}^{x_3} \partial_3(\eta\psi)(y_1, y_2, \xi_3, x_4, \dots, x_{d-1}, x_d)\, \mathrm{d}\xi_3 \\
&\quad \vdots \\
&\quad + \int_{y_{d-1}}^{x_{d-1}} \partial_{d-1}(\eta\psi)(y_1, y_2, y_3, y_4, \dots, \xi_{d-1}, x_d)\, \mathrm{d}\xi_{d-1} \\
&\quad + \int_{y_d}^{x_d} \partial_d(\eta\psi)(y_1, y_2, y_3, y_4, \dots, y_{d-1}, \xi_d)\, \mathrm{d}\xi_d \\
&= \int_{y_1}^{x_1} \int_{o_2-2a}^{x_2} \int_{o_3-2a}^{x_3} \int_{o_4-2a}^{x_4} \cdots \int_{o_{d-1}-2a}^{x_{d-1}} \int_{o_d-2a}^{x_d} \partial_d\partial_{d-1} \dots \partial_4\partial_3\partial_2\partial_1(\eta\psi)(\xi)\, \mathrm{d}\xi \\
&\quad + \int_{o_1-2a}^{y_1} \int_{y_2}^{x_2} \int_{o_3-2a}^{x_3} \int_{o_4-2a}^{x_4} \cdots \int_{o_{d-1}-2a}^{x_{d-1}} \int_{o_d-2a}^{x_d} \partial_d\partial_{d-1} \dots \partial_4\partial_3\partial_1\partial_2(\eta\psi)(\xi)\, \mathrm{d}\xi \\
&\quad + \int_{o_1-2a}^{y_1} \int_{o_2-2a}^{y_2} \int_{y_3}^{x_3} \int_{o_4-2a}^{x_4} \cdots \int_{o_{d-1}-2a}^{x_{d-1}} \int_{o_d-2a}^{x_d} \partial_d\partial_{d-1} \dots \partial_4\partial_2\partial_1\partial_3(\eta\psi)(\xi)\, \mathrm{d}\xi \\
&\quad \vdots \\
&\quad + \int_{o_1-2a}^{y_1} \int_{o_2-2a}^{y_2} \int_{o_3-2a}^{y_3} \int_{o_4-2a}^{y_4} \cdots \int_{y_{d-1}}^{x_{d-1}} \int_{o_d-2a}^{x_d} \partial_d\partial_{d-2} \dots \partial_4\partial_2\partial_1\partial_{d-1}(\eta\psi)(\xi)\, \mathrm{d}\xi \\
&\quad + \int_{o_1-2a}^{y_1} \int_{o_2-2a}^{y_2} \int_{o_3-2a}^{y_3} \int_{o_4-2a}^{y_4} \cdots \int_{o_{d-1}-2a}^{y_{d-1}} \int_{y_d}^{x_d} \partial_{d-1}\partial_{d-2} \dots \partial_4\partial_2\partial_1\partial_d(\eta\psi)(\xi)\, \mathrm{d}\xi\,.
\end{aligned}$$

Consequently, by differentiating the product $\eta\psi$ and using the Schwarz inequality together with elementary estimates, we deduce that there is a positive constant C_2 depending on d, a and $\|\eta\|_{C^d(\overline{Q_a(o)})}$ such that

$$|\psi(x) - \psi(y)| \leq C_2\, \|\psi\|_{W^{d,2}(\mathbb{R}^d)} \Big(|x_1 - y_1|^{1/2} + \dots + |x_d - y_d|^{1/2} \Big) \leq C_2\, \|\psi\|_{W^{d,2}(\mathbb{R}^d)}\, |x - y|^{1/2}\,.$$

Since the choice of the point o is arbitrary and the constant C_2 does not depend on this choice, the obtained inequality extends to all points x, y lying in a cube of sides of length $2a$ (not necessarily $Q_a(o)$). This establishes that any function $\psi \in W^{d,2}(\mathbb{R}^d)$ is necessarily continuous. If the distance between the points x, y is such that they cannot be placed inside a cube of sides of length $2a$, then $|x-y| \geq 2a$ and we trivially have

$$|\psi(x) - \psi(y)| \leq \frac{2\,C_1}{(2a)^{1/2}}\, \|\psi\|_{W^{d,2}(\mathbb{R}^d)}\, |x - y|^{1/2}$$

due to (3.37). Altogether, there is a positive constant C_3 independent of ψ such that

$$\sup_{\substack{x,y\in\mathbb{R}^d \\ x\neq y}} \frac{|\psi(x) - \psi(y)|}{|x-y|^{1/2}} \leq C_3\, \|\psi\|_{W^{d,2}(\mathbb{R}^d)} \sup_{\substack{x,y\in\mathbb{R}^d \\ x\neq y}} \frac{|x-y|^{1/2}}{|x-y|^{1/2}} = C_3\, \|\psi\|_{W^{d,2}(\mathbb{R}^d)}\,.$$

This shows that any function $\psi \in W^{d,2}(\mathbb{R}^d)$ is necessarily uniformly Hölder continuous with exponent 1/2 in $\mathbb{R}^d$. In particular, it is uniformly continuous. $\square$

Coming back to eigenfunctions of $-\Delta_D^\Omega$, the local $W^{k,2}$-regularity for every $k \in \mathbb{N}$ shows that the eigenfunctions are actually infinitely smooth in the interior of Ω.

Theorem 3.31. *Let ψ be any eigenfunction of $-\Delta_D^\Omega$, where $\Omega \subset \mathbb{R}^d$ is an arbitrary open set. Then*

$$\psi \in C^\infty(\Omega)\,.$$

Note carefully that we are not stating any result about the boundary regularity of the eigenfunctions. However, it is true that $\psi \in C^\infty(\overline{\Omega})$ provided that Ω is (infinitely) smooth.

3.10.2 Positivity of the ground state

An operator H in a complex Hilbert space $\mathcal{H}$ is called *real* if

$$[H, \mathcal{T}] = 0\,,$$

where $\mathcal{T}\psi := \bar{\psi}$ is the complex conjugation. The commutation relation means two properties:

(i) $\psi \in \operatorname{dom} H \quad \Longrightarrow \quad \bar{\psi} \in \operatorname{dom} H$;

(ii) $\overline{H\psi} = H\bar{\psi}$ for every $\psi \in \operatorname{dom} H$.

It is easy to see that the spectrum of any real operator is symmetric with respect to the real axis, *i.e.*, $\lambda \in \sigma(H)$ implies $\bar{\lambda} \in \sigma(H)$.

Proposition 3.32. *Let λ be a real eigenvalue of a real operator H. Then the corresponding eigenvector can be chosen to be real.*

Proof. Let ψ be any eigenfunction of H corresponding to λ. Then the eigenvalue equation $H\psi = \lambda\psi$ and the property that H is real as well as that λ is real imply $H\bar{\psi} = \lambda\bar{\psi}$. Hence, the conjugation $\bar{\psi}$ is also an eigenvector of H corresponding to λ. Consequently, either the real part $\Re\psi$ or the imaginary part $\Im\psi$ (or both) are the desired real eigenvectors. Indeed, if $\Im\psi = 0$ identically (respectively, $\Re\psi = 0$ identically), then $\psi = \Re\psi$ (respectively, $-i\psi = \Im\psi$) is the desired real eigenvector. If $\Re\psi \neq 0$ (respectively, $\Im\psi \neq 0$), then $\Re\psi$ (respectively, $\Im\psi$) is the desired real eigenvector. It is also possible that $\Re\psi \neq 0$ and $\Im\psi \neq 0$ simultaneously, in which case both $\Re\psi$ and $\Im\psi$ are the desired eigenvectors. ☐

It is easy to verify that the Dirichlet Laplacian $-\Delta_D^\Omega$ is a real operator. Since it is self-adjoint, all its eigenvalues (if any) are real. Consequently, also the eigenfunctions of $-\Delta_D^\Omega$ can be chosen real.

It is a highly non-trivial fact that if the lowest point in the spectrum of $-\Delta_D^\Omega$ is an eigenvalue, then it possesses an eigenfunction which does not change sign. Moreover, the eigenspace is one-dimensional.

Theorem 3.33. *Let $\Omega \subset \mathbb{R}^d$ be an arbitrary open connected set. Let $\inf\sigma(-\Delta_D^\Omega)$ be an eigenvalue. Then it is simple and the corresponding eigenfunction can be chosen to be positive.*

Proof. Denote $\lambda_1 := \inf\sigma(-\Delta_D^\Omega) \geq 0$ and let ψ_1 be a corresponding real eigenfunction. By the variational characterisation (3.22), one has

$$\lambda_1 = \inf_{\substack{\psi \in W_0^{1,2}(\Omega) \\ \psi \neq 0}} \frac{\displaystyle\int_\Omega |\nabla\psi|^2}{\displaystyle\int_\Omega |\psi|^2}\,. \tag{3.38}$$

Since λ_1 is an eigenvalue, the infimum is achieved and one also has

$$\lambda_1 = \frac{\int_\Omega |\nabla\psi_1|^2}{\int_\Omega |\psi_1|^2} \,. \tag{3.39}$$

If a real function ψ belongs to $W_0^{1,2}(\Omega)$, then also $|\psi| \in W_0^{1,2}(\Omega)$ and $|\nabla|\psi|| = |\nabla\psi|$. Consequently, the absolute value $|\psi_1|$ is an admissible test function in (3.38) and one has

$$\lambda_1 \leq \frac{\int_\Omega |\nabla|\psi_1||^2}{\int_\Omega ||\psi_1||^2} = \frac{\int_\Omega |\nabla\psi_1|^2}{\int_\Omega |\psi_1|^2} \,.$$

Taking into account (3.39), it follows (*cf* Proposition 3.15) that $|\psi_1|$ is also a minimiser of (3.38). Hence $|\psi_1|$ is a non-negative eigenfunction of $-\Delta_D^\Omega$ corresponding to λ_1.

We claim that $|\psi_1|$ is positive in Ω. By contradiction, let us assume that there exists a point $x_0 \in \Omega$ such that $|\psi_1|(0) = 0$. By Theorem 3.31, we know that $|\psi_1|$ is necessarily infinitely smooth inside Ω. From the differential equation (which can be considered in the classical sense)

$$-\Delta|\psi_1| = \lambda_1|\psi_1| \geq 0 \,,$$

we deduce that $|\psi_1|$ is superharmonic in Ω. Let U is any smooth bounded domain $U \subset \Omega$ containing the point x_0. Since

$$\min_{\bar{U}} |\psi_1| = 0$$

and the minimum is attained *inside* U, the strong maximum principle (see, *e.g.*, [34, Thm. 3.5]) implies that $|\psi_1| = 0$ identically in $\bar{U}$. Using the arbitrariness of U, it follows that $\psi_1 = 0$ identically in Ω, a contradiction. So λ_1 admits the positive eigenfunction $|\psi_1|$.

By the argument above, we have actually shown more, namely that ψ_1 is either positive or negative (because $|\psi_1| > 0$ in Ω). So it impossible that there is another eigenfunction from the same eigenspace which would be orthogonal to ψ_1 in $L^2(\Omega)$. Hence, the eigenvalue λ_1 is simple. $\square$

3.10.3 Nodal domains

For simplicity, let us from now on assume that Ω is a bounded domain, so that the spectrum of $-\Delta_D^\Omega$ is purely discrete. Let us arrange the eigenvalues of $-\Delta_D^\Omega$ in a non-decreasing sequence

$$\sigma(-\Delta_D^\Omega) = \sigma_{\text{disc}}(-\Delta_D^\Omega) = \{\lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots \to +\infty\} \,,$$

where each eigenvalue is repeated according to its multiplicity. Notice that λ_1 is simple due to Theorem 3.33, so the inequality between λ_1 and λ_2 is strict. Let $\{\psi_n\}_{n=1}^\infty$ denote a corresponding set of real eigenfunctions, normalised to one in $L^2(\Omega)$. Since the eigenfunctions are mutually orthogonal and ψ_1 can be chosen to be positive due to Theorem 3.33, the other eigenfunctions are forced to change sign. For $n \geq 2$, it makes thus sense to introduce the *nodal set* of ψ_n by setting

$$\mathcal{N}(\psi_n) := \psi_n^{-1}(0) = \{x \in \Omega : \ \psi_n(x) = 0\} \,.$$

The connected components of $\Omega \setminus \mathcal{N}(\psi_n)$ are called *nodal domains* of ψ_n.

In dimension $d = 1$, the situation is particularly simple. Without loss of generality, we can consider $\Omega := (0, a)$ with $a > 0$. Recalling Section 3.2, one has

$$\psi_n(x) = \sqrt{\frac{1}{a}} \sin\left(\frac{n\pi}{a}x\right) \,.$$

Consequently,

$$\mathcal{N}(\psi_n) = \left\{a\frac{k}{n}\right\}_{k=1}^{n-1}$$

and each ψ_n has exactly n nodal domains, see Figure 3.8.

Figure 3.8: Nodal sets (points) of the eigenfunctions in the segment corresponding to the lowest four eigenvalues. The n^{th} eigenfunction has exactly n nodal domains.

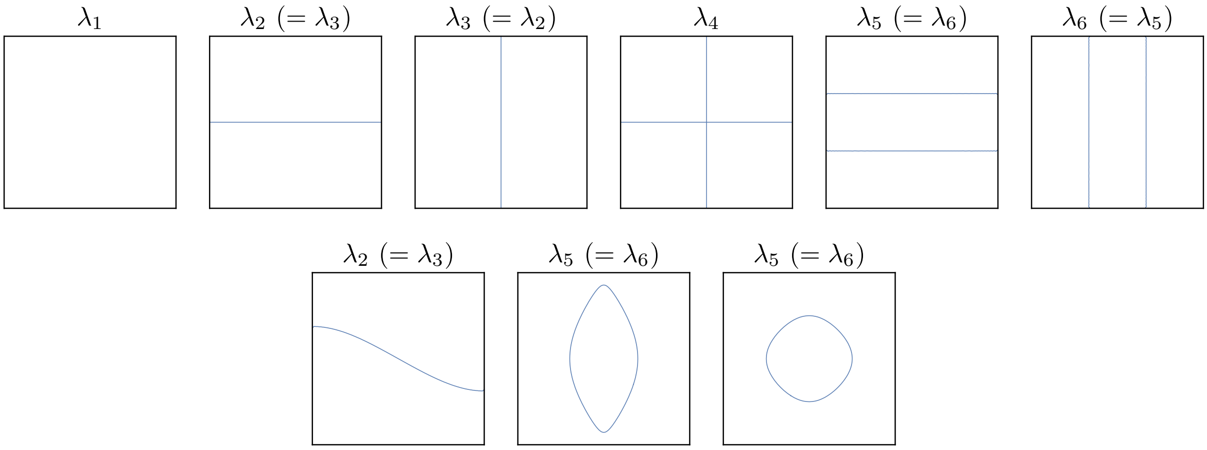


Figure 3.9: Nodal lines of the eigenfunctions in the square corresponding to the lowest six eigenvalues. The first row depicts the nodal lines for the eigenfunctions as obtained by a separation of variables. The second row combines the eigenfunctions corresponding to multiple eigenvalues in a non-trivial way. The fifth eigenfunction is the lowest eigenfunction of the square which admits a closed nodal line.

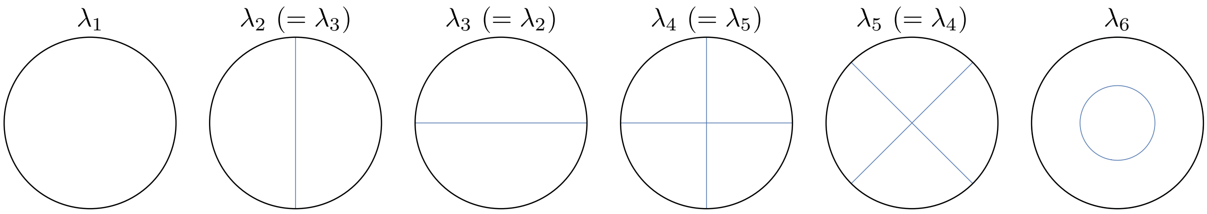


Figure 3.10: Nodal lines of the eigenfunctions in the disk corresponding to the lowest six eigenvalues. The first row depicts the nodal lines for the eigenfunctions as obtained by a separation of variables. The second row combines the eigenfunctions corresponding to multiple eigenvalues in a non-trivial way. The sixth eigenfunction is the lowest eigenfunction of the disk which admits a closed nodal line.

In dimension $d = 2$, the sets $\mathcal{N}(\psi_n)$ are called *nodal lines* and they form spectacular crossing curves or closed loops (*Chladni's patterns*), see Figures 3.9 and 3.10.

In particular, and this fact extends to dimensions $d \geq 2$, it is no longer true that ψ_n has *exactly* n nodal domains. Anyway, the examples suggest that ψ_n has *at most* n nodal domains. This observation holds in the full generality.

Theorem 3.34 (Courant's nodal domain theorem)**.** *Let Ω be an arbitrary bounded domain. For every $n \geq 1$,*

$$\psi_n \textit{ has at most } n \textit{ nodal domains.}$$

Proof. This theorem is originally announced and proved for $d = 2$ in [18, Sec. VI.6]. In higher dimensions, not all the existing proofs meet the necessary mathematical rigour (*cf* [7, Rem. 6 in App. D]). On the other hand, the general rigorous approach of [4] requires apparently unnecessary hypotheses about the regularity of Ω. We rely on some arguments of [7, App. D] used to prove the theorem on manifolds.

The case $n = 1$ is trivial due to the positivity of ψ_1. Henceforth we therefore assume $n \geq 2$. Let $\Omega_1, \dots, \Omega_k$ be the nodal domains of ψ_n. Suppose, by contradiction, that $k > n$. We abbreviate $u_j := \psi_n \chi_{\Omega_j}$, the restriction of ψ_n to its j^{th} nodal domain. Let us consider the function

$$\psi := \sum_{j=1}^{k-1} c_j \, u_j \,,$$

where $c_1, \dots, c_{k-1} \in \mathbb{R}$ are constants to be chosen later.

First of all, we claim that $\psi \in W_0^{1,2}(\Omega)$, so it is an admissible test function in the variational characterisation of the eigenvalues of $-\Delta_D^\Omega$ given by Theorem 3.11. To verify it, we have to be careful when the boundary $\partial\Omega$ is not sufficiently regular. Clearly, it is enough to check that each $u_j \in W_0^{1,2}(\Omega)$. Fix $j \in \{1, \dots, k\}$ and let us assume (without loss of generality) that $u_j > 0$ in Ω_j. For every positive ε, let us introduce the superlevel set $\Omega_j^\varepsilon := \{x \in \Omega_j : u_j > \varepsilon\}$. We set $u^\varepsilon := u - \varepsilon$ in Ω_j^ε and extend it by zero elsewhere. Let $\{\varepsilon_i\}_{i=1}^\infty$ be the set of regular values of u (*i.e.*, $\forall x \in \Omega$, $u(x) = \varepsilon_i \Rightarrow \nabla u(x) \neq 0$) which tend to zero as $i \to \infty$ (by Sard's theorem, critical values form a set of measure zero). Then $\Omega_j^{\varepsilon_i}$ is smooth and since u is smooth and $u^{\varepsilon_i} = 0$ on $\partial\Omega_j^{\varepsilon_i}$, it follows that $u^{\varepsilon_i} \in W_0^{1,2}(\Omega_j^{\varepsilon_i}) \subset W_0^{1,2}(\Omega_j)$. Since the volume $|\Omega_j \setminus \Omega_j^{\varepsilon_i}|$ vanishes as $i \to \infty$, it is straightforward to check that $u^{\varepsilon_i} \to u_j$ in $W^{1,2}(\Omega_j)$ as $i \to \infty$. Since $W_0^{1,2}(\Omega_j)$ is a closed subspace of $W^{1,2}(\Omega_j)$, we have just established that $u_j \in W_0^{1,2}(\Omega_j) \subset W_0^{1,2}(\Omega)$.

Second, we claim that it is possible to choose the constants $c_1, \dots, c_{k-1}$ in such a way that $c_1^2 + \dots + c_{k-1}^2 \neq 0$ (so that ψ is non-trivial) and

$$\forall i = 1, \dots, n-1 \,, \qquad 0 = (\psi_i, \psi) = \sum_{j=1}^{k-1} c_j \int_{\Omega_j} \psi_i \psi_n \,.$$

Indeed, it is enough to notice that we deal with a homogeneous system of linear equations, where the number of unknowns is larger than the number of equations (because $k - 1 \geq n - 1$).

Since ψ is orthogonal to the first $n-1$ eigenfunctions, it follows that $\mathcal{M}_n := \operatorname{span}\{\psi_1, \dots, \psi_{n-1}, \psi\}$ is an n-dimensional subspace of $W_0^{1,2}(\Omega)$. Choosing $\mathcal{L}_n := \mathcal{M}_n$ in (3.19), it follows that

$$\lambda_n \leq \frac{\displaystyle\int_\Omega |\nabla\psi|^2}{\displaystyle\int_\Omega |\psi|^2} = \frac{\displaystyle\sum_{j=1}^{k-1} c_j \int_{\Omega_j} |\nabla\psi_n|^2}{\displaystyle\sum_{j=1}^{k-1} c_j \int_{\Omega_j} |\psi_n|^2} = \frac{\displaystyle\sum_{j=1}^{k-1} c_j \lambda_n \int_{\Omega_j} |\psi_n|^2}{\displaystyle\sum_{j=1}^{k-1} c_j \int_{\Omega_j} |\psi_n|^2} = \lambda_n \,.$$

Consequently (*cf* Proposition 3.15), ψ is an admissible eigenfunction of $-\Delta_D^\Omega$ corresponding to the eigenvalue λ_n. However, $\psi = 0$ on the non-empty open set G_k, which implies that actually $\psi = 0$ on Ω due to the strong maximum principle. This is a contradiction with the fact that ψ has been constructed as a non-trivial function. □

3.10.4 Nodal-line conjecture

For simplicity, let us restrict to dimension $d = 2$, where the nodal set is a one-dimensional object. We continue to assume that Ω is a bounded domain, but the hypotheses that there are two eigenvalues below the essential spectrum would be enough. Since the ground state ψ_1 is positive, the second eigenfunction ψ_2 has at least two nodal domains. It follows by Theorem 3.34 that ψ_2 has *exactly two* nodal domains.

In 1967 Payne conjectured that the nodal line $\mathcal{N}(\psi_2)$ cannot be a closed curve. There are some musical arguments to support this expectation. A reformulation suitable for higher dimensions, too, is that the nodal line touches the boundary.

Conjecture 3.35 (Nodal-line conjecture)**.** *For any domain* Ω*,* $\overline{\mathcal{N}(\psi_2)} \cap \partial\Omega \neq \varnothing$*.*

It is clear from the examples of squares and disks given above that the restriction to the *second* eigenfunction is crucial.

The conjecture has an interesting history. Disregarding results for special domains based on symmetry, the most general result obtained so far was given by Melas in 1992 [57], who showed that the conjecture holds in the case of *convex* domains (see also [3]). Independently, Jerison proved the conjecture in the case of sufficiently *long and thin convex domains* [41] (see also [43]) and, moreover, gave an estimate on its location [42] (see also [36, 37, 38]). As a unique robust result for non-convex domains, in 2008, Freitas and the present author established the validity of the conjecture for sufficiently *thin curved strips* and, moreover, gave an estimate on its location (in fact, for all eigenfunctions) [32] (see also [54]).

On the negative side, in 1997, Hoffmann-Ostenhof squared and N. Nadirashvili constructed a multiply connected counter-example to the conjecture [40] (see also [28, 20]), see Figure 3.11. In 2002, Freitas

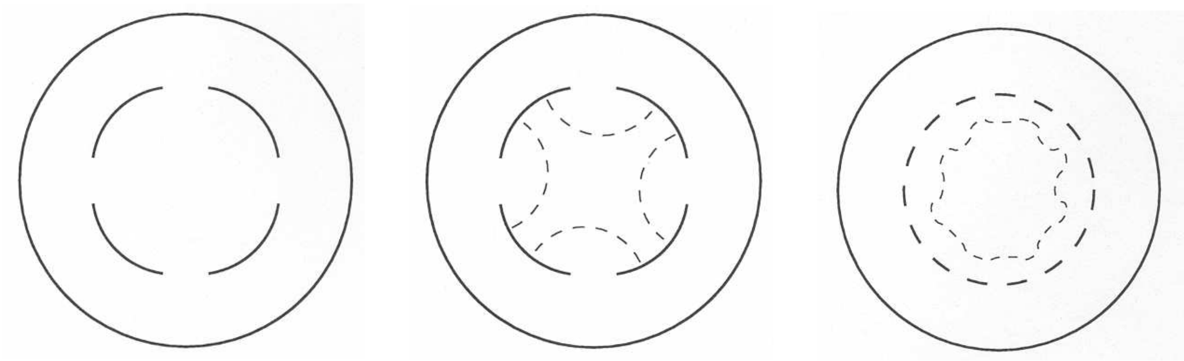


Figure 3.11: The multiply connected domain of [40] for which the nodal line of the second eigenfunction is a closed curve. The idea is to start with two concentric circles; the union of the interior of the inner circle (disk) and the exterior of the inner circle lying inside the outer circle (annulus) forms a disconnected open set. Assuming that the annulus is such that its first eigenvalue is greater than the first eigenvalue of the inner disk and simultaneously smaller than the second eigenvalue of the inner disk, it follows that the second eigenfunction of the disconnected domain is the first eigenfunction in the annulus extended by zero to the inner disk. Digging a sufficient number of small holes in the inner circle will make the set connected and the eigenfunction of the annulus will penetrate in the interior of the inner circle in such a way that it produces a closed nodal line eventually.

showed that the conjecture does not hold for domains on surfaces [30]. In 2007, Freitas and the present author showed that the conjecture does not hold for unbounded domains [31], see Figure 3.12.

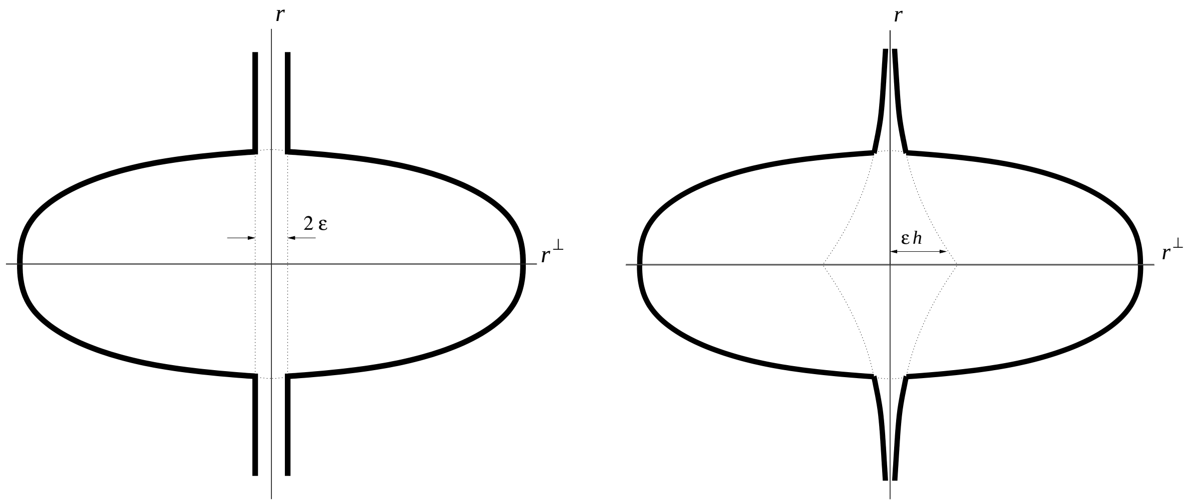


Figure 3.12: Unbounded domains of [31] for which the nodal line of the second eigenfunction does not touch the boundary. The construction starts with a bounded convex domain which is invariant under reflections through two orthogonal lines r and $r^\perp$. Assuming that the bounded domain is sufficiently long in the direction $r^\perp$, its second eigenvalue is simple and has a nodal line coinciding with the axis r inside the domain. Appending two sufficiently thin semi-infinite strips invariant under a reflection through r will make the whole vertical line r to be the nodal line of the obtained unbounded domain. The left (respectively, right) figure represents a quasi-cylindrical (respectively, quasi-bounded) realisation.

The current status is that the validity of the conjecture still constitutes an open problem for simply connected bounded domains in $\mathbb{R}^2$ (in higher dimensions, the restriction to simply connected domains is not enough due to Kennedy [48]).

3.11 Spectral isoperimetric inequalities

In this section, we look at extremal properties of the ground-state eigenvalue as regards the shape of the underlying domain.

Let us begin by recalling some classical geometric facts. For simplicity, you can assume that Ω is a *smooth* bounded domain, in order to have classical definitions of its volume and boundary area, but the domain can be multiply connected, see Figure 3.13.

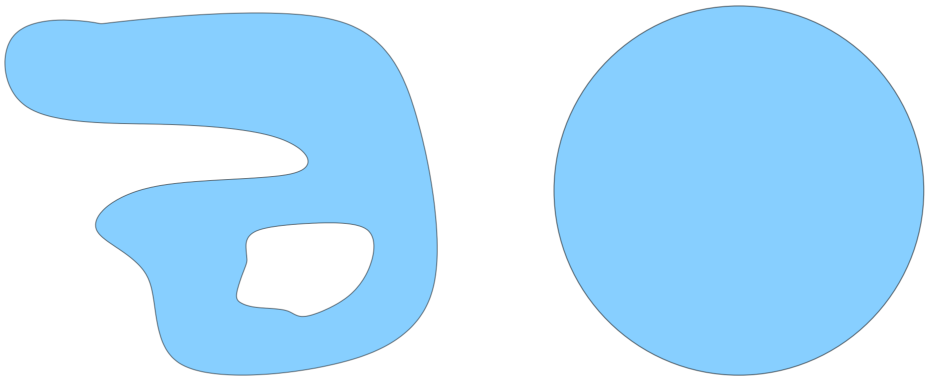


Figure 3.13: An arbitrary smooth bounded domain Ω (left) to be compared with the disk B (right).

3.11.1 Geometric isoperimetric inequalities

The (geometric) *isoperimetric inequality* in two dimensions states that among all planar sets of a given perimeter, the disk has the largest area. That is,

$$\max_{|\partial\Omega|=\mathrm{const}} |\Omega| = |B| \,, \tag{3.40}$$

where the maximum is taken over all bounded domains $\Omega \subset \mathbb{R}^2$ of the fixed perimeter $|\partial\Omega| = \mathrm{const}$, B denotes the disk of the same perimeter as Ω (*i.e.* $|\partial B| = |\partial\Omega| = \mathrm{const}$) and $|\Omega|$ denotes the area of Ω. It is indeed an inequality because (3.40) is equivalent to the statement

$$\forall\Omega,\ |\partial\Omega| = \mathrm{const}, \qquad |\Omega| \le |B| \,. \qquad\qquad (|\partial B| = |\partial\Omega| = \mathrm{const}) \tag{3.41}$$

Moreover, the inequality becomes equality if, and only if, $\Omega = B$.

By scaling, (3.40) is equivalent to the *isochoric inequality* stating that among all planar sets of a given area, the disk has the smallest perimeter. That is,

$$\min_{|\Omega|=\mathrm{const}} |\partial\Omega| = |\partial B| \,, \tag{3.42}$$

where the minimum is taken over all bounded domains $\Omega \subset \mathbb{R}^2$ of a fixed area $|\Omega| = \mathrm{const}$ and now B denotes the disk of the same area as Ω (*i.e.* $|B| = |\Omega| = \mathrm{const}$). Again, one is concerned with an inequality because (3.42) is equivalent to the statement

$$\forall\Omega,\ |\Omega| = \mathrm{const}, \qquad |\partial\Omega| \ge |\partial B| \,. \qquad\qquad (|B| = |\Omega| = \mathrm{const}) \tag{3.43}$$

Moreover, the inequality becomes equality if, and only if, $\Omega = B$.

Since the perimeter and area of a disk is known explicitly, the two inequalities (3.41) and (3.43) can be stated as a unique inequality (without any further constraints on the domain Ω)

$$\forall\Omega, \qquad |\partial\Omega|^2 - 4\pi|\Omega| \ge 0 \,, \tag{3.44}$$

and the inequality becomes equality if, and only if, $\Omega = B$. Indeed, if R denotes the radius of B, then the isoperimetric constraint requires $2\pi R = |\partial\Omega|$, while (3.41) states that $|\Omega| \le \pi R^2$; eliminating R, we arrive at (3.44).

These two classical geometric optimisation problems were known to ancient Greeks (they are usually attributed to the legendary queen of Carthago Dido), but a first rigorous proof appeared only in the 19th century (see [9] for an overview). The analogous statements hold in higher dimensions as well.

3.11.2 The Faber–Krahn inequality

Going from geometric to spectral quantities, one may ask the question whether the ball is the extremal set also when optimising eigenvalues instead of the geometric data. The most celebrated result is certainly the *Faber–Krahn inequality* stating that it is indeed the case for the lowest Dirichlet eigenvalue under the isochoric constraint.

Theorem 3.36 (Spectral isochoric inequality, Dirichlet case)**.** *One has*

$$\min_{|\Omega|=\mathrm{const}} \lambda_1^D(\Omega) = \lambda_1^D(B)\,, \tag{3.45}$$

*where the minimum is taken over all bounded domains $\Omega \subset \mathbb{R}^d$ of a fixed volume $|\Omega| = \mathrm{const}$ and B denotes the ball of the same volume as Ω (*i.e. $|B| = |\Omega| = \mathrm{const}$*).*

This *spectral isochoric inequality* implies a physically expected fact that among all planar membranes of a given area and with fixed edges, the circular membrane produces the lowest fundamental tone. It was conjectured by Lord Rayleigh in 1877 in his famous book *The theory of sound* [59], but proved only by Faber [27] and Krahn [49] almost half a century later.

Before commenting on the proof of Theorem 3.36, let us mention that (3.45) implies the spectral isoperimetric inequality as a corollary.

Corollary 3.37 (Spectral isoperimetric inequality, Dirichlet case)**.** *One has*

$$\min_{|\partial\Omega|=\mathrm{const}} \lambda_1^D(\Omega) = \lambda_1^D(B)\,, \tag{3.46}$$

*where the minimum is taken over all bounded domains $\Omega \subset \mathbb{R}^d$ of a fixed perimeter $|\partial\Omega| = \mathrm{const}$ and B denotes the ball of the same perimeter as Ω (*i.e. $|\partial B| = |\partial\Omega| = \mathrm{const}$*).*

Proof. By Theorem 3.36, one has

$$\lambda_1^D(\Omega) \geq \lambda_1^D(B') \qquad \text{with} \qquad |B'| = |\Omega|\,, \tag{3.47}$$

where B' is the ball of the same volume as Ω. By the geometric isochoric inequality (3.43), one has

$$|\partial\Omega| \geq |\partial B'|\,.$$

Hence, there exists a *larger* ball $B \supset B'$ such that

$$|\partial B| = |\partial\Omega|\,.$$

By the monotonicity of Dirichlet eigenvalues, one has

$$\lambda_1^D(B') \geq \lambda_1^D(B)\,. \tag{3.48}$$

Combining (3.47) and (3.48), we arrive at the desired claim. □

The proof of Theorem 3.36 is based on the following deep result of analysis.

Lemma 3.38 (Rearrangement inequality)**.** *Given any bounded measurable set $S \subset \mathbb{R}^d$, let S^* denote its* symmetric rearrangement *defined by*

$$S^* := B_R(0)\,, \qquad \textit{where} \qquad |B_R(0)| = |S|\,.$$

Given any non-negative function $f \in W_0^{1,2}(\Omega)$ *with* $\Omega \subset \mathbb{R}^d$ *open and bounded, let* f^* *denote its* symmetric-decreasing rearrangement *defined by*

$$f^*(x) := \int_0^\infty \chi_{\{f>t\}^*}(x)\, \mathrm{d}t \,.$$

Then $f^* \in W_0^{1,2}(\Omega^*)$ *and*

(i) $\|f^*\|_{L^2(\Omega^*)} = \|f\|_{L^2(\Omega)}$;

(ii) $\|\nabla f^*\|_{L^2(\Omega^*)} \leq \|\nabla f\|_{L^2(\Omega)}$.

Note that S^* is just the ball centred at the origin of the same volume as S. Instead of going through the formal definition of f^*, we notice that f^* is constructed from f by rearranging the level sets of f in balls of the same volume. Clearly, f^* is non-negative, radially symmetric (*i.e.*, $f^*(x) = f^*(y)$ if $|x| = |y|$) and non-increasing as a function of the distance from the origin (*i.e.*, $f^*(x) \geq f^*(y)$ if $|x| \leq |y|$). Since the functions f and f^* are obviously *equimeasurable* (*i.e.* their level sets have the same measure), we immediately get property (i). Property (ii) is a much more involved result (see, *e.g.*, [55, Lem. 7.17] for a proof); intuitively, we can understand it as the decrease of the derivative after the symmetric rearrangement.

Now we are in a position to prove Theorem 3.36.

Proof. To apply Lemma 3.38, we need to ensure that $\lambda_1^D(\Omega)$ admits a non-negative eigenfunction. By Theorem 3.33, we know that this is true, for it actually admits a positive eigenfunction.

Let ψ_1^* denote the symmetric-decreasing rearrangement of the positive eigenfunction ψ_1. Using it as a test function in the variational characterisation of $\lambda_1^D(B)$ with $B := \Omega^*$, we get

$$\lambda_1^D(B) = \inf_{\substack{\psi \in W_0^{1,2}(\Omega^*) \\ \psi \neq 0}} \frac{\|\nabla\psi\|^2_{L^2(\Omega^*)}}{\|\psi\|^2_{L^2(\Omega^*)}} \leq \frac{\|\nabla\psi_1^*\|^2_{L^2(\Omega^*)}}{\|\psi_1^*\|^2_{L^2(\Omega^*)}} \leq \frac{\|\nabla\psi_1\|^2_{L^2(\Omega)}}{\|\psi_1\|^2_{L^2(\Omega)}} = \lambda_1^D(\Omega) \,.$$

Here the last inequality employs Lemma 3.38. ☐

3.11.3 The Bossel inequality

Next one may ask about analogous optimisation problems for different boundary conditions.

The Neumann case is trivial, because $\lambda_1^N(\Omega) = 0$ for any bounded domain Ω (the corresponding eigenfunction is any non-zero constant). The problem is interesting for the first non-trivial eigenvalue $\lambda_1^N(\Omega)$ (so as it is for higher Dirichlet eigenvalues), but we shall not consider these optimisation problems here.

Instead, we shall look at the case of the lowest eigenvalue of the Robin problem (7). More specifically, we consider the following boundary-value problem

$$\begin{cases} -\Delta\psi = \lambda\psi & \text{in} \quad \Omega \,, \\ \dfrac{\partial\psi}{\partial n} + \alpha\,\psi = 0 & \text{on} \quad \partial\Omega \,, \end{cases} \tag{3.49}$$

where n denotes the outward unit normal vector field of $\partial\Omega$ and $\alpha \in \mathbb{R}$ is a constant. We assume that Ω is a bounded domain with Lipschitz boundary, so that the normal exists almost everywhere. Using the approach of sesquilinear forms in Section 1.4.2, the problem (3.49) should be properly interpreted as a spectral problem for the Robin Laplacian $-\Delta_\alpha^\Omega$ in $L^2(\Omega)$. The spectrum of $-\Delta_\alpha^\Omega$ is purely discrete and we arrange the eigenvalues into a non-decreasing sequence

$$\sigma(-\Delta_\alpha^\Omega) = \{\lambda_1^\alpha(\Omega) \leq \lambda_1^\alpha(\Omega) \leq \dots\} \,,$$

where each eigenvalue is repeated according to its multiplicity. However, we really do not need these facts. We are exclusively interested in the lowest eigenvalue, which can be characterised variationally as follows (multiply the differential equations of (3.49) by $\bar{\psi}$ and integrate by parts using the boundary condition of (3.49)):

$$\lambda_1^\alpha(\Omega) = \inf_{\substack{\psi \in W^{1,2}(\Omega) \\ \psi \neq 0}} \frac{\displaystyle\int_\Omega |\nabla\psi|^2 + \alpha \int_{\partial\Omega} |\psi|^2}{\displaystyle\int_\Omega |\psi|^2} \,. \tag{3.50}$$

From this formula, the influence of the boundary constant α becomes clear. If $\alpha > 0$ (respectively, $\alpha < 0$), we call the Robin boundary conditions *repulsive* (respectively, *attractive*). (The case $\alpha = 0$ corresponds to Neumann boundary conditions.)

The following theorem extends the Faber–Krahn inequality (Theorem 3.36) to repulsive boundary conditions. The proof (much harder than in the Dirichlet case) is due to Bossel [10] in dimension two and due to Daners [21] in all dimensions (see also [13] for an alternative proof).

Theorem 3.39 (Spectral isochoric inequality, repulsive Robin case)**.** *For every $\alpha > 0$, one has*

$$\min_{|\Omega|=\text{const}} \lambda_1^\alpha(\Omega) = \lambda_1^\alpha(B)\,,$$

*where the minimum is taken over all bounded domains $\Omega \subset \mathbb{R}^d$ of a fixed volume $|\Omega| = \text{const}$ and B denotes the ball of the same volume as Ω (*i.e. $|B| = |\Omega| = \text{const}$*).*

Again, by the isoperimetric inequality and scaling, one can also deduce the following analogue of Corollary 3.37.

Corollary 3.40 (Spectral isoperimetric inequality, repulsive Robin case)**.** *For every $\alpha > 0$, one has*

$$\min_{|\partial\Omega|=\text{const}} \lambda_1^\alpha(\Omega) = \lambda_1^\alpha(B)\,,$$

*where the minimum is taken over all bounded domains $\Omega \subset \mathbb{R}^d$ of a fixed perimeter $|\partial\Omega| = \text{const}$ and B denotes the ball of the same perimeter as Ω (*i.e. $|\partial B| = |\partial\Omega| = \text{const}$*).*

In summary, the ball is the minimiser of the lowest eigenvalue of the Laplacian for all repulsive Robin boundary conditions (including the Dirichlet case $\alpha = +\infty$). Surprisingly, the situation changes dramatically if one allows α to be negative.

3.11.4 Bareket's conjecture

Let us now look at attractive Robin boundary conditions, *i.e.* $\alpha < 0$ in (3.49). It seems to be natural to expect that the ball is again the optimal set for the lowest eigenvalue. However, since $\lambda_1^\alpha(\Omega)$ is negative whenever $\alpha < 0$ (indeed, choose a constant trial function in (3.50)), now it makes sense to maximise it. Bareket stated this expectation explicitly in 1977 [6].

Conjecture 3.41 (Spectral isochoric inequality, attractive Robin case)**.** *For every $\alpha < 0$, one has*

$$\max_{|\Omega|=\text{const}} \lambda_1^\alpha(\Omega) = \lambda_1^\alpha(B)\,,$$

*where the maximum is taken over all bounded domains $\Omega \subset \mathbb{R}^d$ of a fixed volume $|\Omega| = \text{const}$ and B denotes the ball of the same volume as Ω (*i.e. $|B| = |\Omega| = \text{const}$*).*

Since we state this spectral isochoric inequality as a conjecture, it might be expected that something goes wrong. Indeed, in collaboration with Freitas [33], we disproved the conjecture by showing that there exists another domain, which is better than the ball, at least if $|\alpha|$ is large, see Figure 3.14.

Theorem 3.42 (Counterexample to Bareket's conjecture)**.** *For every positive numbers $R_1 < R_2$, there exists $\alpha_0 = \alpha_0(R_1, R_2) < 0$ such that, for all $\alpha \leq \alpha_0$,*

$$\lambda_1^\alpha(B_R) < \lambda_1^\alpha(A_{R_1,R_2})\,, \tag{3.51}$$

where $A_{R_1,R_2} := B_{R_2} \setminus \overline{B_{R_2}}$ is a spherical shell *and B_R with $R = R(R_1, R_2)$ is a ball of the same volume as A_{R_1,R_2} (*i.e. $|B_R| = |A_{R_1,R_2}|$*).*

Proof. Because of the rotational symmetry, the spectral problem for the balls and spherical shells can be solved by separation of variables in terms of special (namely, Bessel) functions. Employing the known asymptotics of the Bessel functions, it is tedious but straightforward to establish the following asymptotics:

$$\lambda_1^\alpha(B_R) = -\alpha^2 + \frac{d-1}{R}\,\alpha + o(\alpha)\,,$$
$$\lambda_1^\alpha(A_{R_1,R_2}) = -\alpha^2 + \frac{d-1}{R_2}\,\alpha + o(\alpha)\,,$$

as $\alpha \to -\infty$. Since the condition $|B_R| = |A_{R_1,R_2}|$ implies $R < R_2$ and α is negative, we get the desired inequality (3.51) for all sufficiently large $|\alpha|$. ☐

Theorem 3.42 is remarkable for it provides the first known example where the extremal domain for the lowest eigenvalue of the Robin Laplacian is not a ball. It remains open to show that spherical shells are the maximisers. At the same time, it is still believed (and supported by numerical experiments, see [5]) that the ball is the maximiser within the class of *simply connected* domains (*i.e.*, Bareket's Conjecture 3.41 holds for such domains).

The isoperimetric constraint seems to be much simpler, at least in low dimensions.

Theorem 3.43 (Spectral isoperimetric inequality, attractive Robin case, $d = 2$)**.** *For every $\alpha > 0$, one has*

$$\max_{|\partial\Omega|=\text{const}} \lambda_1^\alpha(\Omega) = \lambda_1^\alpha(B)\,,$$

*where the maximum is taken over all bounded domains $\Omega \subset \mathbb{R}^2$ of a fixed perimeter $|\partial\Omega| = \text{const}$ and B denotes the disk of the same perimeter as Ω (*i.e. $|\partial B| = |\partial\Omega| = \text{const}$*).*

This theorem is due to my collaboration with Antunes and Freitas [5]. It is believed (and supported by numerical experiments, see [5]) that the result extends to higher dimensions as well. In fact, there have been a recent progress showing that the spectral isoperimetric inequality holds in higher dimensions under an extra convexity assumption, see [12].

For the optimisation of the lowest Robin eigenvalue in the *exterior* of compact sets, see [51, 52].

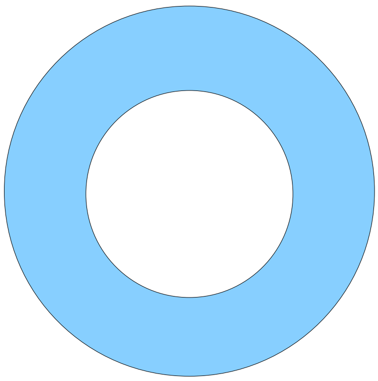


Figure 3.14: Annulus is more optimal than the disk in the spectral isochoric maximisation problem of the attractive Robin problem.

Chapter 4

Quasi-cylindrical domains

Finally, let us consider the class of quasi-cylindrical domains. Spectral analysis of this type of domains is typically the most complicated. The only general result is that there is always some essential spectrum (see Theorem 4.1 below), but there might be also some discrete eigenvalues; schematically:

$$\sigma(-\Delta_D^\Omega) = \underbrace{\sigma_{\rm disc}(-\Delta_D^\Omega)}_{\neq\varnothing?} \cup \underbrace{\sigma_{\rm ess}(-\Delta_D^\Omega)}_{\neq\varnothing}$$

Because of the geometric complexity of quasi-cylindrical domains, we restrict ourselves to a special class: **tubes**, see Figure 4.1. Our motivation is twofold. First, the tubular geometry is rich enough to demonstrate the complexity of quasi-cylindrical domains. Second, the Dirichlet Laplacian in tubes is a reasonable model for the Hamiltonian in quantum-waveguide nanostructures. For simplicity, and also because we have the physical motivation in mind, we restrict to two- and three-dimensional tubes in these lectures.

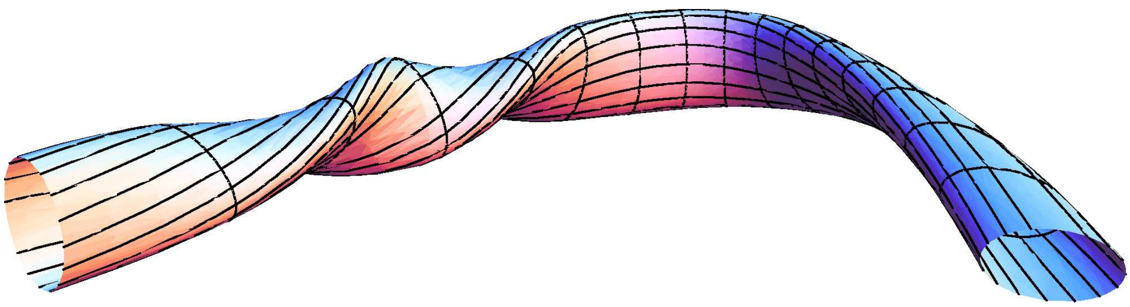


Figure 4.1: An example of a tube of elliptical cross-section. The geometric deformations of twisting and bending are demonstrated on the left and right part of the picture, respectively.

4.1 There is always some essential spectrum

Before considering the special geometric setting of tubes, let us establish a very general result, which is not even restricted to quasi-cylindrical domains.

Theorem 4.1 (General location of the essential spectrum)**.** *Let $\Omega \subset \mathbb{R}^d$ be an arbitrary open set. Set*

$$R_{\max} := \sup\left\{R \,:\, \Omega \text{ contains a sequence of disjoint balls of radius } R\right\}$$

(by convention, we set $R_{\max} := 0$ if there is no such a sequence.) There exists a dimensional constant c_d such that

$$\inf \sigma_{\rm ess}(-\Delta_D^\Omega) \leq \frac{c_d}{R_{\max}^2} \tag{4.1}$$

(by convention, we interpret the right hand side as $+\infty$ or 0 if $R_{\max} := 0$ or $R_{\max} := +\infty$, respectively).

Proof. If $R_{\max} = 0$, the right hand side of (4.1) can be interpreted as $+\infty$ and there is nothing to be proved. Let us therefore assume $R_{\max} > 0$. Let $\{x_n\}_{n\in\mathbb{N}^*} \subset \Omega$ be a set of points such that $\{B_R(x_n)\}_{n\in\mathbb{N}^*} \subset \Omega$ is the set of mutually disjoint balls for all $R \in (0, R_{\max})$. Then there also exists a sequence of cubes $\{Q_a(x_n)\}_{n\in\mathbb{N}^*}$ such that $Q_a(x_n) \subset B_R(x_n)$; in fact, choosing the inscribed cubes, we have the relation $R^2 = da^2$. The idea is to construct a non-compact sequence supported on the disjoint cubes. Let ψ be the first eigenfunction of $-\Delta_D^{Q_a(0)}$, normalised to 1 in $L^2(Q_a(0))$, and recall (*cf* (3.11)) that the corresponding eigenvalue is given by

$$\lambda_1^D(Q_a(0)) = d\left(\frac{\pi}{2a}\right)^2 = \left(\frac{\pi d}{2R}\right)^2 =: \frac{c_d}{R^2}\,.$$

For all $n \in \mathbb{N}^*$, we set

$$\psi_n(x) := \psi(x - x_n)$$

(the first eigenfunction of $-\Delta_D^{Q_a(x_n)}$) and extend it by zero to the whole Ω. Then the functions ψ_n's are mutually orthonormal in $L^2(\Omega)$ and satisfy $\|\nabla\psi_n\|^2_{L^2(\Omega)} = c_d/R^2$. Hence, choosing the n-dimensional subspace $\mathcal{L}_n = \operatorname{span}\{\psi_1, \dots, \psi_n\}$ in the minimax principle (Theorem 3.13), we get

$$\lambda_n^D(\Omega) \le \frac{c_d}{R^2} \tag{4.2}$$

for *all* $n \in \mathbb{N}^*$. Consequently (*cf* (3.23)),

$$\inf \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = \lim_{n\to\infty} \lambda_n^D(\Omega) \le \frac{c_d}{R^2}\,.$$

Since the argument holds for all $R \in (0, R_{\max})$, we conclude with the stated inequality. □

As a consequence of Theorem 4.1, we get the following implications:

$$\begin{array}{lcr} \Omega \text{ is quasi-conical} & \Longrightarrow & \inf \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = 0\,, \\ \Omega \text{ is quasi-cylindrical} & \Longrightarrow & \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) \neq \varnothing\,, \\ \Omega \text{ is quasi-bounded} & \Longleftarrow & \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = \varnothing\,. \end{array}$$

The first implication (in fact, much more) has been established previously, see Theorem 2.3. The last implication says that the quasi-boundedness is a *necessary* condition for the discreteness of the spectrum of the Dirichlet Laplacian (by Theorem 3.8, the boundedness is a sufficient condition). It is the middle implication which is of interest for us as regards quasi-cylindrical domains. Let us highlight it as a corollary.

Corollary 4.2. *Let $\Omega \subset \mathbb{R}^d$ be any quasi-cylindrical domain. Then*

$$\sigma_{\mathrm{ess}}(-\Delta_D^\Omega) \neq \varnothing\,.$$

Proof. Although the result follows directly from the quantitative Theorem 4.1, we provide an alternative proof, which does not use (3.23). Let us assume, by contradiction, that the spectrum of $-\Delta_D^\Omega$ is purely discrete. Then, proceeding as in the proof of Theorem 4.1, we get

$$\lim_{n\to\infty} \lambda_n^D(\Omega) \le \frac{c_d}{R_{\max}^2}\,.$$

Indeed, this asymptotic estimate follows directly from the uniform bound (4.2) and the arbitrariness of $R \in (0, R_{\max})$. That is, the eigenvalues of $-\Delta_D^\Omega$, abbreviated as $\lambda_n := \lambda_n^D(\Omega)$, accumulate at a finite point $\lambda_\infty < +\infty$. Since the corresponding eigenfunctions form a complete orthonormal set $\{\psi_n\}_{n\in\mathbb{N}^*}$

(*cf* Theorem 3.10), we have the decomposition

$$
\begin{aligned}
\forall \psi \in \operatorname{dom}(-\Delta_D^\Omega)\,, \qquad (\psi, -\Delta_D^\Omega \psi) &= \sum_{n,m=1}^{\infty} \big((\psi_n,\psi)\psi_n, (\psi_m, -\Delta\psi)\psi_m\big) \\
&= \sum_{n,m=1}^{\infty} \big((\psi_n,\psi)\psi_n, (\nabla\psi_m, \nabla\psi)\psi_m\big) \\
&= \sum_{n,m=1}^{\infty} \big((\psi_n,\psi)\psi_n, \lambda_m(\psi_m, \psi)\psi_m\big) \\
&= \sum_{n=1}^{\infty} \lambda_n \, |(\psi_n,\psi)|^2 \\
&\leq \lambda_\infty \sum_{n=1}^{\infty} |(\psi_n,\psi)|^2 \\
&= \lambda_\infty \, \|\psi\|^2 \,.
\end{aligned}
$$

On the other hand, given any non-trivial $\varphi \in C_0^2(\Omega)$ and defining $\varphi_N(x) := \varphi(Nx)$ with $N \in \mathbb{N}$, we have $\operatorname{supp}\varphi_N = N^{-1}\operatorname{supp}\varphi$ (the support is diminishing) and $\Delta\varphi_N(x) = N^2\Delta\varphi(Nx)$ (each derivative produces a factor N). Consequently, $\varphi_N \in C_0^2(\Omega) \subset \operatorname{dom}(-\Delta_D^\Omega)$ and

$$
\begin{aligned}
(\varphi_N, -\Delta_D^\Omega \varphi_N) &= N^2 \int_{\operatorname{supp}\varphi_N} |\nabla\varphi(Nx)|^2 \, \mathrm{d}x = N^2 N^{-d} \int_{\operatorname{supp}\varphi} |\nabla\varphi(y)|^2 \, \mathrm{d}y \,, \\
\|\varphi_N\|^2 &= \int_{\operatorname{supp}\varphi_N} |\varphi(Nx)|^2 \, \mathrm{d}x = N^{-d} \int_{\operatorname{supp}\varphi} |\varphi(y)|^2 \, \mathrm{d}y \,.
\end{aligned}
$$

That is,

$$
\lim_{N\to\infty} \frac{(\varphi_N, -\Delta_D^\Omega\varphi_N)}{\|\varphi_N\|^2} = \infty \,,
$$

which contradicts the previously established property that the quotient is bounded by λ_∞. $\square$

4.2 Ground-state variational formula

We also need a highly useful tool, which is an extension of the variational characterisation (3.20) of the lowest eigenvalue of an operator with purely discrete spectrum to the general case. In fact, it is the corollary (3.22) of the general minimax principle (Theorem 3.13), but we like to present a proof which does not use the spectral theorem.

Theorem 4.3. *Let H be a non-negative self-adjoint operator in $\mathcal{H}$ and let h denote its associated sesquilinear form. Then*

$$
\inf \sigma(H) = \inf_{\substack{\psi \in \operatorname{dom} h \\ \psi \neq 0}} \frac{h[\psi]}{\|\psi\|^2} \,. \tag{4.3}
$$

Proof. Let us abbreviate

$$
\lambda_1 := \inf\sigma(H) \qquad \text{and} \qquad \tilde\lambda_1 := \inf_{\substack{\psi \in \operatorname{dom} h \\ \psi \neq 0}} \frac{h[\psi]}{\|\psi\|^2} \,.
$$

$\boxed{\lambda_1 \geq \tilde\lambda_1}$ Let $\{\psi_n\}_{n\in\mathbb{N}} \subset \operatorname{dom} H \subset \operatorname{dom} h$ denote the (approximate) eigenfunction of H corresponding to λ_1 (recall that $\|\psi_n\| = 1$ is part of the property). Then

$$
\tilde\lambda_1 \leq h[\psi_n] = (\psi_n, H\psi_n) = (\psi_n, H\psi_n - \lambda_1\psi_n) + \lambda_1 \leq \|H\psi_n - \lambda_1\psi_n\| + \lambda_1 \,.
$$

Sending n to infinity, we arrive at the desired inequality.

$\boxed{\lambda_1 \leq \tilde{\lambda}_1}$ To prove the converse inequality, let us assume by contradiction that $\lambda_1 > \tilde{\lambda}_1$, so that in particular $\tilde{\lambda}_1$ does not belong to the spectrum of H. Let $\{\psi_n\}_{n\in\mathbb{N}} \subset \operatorname{dom} h$ be a minimising sequence for the infimum defining $\tilde{\lambda}_1$, *i.e.*,

$$\forall n \in \mathbb{N}, \quad \|\psi_n\| = 1 \qquad \text{and} \qquad \lim_{n\to\infty} h[\psi_n] = \tilde{\lambda}_1 \,. \tag{4.4}$$

We set

$$u_n := (H+I)^{-1/2}\psi_n$$

and argue that $\{u_n\}_{n\in\mathbb{N}}$ is an (approximate) eigenfunction of H corresponding to $\tilde{\lambda}_1$, a contradiction.

• $\underline{u_n \in \operatorname{dom} H.}$ First of all, notice that $u_n \in \operatorname{dom} H$ for every $n \in \mathbb{N}$. Indeed, for every $\phi \in \operatorname{dom} h$, one has

$$h(\phi, u_n) = \big(H^{1/2}\phi, H^{1/2}u_n\big) = \big(H^{1/2}\phi, (H+I)^{-1/2}H^{1/2}\psi_n\big) = \big(\phi, H^{1/2}(H+I)^{-1/2}H^{1/2}\psi_n\big)\,,$$

where $\|H^{1/2}(H+I)^{-1/2}\| = 1$ and $4\|H^{1/2}\psi_n\|$ is uniformly bounded in n because

$$\|H^{1/2}\psi_n\| = h[\psi_n] \xrightarrow[n\to\infty]{} \tilde{\lambda}_1 \,.$$

• $\underline{\|u_n\|.}$ Second, let us argue that u_n can be uniformly normalised to 1, *i.e.*, its norm does not converge to zero as $n \to \infty$. In fact, we shall determine the value of the limit. As for the lower bound, we have

$$\begin{aligned}
\|u_n\| &= \|(H+I)^{-1/2}\psi_n\| \\
&= \sup_{\substack{\varphi\in\mathcal{H}\\ \varphi\neq 0}} \frac{|(\varphi, (H+I)^{-1/2}\psi_n)|}{\|\varphi\|} \\
&= \sup_{\substack{\phi\in\operatorname{dom} h\\ \phi\neq 0}} \frac{|(\phi, \psi_n)|}{\|(H+I)^{1/2}\phi\|} \\
&= \sup_{\substack{\phi\in\operatorname{dom} h\\ \phi\neq 0}} \frac{|(\phi, \psi_n)|}{\sqrt{h[\phi] + \|\phi\|^2}} \\
&\geq \frac{\|\psi_n\|^2}{\sqrt{h[\psi_n] + \|\psi_n\|^2}} \\
&\xrightarrow[n\to\infty]{} \frac{1}{\sqrt{\tilde{\lambda}_1 + 1}}
\end{aligned}$$

where the third equality employs the fact that $(H+I)^{-1/2} : \mathcal{H} \to \operatorname{dom} h$ is an isomorphism and the limit is due to (4.4). On the other hand, since (4.4) implies $h[\psi] \geq \tilde{\lambda}_1\|\psi\|^2$ for every $\psi \in \operatorname{dom} h$, we have

$$\begin{aligned}
\|u_n\| &= \sup_{\substack{\phi\in\operatorname{dom} h\\ \phi\neq 0}} \frac{|(\phi, \psi_n)|}{\sqrt{h[\phi] + \|\phi\|^2}} \\
&\leq \sup_{\substack{\phi\in\operatorname{dom} h\\ \phi\neq 0}} \frac{|(\phi, \psi_n)|}{\sqrt{\tilde{\lambda}_1 + 1}\,\|\phi\|} \\
&= \frac{\|\psi_n\|}{\sqrt{\tilde{\lambda}_1 + 1}} = \frac{1}{\sqrt{\tilde{\lambda}_1 + 1}}\,,
\end{aligned}$$

where the last but one equality is due to the fact that $\operatorname{dom} h$ is dense in $\mathcal{H}$. Altogether, we have established the limit

$$\lim_{n\to\infty} \|u_n\| = \frac{1}{\sqrt{\tilde{\lambda}_1 + 1}} \,. \tag{4.5}$$

• $\underline{\|Hu_n - \tilde{\lambda}_1 u_n\|.}$ Finally, we establish the required convergence

$$\begin{aligned}
\|Hu_n - \tilde{\lambda}_1 u_n\|^2 &= \|(H+I)u_n - (\tilde{\lambda}_1 + 1)u_n\|^2 \\
&= \|(H+I)^{1/2}\psi_n\|^2 + (\tilde{\lambda}_1 + 1)^2\|u_n\|^2 - 2\,(\tilde{\lambda}_1 + 1)\|\psi_n\|^2 \\
&= h[\psi_n] + 1 + (\tilde{\lambda}_1 + 1)^2\|u_n\|^2 - 2\,(\tilde{\lambda}_1 + 1) \\
&\xrightarrow[n\to\infty]{} 0\,,
\end{aligned}$$

where the last step is due to (4.4) and (4.5). $\square$

4.3 Straight tubes

The special class of quasi-cylindrical domains we shall consider are obtained as a "local" perturbation of the *straight tube*

$$\Omega_0 := \mathbb{R} \times \omega \,, \tag{4.6}$$

where $\omega \subset \mathbb{R}^{d-1}$ is an arbitrary bounded domain (the *cross-section* of a waveguide modelled by Ω).

Since Ω_0 is a Cartesian product of two domains, it can be shown that

$$-\Delta_D^{\Omega_0} \cong -\Delta_D^{\mathbb{R}} \otimes I_\omega + I_{\mathbb{R}} \otimes -\Delta_D^{\omega} \qquad \text{in} \qquad L^2(\Omega_0) \cong L^2(\mathbb{R}) \times L^2(\omega) \,, \tag{4.7}$$

where $I_{\mathbb{R}}$ and I_ω denote the identity operators on $L^2(\mathbb{R})$ and $L^2(\omega)$, respectively. This is the precise statement of the "separation of variables" in Ω_0. Since the real axis $\mathbb{R}$ is a quasi-conical domain, its Dirichlet spectrum is purely essential (see Theorem 2.3)

$$\sigma(-\Delta_D^{\mathbb{R}}) = \sigma_{\mathrm{ess}}(-\Delta_D^{\mathbb{R}}) = [0, \infty) \,.$$

On the other hand, since ω is bounded, its Dirichlet spectrum is purely discrete (see Theorem 3.8)

$$\sigma(-\Delta_D^{\omega}) = \sigma_{\mathrm{disc}}(-\Delta_D^{\omega}) =: \{E_1 \leq E_2 \leq \dots\} \,.$$

Since the spectrum of the operator on the right-hand side of (4.7) is obtained as the sum of the individual spectra, it follows that the spectrum of $-\Delta_D^{\Omega_0}$ coincides with the semi-axis $[E_1, \infty)$. In particular, it is purely essential.

Theorem 4.4. *Let $\omega \subset \mathbb{R}^{d-1}$ be an arbitrary bounded open domain. Then*

$$\sigma(-\Delta_D^{\Omega_0}) = \sigma_{\mathrm{ess}}(-\Delta_D^{\Omega_0}) = [E_1, \infty) \,, \tag{4.8}$$

where E_1 denotes the lowest eigenvalue of $-\Delta_D^{\omega}$.

Proof. Here we provide an alternative proof for those who want to avoid the usage of the formula (4.7).

$\boxed{\sigma(-\Delta_D^{\Omega_0}) \subset [E_1, \infty)}$ Let h denote the sesquilinear form associated with $-\Delta_D^{\Omega}$, *i.e.*, $h(\phi, \psi) = (\nabla\phi, \nabla\psi)$ and $\operatorname{dom} h = W_0^{1,2}(\Omega)$. Since E_1 is the lowest point of the spectrum of $-\Delta_D^{\omega}$, the variational formula (4.3) implies

$$\forall \phi \in W_0^{1,2}(\omega) \,, \qquad \int_\omega |\nabla\phi(y)|^2 \, \mathrm{d}y \geq E_1 \int_\omega |\phi(y)|^2 \, \mathrm{d}y \,.$$

Consequently, using in addition Fubini's theorem, we have

$$\begin{aligned}
\forall \psi \in \operatorname{dom} h \,, \qquad h[\psi] &= \int_{\Omega_0} \left(|\partial_x \psi(x,y)|^2 + |\nabla_y \psi(x,y)|^2 \right) \mathrm{d}x \, \mathrm{d}y \\
&\geq \int_{\mathbb{R}} \int_\omega |\nabla_y \psi(x,y)|^2 \, \mathrm{d}y \, \mathrm{d}x \\
&\geq E_1 \int_{\mathbb{R}} \int_\omega |\psi(x,y)|^2 \, \mathrm{d}y \, \mathrm{d}x \\
&= E_1 \, \|\psi\|^2 \,.
\end{aligned}$$

By Theorem 4.3, it follows that $\inf \sigma(-\Delta_D^{\Omega_0}) \geq E_1$.

$\boxed{\sigma(-\Delta_D^{\Omega_0}) \supset [E_1, \infty)}$ The proof of the converse inclusion is based on an explicit construction of the approximate eigenfunctions of $-\Delta_D^{\Omega_0}$ corresponding to $k^2 + E_1$ with any $k \in \mathbb{R}$. For every $n \in \mathbb{N}^*$, we set

$$\psi_n(x,y) := \phi_n(x) \, \mathcal{J}_1(y) \qquad \text{with} \qquad \phi_n(x) := \varphi_n(x) \, e^{ikx} \,,$$

where $\mathcal{J}_1$ is the eigenfunction of $-\Delta_D^{\omega}$ normalised to one in $L^2(\omega)$ and (*cf* proof of Theorem 2.3)

$$\varphi_n(x) := n^{-1/2} \, \varphi\left(\frac{x-n}{n}\right)$$

with $\varphi \in C_0^2((0,\infty))$ being normalised to one in $L^2(\mathbb{R})$. Recall that $\{\phi_n\}_{n\in\mathbb{N}^*}$ is an approximate eigenfunction of $-\Delta_D^{\mathbb{R}}$ corresponding to k^2. Using in addition that $-\Delta\mathcal{J}_1 = E_1\mathcal{J}_1$ in ω, we get

$$\| -\Delta_D^{\Omega_0}\psi_n - (k^2+E_1)\psi_n\|_{L^2(\Omega_0)}^2 = \| -\Delta\phi_n - k^2\phi_n\|_{L^2(\mathbb{R})} \xrightarrow[n\to\infty]{} 0\,.$$

At the same time,

$$\|\psi_n\|_{L^2(\Omega_0)} = \|\phi_n\|_{L^2(\mathbb{R})}\,\|\mathcal{J}_1\|_{L^2(\omega)} = 1\,,$$

so $\{\psi_n\}_{n\in\mathbb{N}^*}$ is indeed an approximate eigenfunction of $-\Delta_D^{\Omega_0}$ corresponding to k^2+E_1.

$\boxed{\sigma(-\Delta_D^{\Omega_0}) = \sigma_{\mathrm{ess}}(-\Delta_D^{\Omega_0})}$ Finally, let us show that $\{\psi_n\}_{n\in\mathbb{N}^*}$ is the singular sequence, *i.e.*, it is weakly converging to zero. Since $\{\psi_n\}_{n\in\mathbb{N}^*}$ is bounded in $L^2(\Omega_0)$ (recall that the sequence is normalised to one), it is enough to verify that

$$\lim_{n\to\infty}(\phi,\psi_n) = 0$$

for every ϕ from a *dense subspace* of $L^2(\Omega_0)$ (see Exercise 4d). The space

$$L_0^2(\Omega_0) := \{\psi \in L^2(\Omega_0) :\ \exists N>0,\ \operatorname{supp}\psi \subset [-N,N]\times\overline{\omega}\} \tag{4.9}$$

is such a dense subspace (see Exercise 13). Taking any $\phi \in L_0^2(\Omega_0)$, however, it is clear that $(\phi,\psi_n) = 0$ for all sufficiently large n, because the support of ψ_n tends to infinity, namely (*cf* (2.4))

$$\inf\operatorname{supp}\varphi_n = n + n\,\inf\operatorname{supp}\varphi \geq n\,. \tag{4.10}$$

This concludes the proof of the theorem. □

Notice that $E_1 > 0$ (otherwise $\int_\omega |\nabla\mathcal{J}_1|^2 = 0$, which would imply $\mathcal{J}_1 = $ const almost everywhere in ω, and the constant would have to be equal to zero due to the Dirichlet boundary conditions). Hence, the structure of the spectrum (4.8) suggests that we deal with a reasonable model for semiconductor waveguide nanostructure (the ionisation energy E_1 is strictly positive).

4.4 Stability of the essential spectrum

Recall that the essential spectrum typically contains propagating states. Intuitively, the propagation is associated with phenomena taking part at infinity. Due to these heuristic considerations, it is expected that **the essential spectrum is determined by the behaviour at infinity only**. This is a completely imprecise statement, but it can be justified in many geometric as well as analytic settings. Here we provide the justification in the case of locally deformed tubes.

Definition 4.5. We say that a domain $\Omega \subset \mathbb{R}^d$ is a *local deformation* of the straight tube Ω_0 if there exists a cube $Q \subset \mathbb{R}^d$ such that

$$\Omega \setminus Q = \Omega_0 \setminus Q\,. \tag{4.11}$$

Obviously, the unbounded parts of Ω and Ω_0 are the same, so the following theorem is very expected.

Theorem 4.6. *Let $\Omega \subset \mathbb{R}^d$ be a local deformation of the straight tube Ω_0. Then*

$$\sigma_{\mathrm{ess}}(-\Delta_D^{\Omega}) = \sigma_{\mathrm{ess}}(-\Delta_D^{\Omega_0}) = [E_1,\infty)\,. \tag{4.12}$$

Proof. As usual, we divide the proof into two steps.

$\boxed{\sigma_{\mathrm{ess}}(-\Delta_D^{\Omega}) \supset [E_1,\infty)}$ This part is identical with the second step of the proof of Theorem 4.4. Indeed, the singular sequence $\{\psi_n\}_{n\in\mathbb{N}^*}$ is "localised at infinity" (*cf* (4.10)), so it works just the same for Ω due to (4.11).

$\boxed{\sigma_{\mathrm{ess}}(-\Delta_D^\Omega) \subset [E_1,\infty)}$ One possibility how to establish the opposite inclusion is to use the so-called *Neumann bracketing*. By the minimax principle (extended to operators with an essential spectrum, see Theorem 3.13), one has

$$\inf \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = \lim_{k\to\infty} \lambda_k(\Omega)\,, \tag{4.13}$$

where $\{\lambda_k(\Omega)\}_{k=1}^\infty$ is the non-decreasing sequence defined by

$$\lambda_k(\Omega) := \inf_{\substack{\mathcal{L}_k \subset W_0^{1,2}(\Omega)\\ \dim \mathcal{L}_k = k}} \sup_{\substack{\psi\in\mathcal{L}_k\\ \psi\neq 0}} \frac{\displaystyle\int_\Omega |\nabla\psi|^2}{\displaystyle\int_\Omega |\psi|^2}\,.$$

By Definition 4.5, there exists $R>0$ such that

$$\Omega = \Omega_{\mathrm{left}} \cup \Sigma_{\mathrm{left}} \cup \Omega_{\mathrm{centre}} \cup \Sigma_{\mathrm{right}} \cup \Omega_{\mathrm{right}}\,,$$

where

$$\begin{aligned} \Omega_{\mathrm{left}} &:= (-\infty,-R)\times\omega\,, & \Omega_{\mathrm{right}} &:= (+R,+\infty)\times\omega\,,\\ \Sigma_{\mathrm{left}} &:= \{-R\}\times\omega\,, & \Sigma_{\mathrm{right}} &:= \{+R\}\times\omega\,, \end{aligned} \qquad \Omega_{\mathrm{centre}} := \Omega\cap(-R,R)^d\,.$$

Notice that Σ_{left} and Σ_{right} are sets of measure zero. We introduce spaces of restrictions

$$\mathcal{W}(\Omega_\iota) := \{\psi \restriction \Omega_\iota :\ \psi\in W_0^{1,2}(\Omega)\}\,, \qquad \iota\in\{\text{left},\text{centre},\text{right}\}\,,$$

and set

$$\mathcal{D}(\Omega) := \mathcal{W}(\Omega_{\mathrm{left}}) \oplus \mathcal{W}(\Omega_{\mathrm{centre}}) \oplus \mathcal{W}(\Omega_{\mathrm{right}})\,. \tag{4.14}$$

Notice that

$$\mathcal{D}(\Omega) \supset W_0^{1,2}(\Omega)\,,$$

because the functions from $\mathcal{D}(\Omega)$ may be discontinuous on the interfaces Σ_{left} and Σ_{right}, while $W_0^{1,2}(\Omega)$ is a more regular space. Consequently, defining

$$\lambda_k^N(\Omega) := \inf_{\substack{\mathcal{L}_k \subset \mathcal{D}(\Omega)\\ \dim \mathcal{L}_k = k}} \sup_{\substack{\psi\in\mathcal{L}_k\\ \psi\neq 0}} \frac{\displaystyle\int_\Omega |\nabla\psi|^2}{\displaystyle\int_\Omega |\psi|^2}\,,$$

we get the inequalities (just because the infimum is taken over larger subspaces)

$$\forall k\in\mathbb{N}^*\,, \qquad \lambda_k(\Omega) \geq \lambda_k^N(\Omega)\,. \tag{4.15}$$

Here the superscript stands for "Neumann" and the relationship to Neumann boundary conditions is that the space $\mathcal{D}(\Omega)$ is the domain of the sesquilinear form associated with the operator which acts as the Laplacian in Ω and satisfies Neumann boundary conditions on Σ_{left} and Σ_{right} and Dirichlet boundary conditions on $\partial\Omega$. In other words, imposing Neumann boundary conditions means to impose no boundary conditions on the level of forms.

Because of the direct-sum structure (4.14) of the space $\mathcal{D}(\Omega)$, we clearly have

$$\{\lambda_k^N(\Omega)\}_{k=1}^\infty = \{\lambda_k^N(\Omega_{\mathrm{left}})\}_{k=1}^\infty \cup \{\lambda_k^N(\Omega_{\mathrm{centre}})\}_{k=1}^\infty \cup \{\lambda_k^N(\Omega_{\mathrm{right}})\}_{k=1}^\infty\,, \tag{4.16}$$

where

$$\lambda_k^N(\Omega_\iota) := \inf_{\substack{\mathcal{L}_k \subset \mathcal{W}(\Omega_\iota)\\ \dim \mathcal{L}_k = k}} \sup_{\substack{\psi\in\mathcal{L}_k\\ \psi\neq 0}} \frac{\displaystyle\int_{\Omega_\iota} |\nabla\psi|^2}{\displaystyle\int_{\Omega_\iota} |\psi|^2}\,, \qquad \iota\in\{\text{left},\text{centre},\text{right}\}\,.$$

Since Ω_{centre} is bounded and the Neumann boundary conditions are imposed on smooth (in fact, straight) parts of the boundary, it can be shown that the spectrum of the Laplacian in Ω_{centre} with the combined boundary conditions is purely discrete. In other words,

$$\lim_{k\to\infty} \lambda_k^N(\Omega_{\mathrm{centre}}) = +\infty\,.$$

(Alternatively, one can employ the monotonicity of eigenvalues when extending over the parts of the boundary $\partial\Omega_{\text{centre}}$ where Dirichlet boundary conditions are imposed and a subsequent lower bound through eigenvalues of the Neumann Laplacian in the cube Q.) On the other hand, by a separation of variables, it is easy to see that

$$\forall k \in \mathbb{N}^* , \qquad \lambda_k^N(\Omega_{\text{left}}) = \lambda_k^N(\Omega_{\text{right}}) = E_1 .$$

Consequently, arranging the right-hand side of (4.16) into the non-decreasing sequence standing on the left-hand side, we notice that the elements of $\{\lambda_k^N(\Omega_{\text{centre}})\}_{k=1}^\infty$ greater than E_1 do not count, while $\{\lambda_k^N(\Omega_{\text{left}})\}_{k=1}^\infty$ and $\{\lambda_k^N(\Omega_{\text{right}})\}_{k=1}^\infty$ are stationary non-compact sequences. Altogether, we thus arrive at

$$\lim_{k\to\infty} \lambda_k^N(\Omega) = E_1 . \tag{4.17}$$

Combining (4.13), (4.15) and (4.17), we finally get the desired lower bound

$$\inf \sigma_{\text{ess}}(-\Delta_D^\Omega) = \lim_{k\to\infty} \lambda_k(\Omega) \geq \lim_{k\to\infty} \lambda_k^N(\Omega) = E_1 .$$

This concludes the proof of the theorem. ☐

The stability of the essential spectrum is actually true under much more general definitions of "local deformations". Indeed, it is clear from the proof that we do not really need that $\Omega \setminus Q$ coincides with $\Omega_0 \setminus Q$; it would be enough to assume that Ω has (possibly just one or more than two) unbounded ends each congruent to the straight half-tube $\{x \in \mathbb{R}^d : \ x_1 > 0\}$. More generally, it is enough to assume that this straight half-tube is just "approached at infinity" in a suitable sense, but we do not want to go into much technical details here.

4.5 Tubes with protrusions and intrusions

From now on, we restrict ourselves to the two-dimensional setting when

$$\Omega_0 := \mathbb{R} \times (0, a) \qquad \text{with} \qquad a > 0$$

is an unbounded strip of width a. So the cross-section of the tube is just the interval $(0, a)$. Recalling (3.9) and (3.10), we have

$$E_1 = \left(\frac{\pi}{a}\right)^2 \qquad \text{and} \qquad \mathcal{J}_1(y) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a} y\right) \tag{4.18}$$

in the present notation.

We focus on very special local deformations of the straight strip Ω_0, namely those obtained by locally enlarging or diminishing the cross-section.

Definition 4.7. Given any continuous function $\theta : \mathbb{R} \to \mathbb{R}$ satisfying $\theta > -a$, we define a *deformed tube* by setting

$$\Omega := \left\{(x, y) \in \mathbb{R}^d : \ x \in \mathbb{R} \ \wedge \ 0 < y < a + \theta(x)\right\} . \tag{4.19}$$

The condition $\theta > -a$ ensures that Ω has a geometrical meaning of a non-self-intersecting strip of variable cross-section of positive width $a + \theta(x)$. To have a *local* deformation of Ω_0, we clearly have to additionally assume that θ is compactly supported.

The part of the tube Ω where $\theta(x) > 0$ (respectively, $\theta(x) < 0$) is called a *protrusion* (respectively, *intrusion*). We shall see that these respective geometric deformations have quite opposite impacts on spectral properties of the Dirichlet Laplacian $-\Delta_D^\Omega$.

In this context, we think of $-\Delta_D^\Omega$ as the Hamiltonian of a quantum (quasi-)particle constrained to a waveguide-type nanostructure of shape Ω with hard-wall boundaries. The straight strip Ω_0 is an ideal quantum waveguide, while the deformations due to protrusions and intrusions represent perturbations (either unwanted or intentionally created).

4.6 Bound states due to protrusions

In this section we investigate the effect of protrusions. The following theorem is originally due to [14].

Theorem 4.8. *Let $\theta \in C_0^0(\mathbb{R})$ be a non-trivial function. Then*

$$\theta \geq 0 \qquad \Longrightarrow \qquad \inf \sigma(-\Delta_D^\Omega) < E_1 \,.$$

Consequently, if Ω has a protrusion, then $-\Delta_D^\Omega$ possesses a discrete eigenvalue below the essential spectrum $[E_1, \infty)$.

Proof. First of all, notice that there exists another non-trivial function $\vartheta : \mathbb{R} \to \mathbb{R}$ satisfying

$$\vartheta_\varepsilon \in C_0^1(\mathbb{R}) \qquad \text{and} \qquad 0 \leq \vartheta \leq \theta \,.$$

For every $\varepsilon \in (0,1]$, we introduce the scaled function $\vartheta_\varepsilon := \varepsilon\vartheta$ and consider the domain Ω_ε which is defined by (4.19) with θ being replaced by ϑ_ε. Since $\vartheta_\varepsilon \leq \theta$, one has $\Omega_\varepsilon \subset \Omega$. Since $W_0^{1,2}(\Omega) \supset W_0^{1,2}(\Omega_\varepsilon)$ (by extending the function from $W_0^{1,2}(\Omega_\varepsilon)$ by zero outside Ω_ε, *cf* (3.17)), Theorem 4.3 implies (*cf* Proposition 3.16)

$$\inf \sigma(-\Delta_D^\Omega) \leq \inf \sigma(-\Delta_D^{\Omega_\varepsilon}) \,.$$

Hence, it is enough to prove the theorem for the more regular function ϑ_ε. Notice that $\operatorname{supp} \vartheta_\varepsilon = \operatorname{supp} \vartheta$.

The proof is similar to that of Theorem 2.9. We introduce the quadratic form

$$Q_\varepsilon[\psi] := \|\nabla\psi\|^2_{L^2(\Omega_\varepsilon)} - E_1 \, \|\psi\|^2_{L^2(\Omega_\varepsilon)} \,, \qquad \operatorname{dom} Q_\varepsilon := W_0^{1,2}(\Omega) \,.$$

By Theorem 4.3, it is enough to find a test function $\psi \in W_0^{1,2}(\Omega_\varepsilon)$ such that $Q_\varepsilon[\psi] < 0$. We set

$$\psi_n(x,y) := \varphi_n(x) \, \sin\left(\frac{\pi}{a + \vartheta_\varepsilon(x)} \, y\right) \qquad \text{with} \qquad \varphi_n(x) := \varphi\left(\frac{x}{n}\right) ,$$

where $\varphi \in C_0^1(\mathbb{R})$ is such that

$$0 \leq \varphi \leq 1 \,, \qquad \varphi = 1 \quad \text{on} \quad [-1,1] \,, \qquad \varphi = 0 \quad \text{outside} \quad [-2,2] \,,$$

and the argument of the sine function is motivated by the transverse ground state (4.18). We write $Q_\varepsilon = Q_\varepsilon^{(1)} + Q_\varepsilon^{(2)}$ with

$$Q_\varepsilon^{(1)}[\psi] := \|\partial_1\psi\|^2_{L^2(\Omega_\varepsilon)} \,, \qquad Q_\varepsilon^{(2)}[\psi] := \|\partial_2\psi\|^2_{L^2(\Omega_\varepsilon)} - E_1 \, \|\psi\|^2_{L^2(\Omega_\varepsilon)} \,,$$

and consider the individual forms separately.

$\boxed{Q_\varepsilon^{(2)}}$ Integrating by parts in y, we get

$$\begin{aligned}
Q_\varepsilon^{(2)}[\psi_n] &= \int_{\mathbb{R}} \int_0^{a+\vartheta_\varepsilon(x)} \left[\left(\frac{\pi}{a+\vartheta_\varepsilon(x)}\right)^2 - \left(\frac{\pi}{a}\right)^2\right] |\psi_n(x,y)|^2 \, \mathrm{d}y \, \mathrm{d}x \\
&= \int_{\operatorname{supp}\vartheta} \int_0^{a+\vartheta_\varepsilon(x)} \left[\left(\frac{\pi}{a+\vartheta_\varepsilon(x)}\right)^2 - \left(\frac{\pi}{a}\right)^2\right] \sin^2\left(\frac{\pi}{a+\vartheta_\varepsilon(x)} \, y\right) \mathrm{d}y \, \mathrm{d}x \\
&= \int_{\operatorname{supp}\vartheta} \left[\left(\frac{\pi}{a+\vartheta_\varepsilon(x)}\right)^2 - \left(\frac{\pi}{a}\right)^2\right] \frac{a+\vartheta_\varepsilon(x)}{2} \, \mathrm{d}x \,,
\end{aligned}$$

where the second equality is valid for all n large enough (so that $\varphi_n = 1$ on the support of ϑ; notice that the square bracket equals zero outside the support of ϑ). Hence, there exists $n_0 > 0$ such that, for every $n \geq n_0$ and $\varepsilon > 0$,

$$Q_\varepsilon^{(2)}[\psi_n] = \frac{\pi^2}{2a^2} \int_{\operatorname{supp}\vartheta} \frac{-2a\,\vartheta_\varepsilon(x) - \vartheta_\varepsilon(x)^2}{a+\vartheta_\varepsilon(x)} \, \mathrm{d}x \leq -\frac{\pi^2\,\varepsilon}{a(a+\max\theta)} \int_{\operatorname{supp}\vartheta} \vartheta(x) \, \mathrm{d}x =: -c_1\varepsilon$$

where c_1 is a positive constant independent of both n and ε.

$\boxed{Q_\varepsilon^{(1)}}$ For the first form, we have

$$\begin{aligned}
Q_\varepsilon^{(1)}[\psi_n] &= \int_{\mathbb{R}} \int_0^{a+\vartheta_\varepsilon(x)} \left| \frac{1}{n}\varphi'\left(\frac{x}{n}\right) \sin\left(\frac{\pi}{a+\vartheta_\varepsilon(x)}\, y\right) - \varphi\left(\frac{x}{n}\right) \frac{\pi\, y\, \vartheta_\varepsilon'(x)}{[a+\vartheta_\varepsilon(x)]^2} \cos\left(\frac{\pi}{a+\vartheta_\varepsilon(x)}\, y\right)\right|^2 \mathrm{d}y\, \mathrm{d}x \\
&\leq 2 \int_{\mathbb{R}} \int_0^{a+\vartheta_\varepsilon(x)} \left[\frac{1}{n^2}\varphi'\left(\frac{x}{n}\right)^2 \sin^2\left(\frac{\pi}{a+\vartheta_\varepsilon(x)}\, y\right) + \varphi\left(\frac{x}{n}\right)^2 \frac{\pi^2\, \vartheta_\varepsilon'(x)^2}{[a+\vartheta_\varepsilon(x)]^2} \cos^2\left(\frac{\pi}{a+\vartheta_\varepsilon(x)}\, y\right)\right] \mathrm{d}y\, \mathrm{d}x \\
&= \int_{\mathbb{R}} \left[\frac{1}{n^2}\varphi'\left(\frac{x}{n}\right)^2 [a+\vartheta_\varepsilon(x)] + \varphi\left(\frac{x}{n}\right)^2 \frac{\pi^2\, \vartheta_\varepsilon'(x)^2}{a+\vartheta_\varepsilon(x)}\right] \mathrm{d}x \\
&\leq \frac{a+\max\theta}{n} \int_{\mathbb{R}} |\varphi'(x)|^2\, \mathrm{d}x + \frac{\pi^2\, \varepsilon^2}{a} \int_{\operatorname{supp}\vartheta} |\vartheta'(x)|^2\, \mathrm{d}x \\
&=: \frac{c_2}{n} + c_3\varepsilon^2 \,,
\end{aligned}$$

where c_2 and c_3 are positive constants independent of both n and ε.

In summary,

$$Q_\varepsilon[\psi_n] = \frac{c_2}{n} + c_3\varepsilon^2 - c_1\varepsilon \,.$$

First, we choose ε so small that the sum of the last two terms on the right-hand side is negative (namely, $\varepsilon < c_1/c_3$). Then we can choose n so large that the entire right-hand side becomes negative. This concludes the proof of the inequality $\inf\sigma(-\Delta_D^\Omega) < E_1$.

The inequality implies that $-\Delta_D^\Omega$ possesses *a* spectrum below E_1. By Theorem 4.6, the essential spectrum starts by E_1, because Ω is a local perturbation of Ω_0 due to the compact support of θ. Consequently, $\inf\sigma(-\Delta_D^\Omega)$ must be a discrete eigenvalue. This concludes the proof of the theorem. □

The theorem implies that a quantum particle (say, electron) get trapped inside the waveguide Ω whenever there is a protrusion. More specifically, the Schrödinger equation admits a stationary solution. In quantum mechanics, this phenomenon is known as the existence of *bound states* (the same terminology is kept for the eigenfunctions corresponding to the discrete eigenvalues). We regard it as a negative impact on the transport, because an arbitrarily small defect *à la* protrusion immediately creates at least one bound state.

From a different perspective,

the protrusion acts as an attractive interaction

in the sense that it diminishes the spectrum (*i.e.* the spectrum of Ω starts below the spectral threshold of the straight waveguide Ω_0).

4.7 Hardy inequalities due to intrusions

It turns out that the effect of intrusions is quite opposite. To quantify it, we establish the following lower bound.

Theorem 4.9. *Let $\theta \in C^0(\mathbb{R})$ be such that $\theta > -a$. Then*

$$\forall \psi \in W_0^{1,2}(\Omega), \qquad \int_\Omega |\nabla\psi|^2 - E_1 \int_\Omega |\psi|^2 \geq \int_\Omega \left[\left(\frac{\pi}{a+\theta(x)}\right)^2 - \left(\frac{\pi}{a}\right)^2\right] |\psi(x,y)|^2\, \mathrm{d}x\, \mathrm{d}y\,. \tag{4.20}$$

Proof. Given any bounded open interval $I \subset \mathbb{R}$, recall (*cf* Section 3.2) that $(\pi/|I|)^2$ is the lowest eigenvalue of the Dirichlet Laplacian in $L^2(I)$. As a consequence of the variational formula (4.3), we thus get the inequality

$$\forall \phi \in W_0^{1,2}(I), \qquad \int_I |\phi'|^2 \geq \left(\frac{\pi}{|I|}\right)^2 \int_I |\phi|^2 \,. \tag{4.21}$$

By means of Fubini's theorem, we therefore obtain

$$\forall\psi \in W_0^{1,2}(\Omega)\,, \qquad \begin{aligned} \int_\Omega |\nabla\psi|^2 &= \int_{\mathbb{R}} \int_0^{a+\theta(x)} \left(|\partial_x\psi(x,y)|^2 + |\partial_y\psi(x,y)|^2\right) \, \mathrm{d}y\, \mathrm{d}x \\ &\geq \int_{\mathbb{R}} \int_0^{a+\theta(x)} |\partial_y\psi(x,y)|^2 \, \mathrm{d}y\, \mathrm{d}x \\ &\geq \int_{\mathbb{R}} \left(\frac{\pi}{a+\theta(x)}\right)^2 \int_0^{a+\theta(x)} |\psi(x,y)|^2 \, \mathrm{d}y\, \mathrm{d}x \\ &= \int_\Omega \left(\frac{\pi}{a+\theta(x)}\right)^2 |\psi(x,y)|^2 \, \mathrm{d}x\, \mathrm{d}y\,. \end{aligned}$$

It remains to recall the definition (4.18) of E_1. □

Notice that the square bracket of (4.20) is non-positive (respectively, non-negative) if $\theta \geq 0$ (respectively, $\theta \leq 0$). The inequality is therefore uninteresting for protrusions. On the other hand, it is a non-trivial result for intrusions.

Corollary 4.10. *Let $\theta \in C_0^0(\mathbb{R})$ be a non-trivial function satisfying $\theta > -a$. Then*

$$\theta \leq 0 \qquad \Longrightarrow \qquad -\Delta_D^\Omega - E_1 I \quad \textit{is subcritical}.$$

Proof. The inequality (4.20) is equivalent to the Hardy-type inequality

$$-\Delta_D^\Omega - E_1 I \geq \left(\frac{\pi}{a+\theta}\right)^2 - \left(\frac{\pi}{a}\right)^2 \tag{4.22}$$

in the sense of forms in $L^2(\Omega)$, where the right-hand side is non-negative and non-trivial under the stated hypotheses. (Here we denote by the same symbol θ the function $\theta \otimes 1$ in $\Omega \subset \mathbb{R}\times\mathbb{R}$) □

The implication holds without the assumption that θ is compactly supported. It is this situation, however, which is of special interest, because than Ω is a local deformation of Ω_0. Then Theorem 4.6 implies that the essential spectrum equals the interval $[E_1,\infty)$ and Corollary 4.10 ensures that there is no spectrum below E_1. What is more,

the intrusion acts as a repulsive interaction

in the sense that the right-hand side of (4.22) is non-negative and non-trivial. It is important to notice that such a scenario does not happen for the straight strip.

Proposition 4.11. *The operator $-\Delta_D^{\Omega_0} - E_1 I$ is critical.*

Proof. It is enough to prove that the spectrum of $-\Delta_D^{\Omega_0} - \rho$ starts below E_1 for any non-trivial bounded function $\rho : \Omega_0 \to [0,\infty)$. The proof is similar to the proof of Theorem 2.9 concerning the criticality of $-\Delta^{\mathbb{R}}$ and it is left to the reader (*cf* Exercise 14). □

If the intrusion is not local (or, less restrictively, $\theta(x)$ does not go to zero as $|x| \to \infty$), it might happen that the essential spectrum starts above E_1. What is more, an extreme global intrusion may even annihilate the essential spectrum completely, so that one actually deals with a quasi-bounded domain.

Corollary 4.12. *Let $\theta \in C^0(\mathbb{R})$ be a non-trivial function satisfying $\theta > -a$. Then*

$$\lim_{|x|\to\infty} \theta(x) = -a \qquad \Longrightarrow \qquad \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = \varnothing\,.$$

Proof. Proceeding in the same way as in the proof of Theorem 4.6, we obtain that

$$\inf \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) \geq \min\{\lambda_{\mathrm{left}}, \lambda_{\mathrm{right}}\}\,, \tag{4.23}$$

where

$$\lambda_\iota := \inf_{\substack{\psi \in \mathcal{W}(\Omega_\iota)\\ \psi \neq 0}} \frac{\displaystyle\int_{\Omega_\iota} |\nabla\psi|^2}{\displaystyle\int_{\Omega_\iota} |\psi|^2}\,, \qquad \iota \in \{\mathrm{left}, \mathrm{right}\}\,, \qquad \begin{aligned} \Omega_{\mathrm{left}} &:= [(-\infty, -R) \times \mathbb{R}] \cap \Omega\,, \\ \Omega_{\mathrm{right}} &:= [(+R, +\infty) \times \mathbb{R}] \cap \Omega\,. \end{aligned}$$

Proceeding as in the proof of Theorem 4.9, we get

$$\begin{aligned} \forall \psi \in \mathcal{W}(\Omega_{\mathrm{right}})\,, \qquad \int_{\Omega_{\mathrm{right}}} |\nabla\psi|^2 &\geq \int_{\Omega_{\mathrm{right}}} \left(\frac{\pi}{a+\theta(x)}\right)^2 |\psi(x,y)|^2 \,\mathrm{d}x\,\mathrm{d}y \\ &\geq \left(\frac{\pi}{a + \inf\limits_{(R,\infty)} \theta}\right)^2 \int_{\Omega_{\mathrm{right}}} |\psi|^2\,, \end{aligned}$$

and similarly for Ω_{left}. Consequently,

$$\lambda_{\mathrm{left}} \geq \left(\frac{\pi}{a + \inf\limits_{(-\infty,-R)} \theta}\right)^2 \qquad \text{and} \qquad \lambda_{\mathrm{right}} \geq \left(\frac{\pi}{a + \inf\limits_{(R,\infty)} \theta}\right)^2 .$$

Because of our hypothesis, both λ_{left} and λ_{right} tend to ∞ as $R \to \infty$. Since the left-hand side of (4.23) is independent of R and the right-hand side can made arbitrarily large by taking R large, it follows that $\inf \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = \infty$. □

4.8 Twisting versus bending in curved tubes

Instead of considering straight tubes with varying cross-section, it is interesting to consider *curved* tubes of uniform cross-section, see Figure 4.1. Without going into technical details, let us mention that it can be shown, by the same techniques as above, that:

bending acts as an attractive interaction

twisting acts as a repulsive interaction

This is a brief summary of many results established in recent years (see [50] for an overview). Here it is interesting that the existence of bound states in bent waveguides is a purely quantum effect, without a classical counterpart. The moral is that, in order to make the transport in modern quantum wires stable, one should use twisted geometries.

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Appendix A

Notation

Here we point out some special notation used in the lectures.

- $\mathbb{N}^* := \mathbb{N} \setminus \{0\}$, where $\mathbb{N} = \{0, 1, 2, \dots\}$ are natural numbers (including zero).
- $\mathbb{R}_+ := (0, +\infty)$, $\mathbb{R}_- := (-\infty, 0)$.
- $B_R(x_0) := \{x \in \mathbb{R}^d : \ |x - x_0| < R\}$ (ball of radius R and centre x_0), where $x_0 \in \mathbb{R}^d$ and $R > 0$.
- $B_R := B_R(0)$ (ball of radius R centred at the origin).
- $Q_a := (-a, a)^d$ (hyper(cube) of side $2a$), where $a > 0$. $Q_a(x_0) := x_0 + Q_a$, where $x_0 \in \mathbb{R}^d$.
- $\chi_S(x) := \begin{cases} 1 & \text{if} \quad x \in S\,, \\ 0 & \text{otherwise}\,, \end{cases}$ (characteristic function of a set S), where $S \subset \mathbb{R}^d$.
- If $a \in \mathbb{C}^d$ and $A \in \mathbb{C}^{d \times d}$ is a vector and a matrix, respectively, we use the common notation
$$|a| := \sqrt{\sum_{j=1}^{d} |a_j|^2} \qquad \text{and} \qquad |A| := \sqrt{\sum_{j,k=1}^{d} |A_{jk}|^2}\,.$$
for the Euclidean and Frobenius norm, respectively.
- The elements of the gradient $\nabla\psi$ are regarded as being arranged in the Euclidean vector
$$\big(\partial_1\psi(x), \dots, \partial_d\psi(x)\big) \in \mathbb{C}^d$$
and we abbreviate $\|\nabla\psi\| := \big\||\nabla\psi|\big\|$.
- The elements of the Hessian $\nabla^2\psi$ are regarded as being arranged in the matrix
$$\begin{pmatrix} \partial_1^2\psi(x) & \dots & \partial_1\partial_d\psi(x) \\ \vdots & \ddots & \vdots \\ \partial_d\partial_1\psi(x) & \dots & \partial_d^2\psi(x) \end{pmatrix} \in \mathbb{C}^{d \times d}$$
and we abbreviate $\|\nabla^2\psi\| := \big\||\nabla^2\psi|\big\|$.
- For two norm spaces $\mathcal{B}, \mathcal{B}'$, we write $\mathcal{B}' \hookrightarrow \mathcal{B}$ if $\mathcal{B}' \subset \mathcal{B}$ and the inclusion map (*embedding*) $\iota : \mathcal{B}' \to \mathcal{B} : \{\psi \mapsto \psi\}$ is a bounded operator. Note that the spaces are allowed to have different topologies. The space $\mathcal{B}'$ is said to be *embedded* in $\mathcal{B}$.

Appendix B

Exercises

More involved exercises are highlighted by an asterisk.

1. Construct an example of a sesquilinear form which is densely defined, symmetric and bounded from below, but **not closable**.
   Solution: In $L^2(\mathbb{R})$, $h[\psi] := |\psi(0)|^2$, $\operatorname{dom} h := W^{1,2}(\mathbb{R})$.

2. Confirm the **independence of injectivity and surjectivity** in infinite-dimensional spaces.

   (a) Give an example of an operator which is injective but not surjective.
   Hint: Consider an operator induced by differentiation with too many boundary conditions.
   Solution: $p := -i\nabla$ in $L^2((0,1))$, $\operatorname{dom} p := W_0^{1,2}((0,1))$.

   (b) Give an example of an operator which is surjective but not injective.
   Hint: Consider an operator induced by differentiation with too few boundary conditions.
   Solution: $p^* = -i\nabla$ in $L^2((0,1))$, $\operatorname{dom} p^* = W^{1,2}((0,1))$.

3. Give an example of an operator which is **closed symmetric but not self-adjoint**.
   Solution: The operator p from Exercise 2.

4. Study the **weak convergence**.

   (a) *Prove that every bounded sequence in a Hilbert space contains a weakly converging subsequence.
   Hint: Use the Bolzano–Weierstrass theorem for the sequence of numbers $\{(\phi, \psi_n)\}_{n\in\mathbb{N}}$, where $\{\psi_n\}_{n\in\mathbb{N}}$ is the bounded sequence and ϕ is an arbitrary vector in the Hilbert space.
   Solution: Proof of [67, Thm. 4.25] or [65, Thm. 4.41-A], but probably the cleanest proof can be found in [62, Sec. 8.3].

   (b) Show that every orthonormal sequence in a Hilbert space weakly converges to zero.
   Hint: Use the Bessel inequality.

   (c) Show that weak convergence does not imply strong convergence in general.
   Hint: Consider an orthonormal sequence in an infinite-dimensional space.

   (d) Let $\{\psi_n\}_{n\in\mathbb{N}}$ be a bounded sequence in $\mathcal{H}$. Prove that to show that $\{\psi_n\}_{n\in\mathbb{N}}$ is weakly converging to zero in $\mathcal{H}$, it is enough to guarantee that $(\phi, \psi_n) \to 0$ as $n \to \infty$ for every ϕ from a dense subspace of $\mathcal{H}$.
   Solution: Proof of [47, Lem. III.1.31].

5. Show that the eigenfunctions (3.10) of $-\Delta_D^{(-a,a)}$ form a **complete orthonormal set** in $L^2((-a,a))$.
   Hint: The orthonormality is easily verified. For the completeness, employ the well known (see, *e.g.*, [63, Sec. 4.24]) completeness of the trigonometric sequence $\{e^{ikx}\}_{k\in\mathbb{Z}}$ in $L^2((0,2\pi))$ and symmetry.

6. Study the low-lying **eigenvalues of the square**.

   (a) Simplify the formula (3.11) in the case of a square of side π.
   Solution: $\sigma_{\mathrm{p}}\big(-\Delta_D^{Q_{\pi/2}}\big) = \big\{k_1^2 + k_2^2\big\}_{k_1,k_2=1}^{\infty}$.

   (b) Identify the first eleven lowest eigenvalues (counting multiplicities) and arrange them in a non-decresing order.
   Solution: $2 < 5 \leq 5 < 8 < 10 \leq 10 < 13 \leq 13 < 17 \leq 17 < 18 < \dots$

(c) What is the highest multiplicity?
Solution: 2 (the 2nd and 3rd; 5th and 6th; 7th and 8th; 9th and 10th eigenvalues are doubly degenerated).

(d) *Can one have a higher degeneracy for higher eigenvalues?
Solution: Yes. (The 31st, 32nd, 33rd eigenvalues are triply degenerated.)

7. Study properties of **compact operators**.

(a) A bounded operator H in $\mathcal{H}$ is compact if, and only if, $Hf_n \to 0$ as $n \to \infty$ for every sequence $\{f_n\}_{n\in\mathbb{N}}$ weakly converging to zero.
Solution: Proof of [67, Thm. 6.3].

(b) If H_1, H_2 are bounded compact operators, then the sum $H_1 + H_2$ is also compact.
Solution: Proof of [67, Thm. 6.4].

(c) Show that H is a bounded operator of rank m (*i.e.*, $\dim \operatorname{ran} H = m$) if, and only if, there exists an othonormal sets $\{f_j\}_{j=1}^m$ and $\{g_j\}_{j=1}^m$ such that $H = \sum_{j=1}^m g_j(f_j, \cdot)$.
Solution: Proof of [67, Thm. 6.1].

(d) Show that any bounded operator *of finite rank* (*i.e.*, $\dim \operatorname{ran} H < \infty$) is compact.
Hint: Use the previous points.

(e) *Show that H is compact if, and only if, there exists a sequence of operators $\{H_N\}_{N\in\mathbb{N}}$ of finite rank which converge in norm to H.
Solution: Proof of [67, Thm. 6.5].

(f) A bounded operator H is compact if, and only if, H^*H is compact.
Solution: Proof of [67, Thm. 6.4].

(g) *Show that $\sigma(H)\setminus\{0\} = \sigma_{\mathrm{disc}}(H)\setminus\{0\}$ for any compact operator H in $\mathcal{H}$. Moreover, $0 \in \sigma_{\mathrm{ess}}(H)$ whenever $\mathcal{H}$ is infinite-dimensional.
Solution: Proof of [67, Thm. 6.7].

8. Study the case of **Neumann boundary conditions** (6). More specifically, consider the boundary-value problem

$$\begin{cases} -\Delta\psi = \lambda\psi & \text{in} \quad \Omega\,, \\ \dfrac{\partial\psi}{\partial n} = 0 & \text{on} \quad \partial\Omega\,, \end{cases} \tag{B.1}$$

where n denotes the outward unit normal vector field of $\partial\Omega$.

(a) Find the eigenvalues and eigenfunctions if $\Omega := (-a, a)$ is a segment of half-width $a > 0$.
Hint: Follow the approach of Section 3.2 in the Dirichlet case.
Solution: See Remark 3.6.

(b) Find the eigenvalues and eigenfunctions if $\Omega := \mathcal{R}_{a_1,\dots,a_d}$ is a rectangular parallelepiped of half-sides $a_1, \dots, a_d > 0$.
Hint: Separation if variables.
Solution: See Remark 3.6.

(c) Find a counterexample to the monotonicity of Neumann eigenvalues, *i.e.*, find domains $\Omega_1 \subset \Omega_2$ such that $\lambda_k^N(\Omega_1) < \lambda_k^N(\Omega_2)$ for some $k \in \mathbb{N}^*$.
Hint: Consider rectangles.
Solution: See Figure 3.4.

9. Study the case of **combined boundary conditions**. More specifically, consider the boundary-value problem

$$\begin{cases} -\psi'' = \lambda\psi & \text{in} \quad (-a, a)\,, \\ \psi(-a) = 0\,, \\ \psi'(a) = 0\,. \end{cases} \tag{B.2}$$

Find the eigenvalues and eigenfunctions.
Hint: Follow the approach of Section 3.2 in the Dirichlet case.
Solution: See Remark 3.7.

10. Show that the numbers $\tilde{\lambda}_k$ defined by the right-hand side of (3.11) (minimax principle) are greater than or equal to the eigenvalues λ_k also for $k \geq 2$. (In the lecture just $k = 1$.)
    Solution: The last part of the proof of Theorem 3.11.

11. Think about **converse isoperimetric optimisation problems**.

    (a) Why do not we consider min instead of max in the isoperimetric inequality (3.40)?
    Hint: Consider thin rectangles.

    (b) Why do not we consider max instead of min in the isochoric inequality (3.42)?
    Hint: Consider thin and long rectangles.

    (c) Why do not we consider max instead of min in the spectral isochoric inequality (3.45)?
    Hint: Consider thin and long rectangles.

    (d) Why do not we consider max instead of min in the spectral isochoric inequality (3.46)?
    Hint: Consider thin rectangles.

12. Study the **symmetric rearrangement** introduced in Lemma 3.38.

    (a) Given $f(x) := \begin{cases} x+1 & \text{if} \quad x \in [-1,0)\,, \\ 1 - \dfrac{x}{2} & \text{if} \quad x \in [0,2)\,, \\ 0 & \text{otherwise}\,, \end{cases}$ how does f^* look?

    (b) Compute $\|f\|$ and $\|f^*\|$, where $\|\cdot\|$ is the norm of $L^2(\mathbb{R})$.

    (c) Compute $\|f'\|$ and $\|f^{*\prime}\|$.

13. Show that the space $L^2_0(\Omega_0)$ defined in (4.9) is dense in $L^2(\Omega_0)$, where Ω_0 is the straight tube (4.6).
    Hint: Given any $\psi \in L^2(\Omega_0)$, use the approximation $\psi_R := \chi_{[-R,R]}\psi$ with $R > 0$.

14. Prove Proposition 4.11.
    Hint: Use $\psi(x,y) = \varphi_n(x)\mathcal{J}_1(y)$ as the test function in the variational characterisation (4.3) of the lowest point in the spectrum of $-\Delta_D^{\Omega_0} - \rho$, where φ_n is the function from the proof of Theorem 4.8 and $\mathcal{J}_1$ is defined in (4.18).