Geometrical aspects of spectral theory

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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.

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?

In [14], I. M. Glazman introduced the following useful classification (see also [10, 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 $\mathbb{R}^2$.

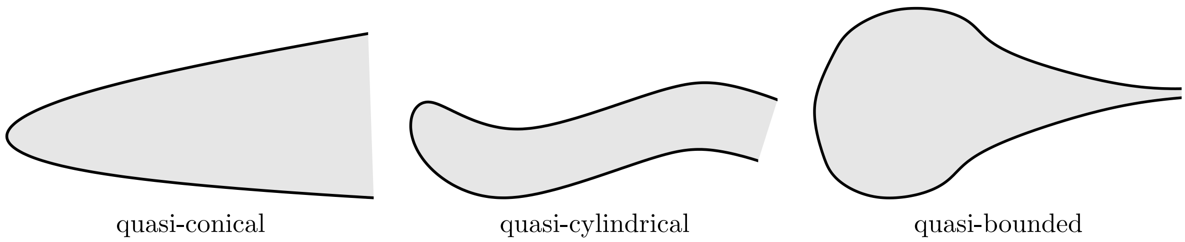


Figure 1: Examples of planar domains as regards the Glazman classification.

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. The plan of our lecture is as follows:

Day 1: Quasi-conical domains or Stability of matter;

Day 2: Quasi-bounded domains or Vibrational systems (or Quantum resonators);

Day 3: Quasi-conical domains or Quantum waveguides.

Before implementing the plan, let us start with rather technical preliminaries.

0.5 The Dirichlet Laplacian

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 precise what an operator is. An operator acts on a space, so we first need to precise what kind of spaces we are interested in.

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*. In summary, we shall always assume:

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

The norm of $\mathcal{H}$ associated with the inner product $(\cdot,\cdot)$ will be denoted by $\|\psi\| := \sqrt{(\psi,\psi)}$.

Example 0.1 (Euclidean space)**.** $\mathbb{C}^n$ with $n \in \mathbb{N}$ is a canonical example of a finite-dimensional complex Hilbert space, with $\dim \mathbb{C}^n = n$. We understand it as equipped with the standard Euclidean scalar product

$$(u,v) := \sum_{j=1}^{n} \overline{u_j} v_j \,, \qquad \text{where} \qquad u = \begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix}, \quad v = \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}.$$

In quantum mechanics, $\mathbb{C}^2$ is the Hilbert space for describing a charged particle of spin $\frac{1}{2}$ at rest interacting with a magnetic field. ◇

Example 0.2 (Lebesgue space)**.** Given any domain $\Omega \subset \mathbb{R}^d$ with $d \geq 1$, 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

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

Here "measurable" refers to the Lebesgue measure in $\mathbb{R}^d$. Following Schechter [24, 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 $L^2(\Omega)$. One has $\dim L^2(\Omega) = \infty$.

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

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.

Example 0.3 (Matrices)**.** Given a matrix $A \in \mathbb{C}^{n\times n}$, the map

$$T_A u := Au \,, \qquad u \in \operatorname{dom} T_A := \mathbb{C}^n \,,$$

where the action is understood in the sense of matrix multiplication, is a linear operator in $\mathbb{C}^n$.

In quantum mechanics, the matrix $\left(\begin{smallmatrix} -1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$ represents the Hamiltonian of a charged particle of spin $\frac{1}{2}$ at rest interacting with a uniform magnetic field. ◇

Example 0.4 (Multiplication operator)**.** Given a domain $\Omega \subset \mathbb{R}^d$, let $V : \Omega \to \mathbb{R}$ be a measurable function. The map

$$\hat{V}\psi := V\psi \,, \qquad \psi \in \operatorname{dom} \hat{V} := \{\psi \in L^2(\Omega) : \ V\psi \in L^2(\Omega)\}$$

is a linear operator in $L^2(\Omega)$. If V is bounded (more generally, $V \in L^\infty(\Omega)$), then $\operatorname{dom} \hat{V} = L^2(\Omega)$. If the function V is unbounded, however, then $\operatorname{dom} \hat{V}$ is necessarily a proper subset of $L^2(\Omega)$.

In quantum mechanics, $\hat{V}$ represents the potential energy of an electron constrained to a nanostructure of shape Ω. ◇

Let $\Omega \subset \mathbb{R}^d$ be a domain. 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

$$\dot{H} := -\Delta\psi\,, \qquad \operatorname{dom}\dot{H} := C_0^2(\Omega) \equiv \{\psi \in C^2(\Omega) : \ \operatorname{supp}\psi \text{ is compact in } \Omega\}\,.$$

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 $\partial\Omega$. It is clear that this choice of the domain 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?

The correct choice of the domain is a delicate matter, which requires the knowledge of rather advanced techniques. The most effective way is to start with the sesquilinear form $\dot{h}$ associated with the operator $\dot{H}$, namely,

$$\dot{h}(\phi,\psi) := (\phi, \dot{H}\psi)\,, \qquad \operatorname{dom}\dot{h} := \operatorname{dom}\dot{H}\,.$$

Integrating by parts, we easily get

$$\dot{h}(\phi,\psi) = (\nabla\phi, \nabla\psi)\,,$$

so the form is well defined even in the larger space $C_0^1(\Omega)$, while still keeping the Dirichlet boundary conditions in the very restrictive sense. To make the domain as large as possible, we introduce the *closed* form

$$h(\phi,\psi) := (\nabla\phi, \nabla\psi)\,, \qquad \operatorname{dom} h := W_0^{1,2}(\Omega) \equiv \overline{C_0^2(\Omega)}^{|\!|\!|\cdot|\!|\!|}\,, \qquad |\!|\!|\psi|\!|\!| := \sqrt{\|\nabla\psi\|^2 + \|\psi\|^2}\,.$$

Here the line denotes the completion of the space of smooth functions with respect to the triple norm $|\!|\!|\cdot|\!|\!|$ (the double norm $\|\cdot\|$ denotes the norm of $L^2(\Omega)$ as above) and the action of the gradient should be interpreted in a distributional sense (*i.e.*, motivated by an integration by parts, $\nabla\psi$ equals a function $g \in L^2(\Omega)^d$ such that $\int_\Omega g \cdot \varphi = -\int_\Omega \psi \operatorname{div}\varphi$ for every $\varphi \in C_0^1(\Omega)^d$). The domain $W_0^{1,2}(\Omega)$ is a *Sobolev space*.

Using an analogue of the Riesz representation theorem in finite-dimensional spaces (*cf* [16, Thm. VI.2.1]), there exists an operator H associated with the form, *i.e.*,

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

It is easy to see that

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

where $-\Delta\psi$ should be interpreted as the distributional Laplacian of ψ (*i.e.*, motivated by an integration by parts, $-\Delta\psi$ equals a function $g \in L^2(\Omega)$ such that $(\varphi, g) = (-\Delta\varphi, \psi)$ for every $\varphi \in C_0^2(\Omega)$). 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* domain (without any requirement on the regularity of the boundary; for example, Ω can have a fractal boundary!).

Definition 0.2. For every open set $\Omega \subset \mathbb{R}^d$, the *Dirichlet Laplacian* is the operator in $L^2(\Omega)$ defined by

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

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 $\partial\Omega \in C^2$ is a nice domain), then

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

Here

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

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. At the same time,

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

if Ω is a nice domain. As expected,

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

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.

0.6 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 an eigenvalue problem.

Definition 0.3. 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 0.3, 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

$$\dim\ker(H - \lambda I) + \dim\operatorname{ran}(H - \lambda I) = \dim\mathcal{H} \, , \tag{8}$$

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 1).

If $\lambda \notin \sigma_p(H)$, 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 0.4. Let H be an operator in a Hilbert space $\mathcal{H}$. The *continuous spectrum* of H is defined by:

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

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

Proposition 0.1. *Let H be an operator in a Hilbert space $\mathcal{H}$. Let $\lambda \notin \sigma_p(H)$. Then*

$$\lambda \in \sigma_c(H) \quad \Longleftrightarrow \quad (H-\lambda I)^{-1} \text{ is unbounded.}$$

Proof. 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 $\lambda \in \sigma_c(H)$, 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 eigenfunction of H corresponding to λ; hence $(H-\lambda I)^{-1}$ is unbounded. 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 $\lambda \in \sigma_c(H)$ by Definition 0.4. □

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

$$\sigma(H) := \sigma_p(H) \cup \sigma_c(H).$$

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 0.2. *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 eigenfunction 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. $\square$

The reader is warned that our Definition 0.5 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.

0.7 Self-adjointness

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 is defined by means of the duality introduced via the inner product

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

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

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

This operator is well (*i.e.* uniquely) defined provided that H is densely defined (*i.e.*, $\operatorname{dom} H$ is a dense subspace of $\mathcal{H}$).

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

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

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.

Example 0.5. The operator T_A of Example 0.3 is self-adjoint if, and only if, the generating matrix A is Hermitian, *i.e.* $A = A^* := \overline{A}^T$. $\diamondsuit$

Example 0.6. The multiplication operator $\hat{V}$ of Example 0.4 is self-adjoint if, and only if, the generating matrix V is real-valued. $\diamondsuit$

Example 0.7. The Dirichlet Laplacian $-\Delta_D^\Omega = H$ of Section 0.5 is self-adjoint for any domain Ω. This follows immediately from the representation theorem [16, Thm. VI.2.1] that we used to define the operator. Notice that the associated form h is symmetric, *i.e.* $h(\phi,\psi) = \overline{h(\psi,\phi)}$ for every $\phi, \psi \in \operatorname{dom} h$. In light terms, the property of $-\Delta_D^\Omega$ being symmetric can be deduced (at least for nice domains) by an integration by parts, using that the boundary terms vanish due to the Dirichlet boundary conditions.

The operator $\dot{H}$ is symmetric (here one can use the integration by parts for any domain), but it is not self-adjoint. In fact, the domain of the adjoint operator $\operatorname{dom} \dot{H}^*$ is much larger than $\operatorname{dom} \dot{H}$. This demonstrates that the self-adjointness is really a delicate matter. $\diamondsuit$

In quantum mechanics, physical observables are represented by self-adjoint operators and their spectrum correspond to outcomes of measuring. A deep reason for self-adjointness is that generators of conservative evolutions associated with the Schrödinger equation (more specifically, of unitary groups) are necessarily self-adjoint operators. In light terms, we can understand this choice due to the fact that the spectrum of self-adjoint operators is necessarily real (which should be the case of physical quantities we measure).

Proposition 0.3. *Let H be a self-adjoint operator in a Hilbert space $\mathcal{H}$. Then*

$$\sigma(H) \subset \mathbb{R}\,.$$

Proof. Let $\lambda \in \sigma(H)$. By Proposition 0.2, there exists a sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset \operatorname{dom} H$ such that $\|\psi_n\| = 1$ for every $n \in \mathbb{N}$ and $H\psi_n - \lambda\psi_n \to 0$ as $n \to \infty$. Hence

$$\begin{aligned}
\lambda &= \lambda\,\|\psi_n\|^2 \\
&= \lim_{n\to\infty} \lambda\,\|\psi_n\|^2 \\
&= \lim_{n\to\infty} (\psi_n, \lambda\psi_n) \\
&= \lim_{n\to\infty} (\psi_n, H\psi_n) \\
&= \lim_{n\to\infty} (H\psi_n, \psi_n) \\
&= \lim_{n\to\infty} (\lambda\psi_n, \psi_n) \\
&= \lim_{n\to\infty} \overline{\lambda}\,\|\psi_n\|^2 \\
&= \overline{\lambda}\,\|\psi_n\|^2 \\
&= \overline{\lambda}\,.
\end{aligned}$$

It follows that the imaginary part of λ equals zero. ◻

Chapter 1

Quasi-conical domains

In this lecture we are concerned with spectral properties of the Dirichlet Laplacian $-\Delta_D^\Omega$ in the situation where Ω is a quasi-conical domain. Recall that Ω is called quasi-conical if it contains an arbitrarily large ball. 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).

1.1 Location of the spectrum

Since Ω is quasi-conical, 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.

1.1.1 The spectrum is non-negative

Let $\lambda \in \sigma(H)$. By our definition of the spectrum (*cf* Proposition 0.2), there exists a sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset \operatorname{dom}(-\Delta_D^\Omega)$ such that $\|\psi_n\| = 1$ for every $n \in \mathbb{N}$ and $-\Delta_D^\Omega\psi_n - \lambda\psi_n \to 0$ as $n \to \infty$. Similarly as in the proof of Proposition 0.3, we have

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

Here the last but one equality follows by the definition of the distributional Laplacian. For nice domains, it can be also understood as a consequence of an integration by parts (or, more specifically, of the divergence theorem):

$$
\begin{aligned}
(\psi_n, -\Delta\psi_n) &= -\int_\Omega \overline{\psi}_n \, \Delta\psi_n \\
&= -\int_\Omega \left\{ \nabla \cdot \left(\overline{\psi}_n \, \nabla\psi_n\right) - |\nabla\psi_n|^2 \right\} \\
&= -\int_{\partial\Omega} \overline{\psi}_n \, \frac{\partial\psi_n}{\partial n} + \int_\Omega |\nabla\psi_n|^2 \\
&= \int_\Omega |\nabla\psi_n|^2 \\
&= \|\nabla\psi_n\|^2 \,,
\end{aligned}
$$

where n denotes the outward unit normal of $\partial\Omega$. Hence, λ is not only real, 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 domain Ω.

Proposition 1.1. *Let $\Omega \subset \mathbb{R}^d$ be any domain. Then*

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

1.1.2 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

$$
-\Delta\psi = \lambda\psi \quad \text{in} \quad \Omega \tag{1.1}
$$

such that $\psi \in W_0^{1,2}(\Omega)$ and $\Delta\psi \in L^2(\Omega)$. The differential equation (1.1) admits a classical solution

$$
w_k(x) := e^{ik\cdot x} \qquad \text{with any} \quad k \in \mathbb{C}^d \quad \text{such that} \quad k^2 := k \cdot k = \lambda \,, \tag{1.2}
$$

where the dot denotes the scalar product in $\mathbb{R}^d$ (notice that $k^2 \neq |k|^2$ unless $k \in \mathbb{R}^d$). This suggests that $\sigma_{\mathrm{p}}(-\Delta_D^\Omega) = \mathbb{C}$, in contradiction with the self-adjointness of $-\Delta_D^\Omega$ (and, in particular, with Proposition 1.1). What is wrong?

Of course, the solutions (1.2) 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 (1.2). Anyway, we can use these classical solutions to construct approximate eigenvalues.

1.1.3 Construction of approximate eigenfunctions

The key observation is that the classical solutions (1.2) are *bounded* for $k \in \mathbb{R}^d$ (plane waves), so that an approximation of these plane-wave solutions by a sequence playing the role of the approximate eigenfunction of Definition 0.4 is possible.

Let φ be a function from $C_0^2(\mathbb{R}^d)$, 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

$$
\|\varphi_n\|_{L^2(\mathbb{R}^d)}^2 = |N_n|^2 \int_{\mathbb{R}^d} \left|\varphi\!\left(\frac{x - a_n}{n}\right)\right|^2 \mathrm{d}x = \int_{\mathbb{R}^d} |\varphi(y)|^2 \, \mathrm{d}y = \|\varphi\|_{L^2(\mathbb{R}^d)}^2 = 1 \,. \tag{1.3}
$$

With respect to the support of φ, the support of φ_n is translated by the vector a_n and scaled by n:

$$\operatorname{supp}\varphi_n = a_n + n \operatorname{supp}\varphi\,. \tag{1.4}$$

By the property of the domain Ω being quasi-conical, for each $n \in \mathbb{N}^*$ there exists $j_n \in \mathbb{N}^*$ such that $\operatorname{supp}\varphi_n \subset B_{j_n} \subset \Omega$ with the choice $a_n := x_{j_n}$. Hence, $\varphi_n \in \operatorname{dom}(-\Delta_D^\Omega)$. For any $n \in \mathbb{N}^*$, we define

$$\psi_n(x) := \varphi_n(x)\, e^{ik\cdot x}\,, \tag{1.5}$$

which also belongs to $\operatorname{dom}(-\Delta_D^\Omega)$. By (1.3), $\|\psi_n\| = 1$ for every $n \in \mathbb{N}^*$.

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 $\psi_n \in C_0^2(\Omega)$, the action of $-\Delta_D^\Omega$ is that of the classical Laplacian. We compute

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

Consequently,

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

and therefore

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

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

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

1.2 The whole Euclidean space

According to Theorem 1.1, 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.

1.2.1 Subcriticality of high dimensions

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

Theorem 1.2 (Hardy inequality)**.** *Let $d \ge 3$. Then*

$$\forall\psi \in W^{1,2}(\mathbb{R}^d)\,, \qquad \int_{\mathbb{R}^d} |\nabla\psi(x)|^2\,\mathrm{d}x \ge \frac{(d-2)^2}{4}\int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|^2}\,\mathrm{d}x\,. \tag{1.6}$$

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

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

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

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

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

Where did we use the requirement $d \geq 3$ in the proof? The inequality (1.6) is trivial if $d = 2$, 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 $\psi \in C_0^1(\mathbb{R}^d \setminus \{0\})$. This is enough because such functions form a dense set in $W^{1,2}(\mathbb{R}^d)$, namely (*cf* [10, Corol. VIII.6.4])

$$W^{1,2}(\mathbb{R}^d) = W_0^{1,2}(\mathbb{R}^d \setminus \{0\}) \qquad \Longleftrightarrow \qquad d \geq 2 \,. \tag{1.7}$$

However, if $d = 1$, it is not true that any function $\psi \in W^{1,2}(\mathbb{R})$ can be approximated by a sequence of smooth functions of compact support which does not intersect the origin (find a counterexample!). Physically, the dimensional difference expresses the fact that it is only in dimension one where the point is able to bear an electric charge. □

The Hardy inequality (1.6) is related to spectral properties of the Dirichlet Laplacian in the following way. The left-hand side of (1.6) is just the quadratic form of the Dirichlet 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 (1.6) is the quadratic form of the operator of multiplication by the function

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

Hence, we can write

$$-\Delta_D^{\mathbb{R}^d} \geq \rho \tag{1.8}$$

in the sense of quadratic forms in $L^2(\mathbb{R}^d)$. By Theorem 1.1, the spectrum of $-\Delta_D^\Omega$ starts by zero, so it is impossible that (1.8) holds with ρ being replaced by a positive constant. Anyway, if $d \geq 3$, inequality (1.8) 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 $d \geq 3$.

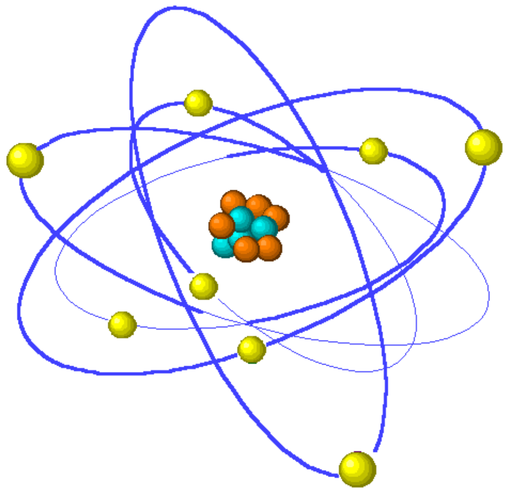
Any self-adjoint operator H in $L^2(\Omega)$ satisfying the inequality $H \geq \rho$ in the sense of quadratic forms in $L^2(\Omega)$ with a positive function ρ is called *subcritical.* If the spectrum of H starts by zero but it does not satisfy the inequality with any positive function ρ, the operator is called *critical.* Hence, the Dirichlet Laplacian $-\Delta_D^{\mathbb{R}^d}$ is subcritical if $d \geq 3$.

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

1.2.2 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 1.1. 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!)



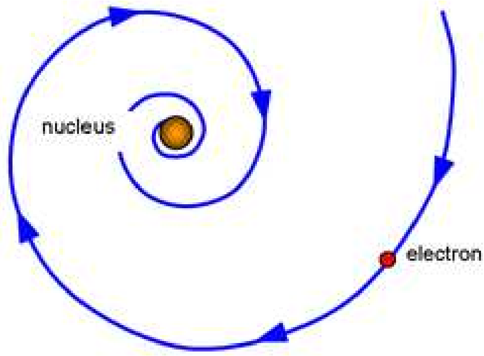


Figure 1.1: Rutherford's planetary model of the atom and its collapse due to classical physics.

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

$$H(x,p) := \frac{|p|^2}{2m} - \frac{e^2}{|x|} \tag{1.9}$$

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.*,

$$\inf_{(x,p)\in\mathbb{R}^3\times\mathbb{R}^3} H(x,p) = -\infty\,, \tag{1.10}$$

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 hydrogen atom is 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 (1.10) 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 (1.6) 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

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

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.*, [15, Sec. 4.2]).

1.2.3 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 (1.8) with a positive function ρ is admissible.

Theorem 1.3. *Let $d = 1, 2$. For any positive function $\rho \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$, one has*

$$\inf_{\substack{\psi \in C_0^1(\mathbb{R}^d) \\ \psi \neq 0}} \left(\int_{\mathbb{R}^d} |\nabla\psi(x)|^2 \, \mathrm{d}x - \int_{\mathbb{R}^d} \rho(x) \, |\psi(x)|^2 \, \mathrm{d}x \right) < 0 \,. \tag{1.11}$$

Before proving the theorem, let us first comment on why the result (1.11) contradicts the validity of the Hardy inequality (1.8). 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

$$Q[\psi] := \int_{\mathbb{R}^d} |\nabla\psi(x)|^2 \, \mathrm{d}x - \int_{\mathbb{R}^d} \rho(x) \, |\psi(x)|^2 \, \mathrm{d}x \tag{1.12}$$

is non-negative. Since $C_0^1(\mathbb{R}^d) \subset W^{1,2}(\mathbb{R}^d)$, it follows that $Q[\psi] \geq 0$ for every $\psi \in C_0^1(\mathbb{R}^d)$. But this is an obvious contradiction with (1.11). So, indeed, no Hardy inequality (1.8) is available in dimensions $d = 1, 2$.

Proof. Clearly, to establish (1.11), it is enough to find a (so-called "test" or "trial") function $\psi \in C_0^1(\mathbb{R}^d)$ 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

$$Q[1] = -\int_{\mathbb{R}^d} \rho(x) \, \mathrm{d}x < 0 \,. \qquad \text{(formally!)} \tag{1.13}$$

Hence, the idea is to use a trial function which approximates 1, but it is still an admissible element of $C_0^1(\mathbb{R}^d)$. We thus look for a sequence $\{\psi_n\}_{n=1}^\infty \subset C_0^1(\mathbb{R}^d)$ 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 $d = 1, 2$.

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

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

Notice that $\psi_n = 1$ on $[-n, n]$ and $\psi_n = 0$ on $[-2n, 2n]$, 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 (1.12) 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 (1.13) 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.

If $d = 2$, we have to use a more refined approximation of 1. We start by picking a function $\eta \in C^1([0,1])$ 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 $n \in \mathbb{N}$, we then define

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

Again $\psi_n \in C_0^1(\mathbb{R}^2)$ for every $n \in \mathbb{N}^*$ and $\psi_n \to 0$ 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 (1.12) again vanishes as $n \to \infty$. The rest of the proof is the same as in the one-dimensional case. $\square$

Let us summarise the dimensional features of the Euclidean space $\mathbb{R}^d$. Due to Theorem 1.1, 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 1.2 and 1.3 can be schematically summarise into the following equivalence:

$$-\Delta_D^{\mathbb{R}^d} \text{ satisfies a Hardy inequality} \qquad \Longleftrightarrow \qquad d \geq 3. \tag{1.14}$$

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 (1.14) through the stability of matter: $\mathbb{R}^3$ is the lowest dimensional Euclidean space for which the atoms and molecules are quantum-mechanically stable.

Chapter 2

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

$$\text{unbounded } \Omega \text{ is quasi-bounded} \qquad \Longleftrightarrow \qquad \lim_{\substack{|x|\to\infty \\ x\in\Omega}} \operatorname{dist}(x,\partial\Omega) = 0\,. \tag{2.1}$$

Figure 2.1 represents a highly irregular unbounded quasi-bounded domain (with empty exterior).

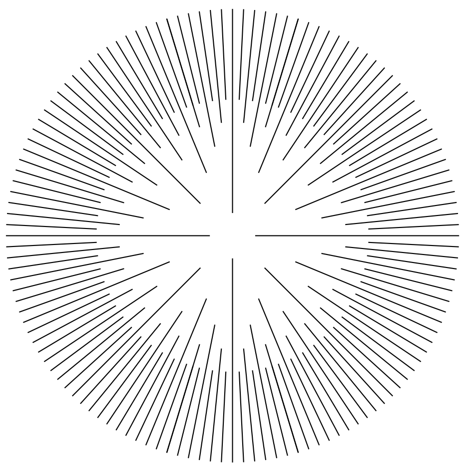


Figure 2.1: *Spiny urchin* as an example of a highly irregular unbounded quasi-bounded domain:
$$\Omega := \mathbb{R}^2 \setminus \bigcup_{k=1}^{\infty} \Big\{ (r\cos\vartheta, r\sin\vartheta) : \quad r \geq k \quad \wedge \quad \vartheta = n\pi/2^k \quad \text{for} \quad n = 1,2,\dots,2^{k+1} \Big\}$$

Recall that the spectrum of the Dirichlet Laplacian $-\Delta_D^\Omega$ is non-negative for any domain $\Omega \subset \mathbb{R}^d$ (*cf* Proposition 1.1). For quasi-conical domains, we have seen that the whole interval $[0,\infty)$ constitutes the spectrum (*cf* Theorem 1.1). 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 lecture we shall 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.

2.1 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 0.6, 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 2.1. Let H be an operator in a Hilbert space $\mathcal{H}$. The *essential spectrum* of H is defined by:

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

The *discrete spectrum* is the rest:

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

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

By definition,

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

and the union is again disjoint.

Notice that contrary to Proposition 0.2, 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 is 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 the 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 $\{\psi_n\}_{n\in\mathbb{N}} \subset \operatorname{dom} H$,

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

Here the logical connective between the vertical statements is *and* (logical conjuction). Self-adjoint operators are closed. (So, in particular, the Dirichlet Laplacian $-\Delta_D^\Omega$ is closed for any domain Ω, *cf* Example 0.7.) For closed operators, we have the following inclusion for the discrete spectrum.

Proposition 2.1. *If H is a closed operator, then*

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

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. $\square$

For self-adjoint operators, we have the complete characterisation

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

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 2.2). 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.

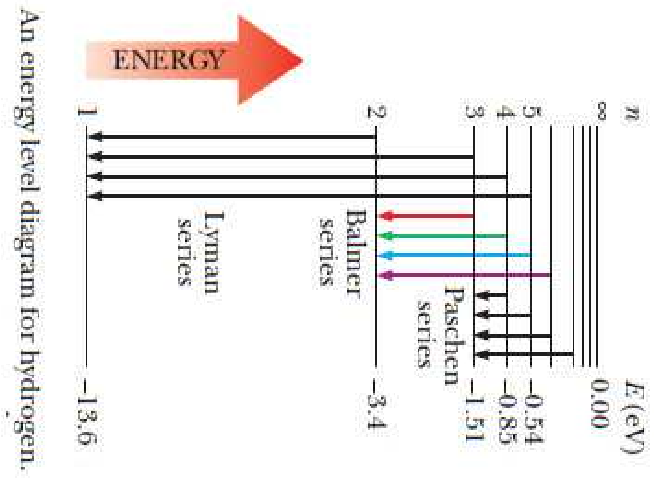


Figure 2.2: Schematic picture of discrete energy levels and the ionisation energy (corresponding the level 0 in the picture) for the hydrogen atom.

If the essential (respectively, discrete) spectrum is empty, we say that the spectrum is *purely discrete* (respectively, *purely essential*). Due to Theorem 1.1, 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 2.2. *For any operator H in a Hilbert space $\mathcal{H}$, one has:*

$$\sigma_{\mathrm{ess}}(H) = \left\{\lambda \in \mathbb{C} : \ \exists \underset{\|\psi_n\|=1}{\{\psi_n\}_{n\in\mathbb{N}}} \subset \operatorname{dom} H, \quad \psi_n \xrightarrow[n\to\infty]{w} 0 \quad \wedge \quad \|H\psi_n - \lambda\psi_n\| \xrightarrow[n\to\infty]{} 0\right\}. \tag{2.2}$$

Proof. 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 $\psi \in \mathcal{H}$. 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 $j \to \infty$.

Conversely, if a sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset \operatorname{dom} H$ satisfies the requirements on the right-hand side of (2.2), 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 $\lambda \in \sigma_{\mathrm{ess}}(H)$. □

2.2 Rectangular parallelepipeds

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

$$\mathcal{R}_{a_1,\dots,a_d} := (a_1, a_1) \times \cdots \times (a_d, a_d) \tag{2.3}$$

denote a *rectangular parallelepiped* 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

$$\begin{cases} -\psi'' = \lambda\psi & \text{in} \quad (-a,a)\,, \\ \quad \psi = 0 & \text{at} \quad \pm\, a\,. \end{cases} \tag{2.4}$$

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* [1, 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.*, [11, Thm. 6.3.6]), any solution of (2.4) belongs to $C^\infty([-a,a])$, so we are actually dealing with a classical boundary-value problem.

Since $-\Delta_D^{(-a,a)}$ is a non-negative operator (*cf* Proposition 1.1), we know that $\lambda \geq 0$. Solving the differential equations of (2.4) in terms of sines and cosines if $\lambda > 0$ (or linear functions if $\lambda = 0$) and subjecting the general solution to the boundary conditions at $\pm a$, we arrive at the equation

$$\sin\left(2\sqrt{\lambda}\, a\right) = 0 \tag{2.5}$$

that the eigenvalues $\lambda > 0$ must satisfy, while $\lambda = 0$ leads just to a trivial solution of (2.4). Consequently,

$$\sigma_{\mathrm{p}}\big(-\Delta_D^{(-a,a)}\big) = \left\{ \left(\frac{k\pi}{2a}\right)^2 \right\}_{k=1}^{\infty} . \tag{2.6}$$

The eigenfunctions corresponding to eigenvalues of $-\Delta_D^{(-a,a)}$, ordered as in (2.6), are given by

$$\psi_k^D(x) := \begin{cases} \sqrt{\dfrac{1}{a}}\, \cos\left(\dfrac{k\pi}{2a}x\right) & \text{if} \quad k \text{ is odd}\,, \\[2ex] \sqrt{\dfrac{1}{a}}\, \sin\left(\dfrac{k\pi}{2a}x\right) & \text{if} \quad k \text{ is even}\,. \end{cases} \tag{2.7}$$

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 parallelepiped 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

$$\sigma_{\mathrm{p}}\big(-\Delta_D^{\mathcal{R}_{a_1,\dots,a_d}}\big)=\left\{\left(\frac{k_1\pi}{2a_1}\right)^2+\dots+\left(\frac{k_d\pi}{2a_d}\right)^2\right\}_{k_1,\dots,k_d=1}^{\infty}\,. \tag{2.8}$$

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,

$$\forall\psi\in L^2(\mathcal{R}_{a_1,\dots,a_d})\,,\qquad \psi=\sum_{k_1,\dots,k_d=1}^{\infty}c_{k_1,\dots,k_d}\,\psi_{k_1,\dots,k_d}^D \qquad\text{with}\qquad c_{k_1,\dots,k_d}:=(\psi_{k_1,\dots,k_d}^D,\psi)\,. \tag{2.9}$$

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). 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. The corresponding set of eigenfunctions will be denoted by $\{\psi_k^D\}_{k\in\mathbb{N}^*}$.

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

Proposition 2.3. $\sigma_{\mathrm{ess}}\big(-\Delta_D^{\mathcal{R}_{a_1,\dots,a_d}}\big)=\varnothing\,.$

Proof. 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 2.2, 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 (2.9), 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

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

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 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. 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, 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 parallelepiped $\mathcal{R}_{a_1,\dots,a_d}$, 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 $\{T\psi_{n_j}\}_{j\in\mathbb{N}}$ 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 6e)

Proposition 2.4. *The resolvent* $\big(-\Delta_D^{\mathcal{R}_{a_1,\dots,a_d}} + I\big)^{-1}$ *is a compact operator.*

Proof. The argument mimicks the proof of [9, Lem. 4.4.1]. For every $N \in \mathbb{N}^*$, define the finite-rank operators H_N by

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

From the formula

$$\big(-\Delta_D^{\mathcal{R}_{a_1,\dots,a_d}}+I\big)^{-1}-H_k=\sum_{k=N+1}^{\infty}(\lambda_k+1)^{-1}\psi_k^D(\psi_k^D,\cdot)$$

and the Bessel inequality, we deduce that, for every $\psi\in L^2(\mathcal{R}_{a_1,\dots,a_d})$,

$$\big\|\big[\big(-\Delta_D^{\mathcal{R}_{a_1,\dots,a_d}}+I\big)^{-1}-H_k\big]\psi\big\|\leq(\lambda_N+1)^{-1}\|\psi\|^2\,.$$

Since $\lambda_N\to\infty$ as $N\to\infty$, we see that H_N converges in norm to $\big(-\Delta_D^{\mathcal{R}_{a_1,\dots,a_d}}+I\big)^{-1}$ as $N\to\infty$. □

By standard argumenrts (see Exercise 6f), it follows that also the square root $\big(-\Delta_D^{\mathcal{R}_{a_1,\dots,a_d}}+I\big)^{-1/2}$ is a compact operator.

Remark 2.1 (Neumann boundary conditions)**.** The spectral problem for the Laplacian in the rectangular parallelepiped $\mathcal{R}_{a_1,\dots,a_d}$, subject to *Neumann* boundary conditions, can be solved in the same way. In the one-dimensional case, one finds

$$\sigma_{\mathrm{p}}\big(-\Delta_N^{(-a,a)}\big)=\left\{\left(\frac{k\pi}{2a}\right)^2\right\}_{k=0}^{\infty}, \tag{2.10}$$

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

$$\psi_k^N(x):=\begin{cases}\sqrt{\dfrac{1}{2a}} & \text{if}\quad k=0\,,\\ \sqrt{\dfrac{1}{a}}\,\cos\left(\dfrac{k\pi}{2a}x\right) & \text{if}\quad k\geq 1 \text{ is even}\,,\\ \sqrt{\dfrac{1}{a}}\,\sin\left(\dfrac{k\pi}{2a}x\right) & \text{if}\quad k\geq 1 \text{ is odd}\,.\end{cases} \tag{2.11}$$

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 (2.10) 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 parallelepiped 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 2.2 (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

$$\sigma_{\mathrm{p}}\big(-\Delta_{DN}^{(-a,a)}\big)=\left\{\left(\frac{(2k-1)\pi}{4a}\right)^2\right\}_{k=1}^{\infty}. \tag{2.12}$$

The corresponding eigenfunctions are given by

$$\psi_k^{DN}(x) := \sqrt{\frac{1}{a}}\,\sin\left(\frac{(2k-1)\pi}{4a}\,x\right) \tag{2.13}$$

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 (2.12) with (2.10) that the clarinet tones are lower than the tones of the flute (if the zero mode is not counted).

2.3 Bounded domains

The main message of this lecture 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, assuming, by contradiction, that $\lambda \in \sigma_{\mathrm{ess}}(-\Delta_D^\Omega)$, where Ω is a bounded domain contained in a large cube Q_a, 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:

$$\tilde\psi_n(x) := \begin{cases} \psi_n(x) & \text{if} \quad x \in \Omega\,, \\ 0 & \text{if} \quad x \notin \Omega\,, \end{cases} \tag{2.14}$$

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 2.1. *Let $\Omega \subset \mathbb{R}^d$ be any bounded domain. Then $\sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = \varnothing$.*

Proof. By contradiction, let us assume that there exists $\lambda \in \sigma_{\mathrm{ess}}(-\Delta_D^\Omega)$. Then there exists a singular sequence $\{\psi_n\}_{n\in\mathbb{N}} \subset \mathrm{dom}(-\Delta_D^\Omega) \subset W_0^{1,2}(\Omega)$ 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 $|(\psi_n, -\Delta_D^\Omega\psi_n - \lambda\psi_n)_{L^2(\Omega)}| \le \|\psi_n\|_{L^2(\Omega)}\| - \Delta_D^\Omega\psi_n - \lambda\psi_n\|_{L^2(\Omega)}$ by the Schwarz inequality). Consequently,

$$\|\nabla\psi_n\|^2 \xrightarrow[n\to\infty]{} \lambda\,. \tag{2.15}$$

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 (2.14). 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 2.4) and compact operators maps weakly converging sequences to strongly converging sequences (see Exercise 6a) 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 (2.15), 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. □

Remark 2.3 (Neumann boundary conditions)**.** As in the Dirichlet case, it is also true that the spectrum of the Neumann Laplacian in any rectangular parallelepiped $\mathcal{R}_{a_1,\dots,a_d}$ is purely discrete. However, this is no longer true for the Neumann Laplacian in an *arbitrary* domain Ω, see Figure 2.3. This defect is intimately related to the absence of the extension property for functions from the Sobolev space $W^{1,2}(\Omega)$, which is the form domain of the Neumann Laplacian. A certain regularity of the boundary $\partial\Omega$ is needed in order to ensure that the essential spectrum of the Neumann Laplacian in a bounded domain Ω is empty.

2.4 The spectral theorem

Our given proof of the discreteness of the spectrum of the Dirichlet Laplacian in 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 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 2.2 (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) in general (for then you have the 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.

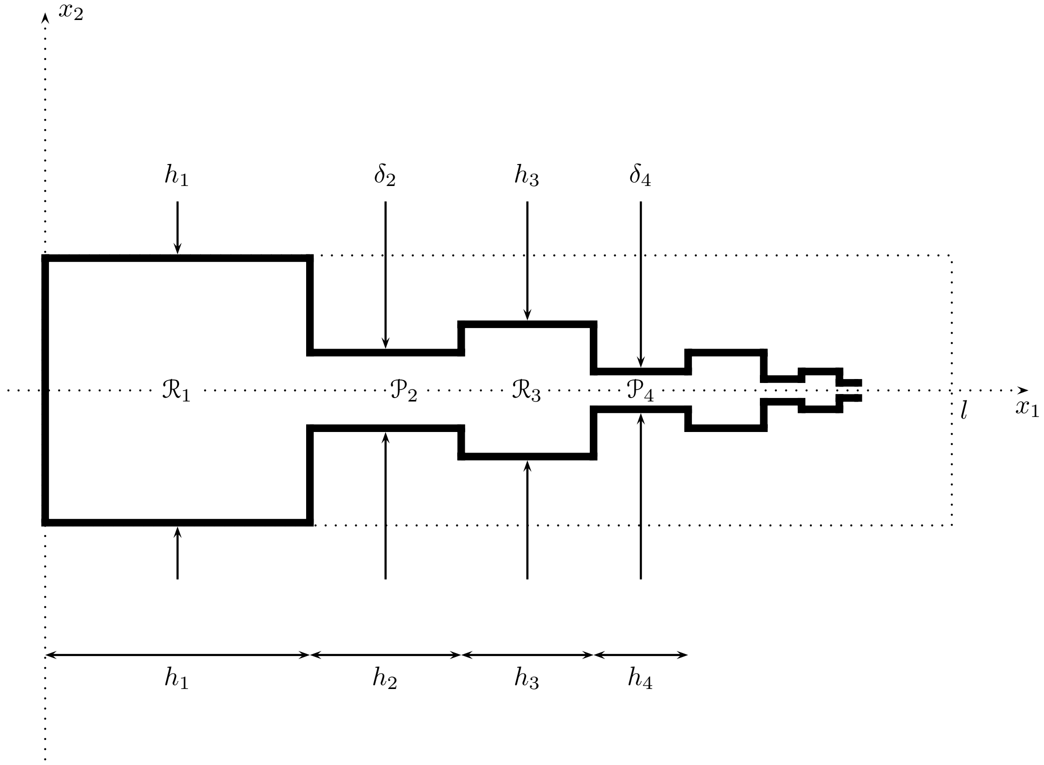


Figure 2.3: *Rooms and passages* as an example of a bounded domain for which the Neumann Laplacian has an essential spectrum. Choosing $h_j := j^{-3/2}$ and $\delta_j := j^{-6}$, it turns out that zero belongs to the essential spectrum (see [10, Sec. V.4.9]).

Theorem 2.3 (Spectral theorem, purely discrete spectrum)**.** *Let H is a self-adjoint operator in a Hilbert space $\mathcal{H}$ with $\dim \mathcal{H} = \infty$. Then*

$$\text{the eigenvectors of } H \text{ form an orthonormal basis in } \mathcal{H} \quad \Longleftrightarrow \quad \sigma_{\text{ess}}(H) = \varnothing\,.$$

The proof of the direction $\Rightarrow$ is analogous to our proof of Proposition 2.3 for rectangular parallelepipeds. The direction $\Leftarrow$ is more 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.

Combining the direction $\Leftarrow$ of Theorem 2.3 with the absence of the essential spectrum in bounded domains (Theorem 2.1), it follows that the Dirichlet Laplacian in any bounded domain indeed possesses an infinite number of discrete eigenvalues.

2.5 The minimax principle

Let us now prove a highly important consequence of Theorem 2.3. We say 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 2.4 (Minimax principle)**.** *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 $k \in \{1, \ldots, N\}$,*

$$\lambda_k = \inf_{\substack{\mathcal{L}_k \subset \operatorname{dom} H \\ \dim \mathcal{L}_k = k}} \sup_{\substack{\psi \in \mathcal{L}_k \\ \psi \neq 0}} \frac{(\psi, H\psi)}{\|\psi\|^2} \,. \tag{2.16}$$

Proof. Let us denote the right-hand side of (2.16) by $\tilde{\lambda}_k$. Our aim is to show that $\tilde{\lambda}_k = \lambda_k$ for every $k \in \{1, \ldots, N\}$. We follow the proof of [9, 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 2.3, they can be normalised in such a way that $\{\psi_k\}_{k=1}^N$ is a complete orthonormal set in $\mathcal{H}$. For every $\psi \in \mathcal{M}_k := \operatorname{span}\{\psi_1, \ldots, \psi_k\}$, 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 (2.16), one gets $\tilde{\lambda}_k \leq \lambda_k$ for every $k \in \{1, \ldots, N\}$.

$\boxed{\tilde{\lambda}_k \geq \lambda_k}$ If $k = 1$, the formula (2.16) 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 $k \in \{2, \ldots, N\}$, 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 $k \in \{1, \ldots, N\}$. ☐

Remark 2.4. Let H be as in Theorem 2.4 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 [9, Thm. 4.5.3]) that the formula (2.16) can be replaced by

$$\lambda_k = \inf_{\substack{\mathcal{L}_k \subset \operatorname{dom} h \\ \dim \mathcal{L}_k = k}} \sup_{\substack{\psi \in \mathcal{L}_k \\ \psi \neq 0}} \frac{h[\psi]}{\|\psi\|^2} \,. \tag{2.17}$$

Theorem 2.4 enables one to compute the spectrum of self-adjoint semi-bounded operators variationally (it is thus interesting even in finite-dimensional vector spaces). What is more, the variational characterisation remains valid for discrete eigenvalues below the essential spectrum (*i.e.*, even if the latter is not empty), see Remark 2.5 below. It then represents an extremely useful tool in practical problems in quantum mechanics (*e.g.*, for computation of eigenvalues of many-body Hamiltonians in quantum chemistry). In these lectures, however, we shall merely use it to establish upper bounds to the eigenvalues of the Dirichlet Laplacian.

Remark 2.5. Since the spectral theorem is not restricted to self-adjoint operators with purely discrete spectrum, there exists a version of Theorem 2.4 even for operators whose essential spectrum is not empty (see [9, Thm. 4.5.2]). In general, the numbers as *defined* by (2.16) coincide with discrete eigenvalues of H *below the essential spectrum.* Hence, we have a complete variational characterisation for such eigenvalues. Then the bottom of the essential spectrum is characterised by the limit

$$\inf \sigma_{\mathrm{ess}}(H) = \lim_{k\to\infty} \lambda_k \tag{2.18}$$

(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.

2.6 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. (We emphasise the dependent 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* (2.14). More generally, we have the natural continuous embedding

$$\Omega_1 \subset \Omega_2 \qquad \Longrightarrow \qquad W_0^{1,2}(\Omega_1) \hookrightarrow W_0^{1,2}(\Omega_2)\,, \tag{2.19}$$

just by extending the functions in $W_0^{1,2}(\Omega_1)$ by zero outside Ω_1. Using (2.17), we therefore get, for every $k \in \mathbb{N}^*$,

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

Let us formulate this crucial monotonicity property into the following proposition.

Proposition 2.5 (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 2.6 (General domains)**.** We have formulated Proposition 2.5 for *bounded* domains only, but the monotonicity actually holds for *any* domains, provided that the numbers λ_k's are interpreted through the formula (2.17). In particular, the monotonicity holds for (discrete) eigenvalues below the essential spectrum.

Proposition 2.5 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 parallelepipeds are known explicitly, see Section 2.2.

Remark 2.7 (Neumann boundary conditions)**.** The **monotonicity result does not hold for Neumann** eigenvalues $\lambda_k^N(\Omega) := \lambda_k(-\Delta_N^\Omega)$ (or more generally Robin eigenvalues), see Figure 2.4.

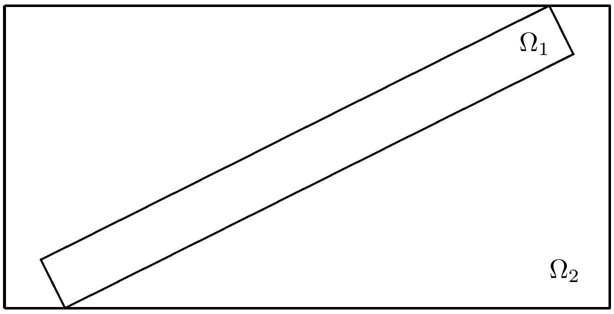


Figure 2.4: A counterexample to the monotonicity of Neumann eigenvalues. If the lengths of the sides of the circumscribed (respectively inscribed) rectangle are $a_2 \geq b_2$ (respectively $a_1 \geq b_1$), then $a_1 = \sqrt{a_2^2 + b_2^2} - b_1 a_2/b_2$ with $b_1 \leq b_2\sqrt{a_2^2 + b_2^2}/(a_2 + b_2)$, so that the second Neumann eigenvalues satisfy $\lambda_2^N(\Omega_2) = (\pi/a_2)^2 > (\pi/a_1)^2 = \lambda_2^N(\Omega_1)$ for all sufficiently small b_1. (On the other hand, if the inscribed rectangle Ω_1 is parallel with respect to Ω_2, we have a reverse inequality $\lambda_2^N(\Omega_2) < \lambda_2^N(\Omega_1)$ for all $a_1 \leq a_2$ and $b_1 \leq b_2$.)

2.7 Spectral isoperimetric inequalities

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.

2.7.1 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,

$$\max_{|\partial\Omega|=\text{const}} |\Omega| = |B| \,, \tag{2.20}$$

where the maximum is taken over all bounded domains $\Omega \subset \mathbb{R}^2$ of the fixed perimeter $|\partial\Omega| = \text{const}$, B denotes the disk of the same perimeter as Ω (*i.e.* $|\partial B| = |\partial\Omega| = \text{const}$) and $|\Omega|$ denotes the area of Ω. It is indeed an inequality because (2.20) is equivalent to the statement

$$\forall\Omega,\ |\partial\Omega| = \text{const}, \qquad |\Omega| \leq |B| \,. \qquad (|\partial B| = |\partial\Omega| = \text{const}) \tag{2.21}$$

Moreover, the inequality becomes equality if, and only if, $\Omega = B$.

By scaling, (2.20) is equivalent to the *isochoric inequality* stating that among all planar sets of a given area, the disk has the smallest perimeter. That is,

$$\min_{|\Omega|=\text{const}} |\partial\Omega| = |\partial B| \,, \tag{2.22}$$

where the minimum is taken over all bounded domains $\Omega \subset \mathbb{R}^2$ of a fixed area $|\Omega| = \text{const}$ and now B denotes the disk of the same area as Ω (*i.e.* $|B| = |\Omega| = \text{const}$). Again, one is concerned with an inequality because (2.22) is equivalent to the statement

$$\forall\Omega,\ |\Omega| = \text{const}, \qquad |\partial\Omega| \geq |\partial B| \,. \qquad (|B| = |\Omega| = \text{const}) \tag{2.23}$$

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 (2.21) and (2.23) can be stated as a unique inequality (without any further constraints on the domain Ω)

$$\forall\Omega, \qquad |\partial\Omega|^2 - 4\pi|\Omega| \geq 0\,, \tag{2.24}$$

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 (2.21) states that $|\Omega| \leq \pi R^2$; eliminating R, we arrive at (2.24).

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 [4] for an overview). The analogous statements hold in higher dimensions as well.

2.7.2 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 2.5 (Spectral isochoric inequality, Dirichlet case)**.** *One has*

$$\min_{|\Omega|=\text{const}} \lambda_1^D(\Omega) = \lambda_1^D(B)\,, \tag{2.25}$$

*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. $|B| = |\Omega| = \text{const}$*).*

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* [22], but proved only by Faber [12] and Krahn [17] almost half a century later.

Before commenting on the proof of Theorem 2.5, let us mention that (2.25) implies the spectral isoperimetric inequality as a corollary.

Corollary 2.1 (Spectral isoperimetric inequality, Dirichlet case)**.** *One has*

$$\min_{|\partial\Omega|=\text{const}} \lambda_1^D(\Omega) = \lambda_1^D(B)\,, \tag{2.26}$$

*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. $|\partial B| = |\partial\Omega| = \text{const}$*).*

Proof. By Theorem 2.5, one has

$$\lambda_1^D(\Omega) \geq \lambda_1^D(B') \qquad \text{with} \qquad |B'| = |\Omega|\,, \tag{2.27}$$

where B' is the ball of the same volume as Ω. By the geometric isochoric inequality (2.23), 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

$$\lambda_1^D(B') \geq \lambda_1^D(B)\,. \tag{2.28}$$

Combining (2.27) and (2.28), we arrive at the desired claim. $\square$

The proof of Theorem 2.5 is based on the following deep result of analysis.

Lemma 2.1 (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.*, [21, 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 2.5.

Proof. To apply Lemma 2.1, we need to ensure that $\lambda_1^D(\Omega)$ admits a non-negative eigenfunction. This follows from the minimax principle. First of all, notice that the Dirichlet Laplacian $-\Delta_D^\Omega$ is a *real* operator (*i.e.*, if ψ lies in $\mathrm{dom}(-\Delta_D^\Omega)$, then its complex conjugate $\overline{\psi}$ also lies in $\mathrm{dom}(-\Delta_D^\Omega)$ and $-\Delta_D^\Omega\overline{\psi} = \overline{-\Delta_D^\Omega\psi}$). Consequently, its eigenfunctions can be chosen to be real-valued. The variational characterisation (2.17) reduces to

$$\lambda_1^D(\Omega) = \inf_{\substack{\psi \in W_0^{1,2}(\Omega)\\ \psi\neq 0}} \frac{\displaystyle\int_\Omega |\nabla\psi|^2}{\displaystyle\int_\Omega |\psi|^2} = \frac{\displaystyle\int_\Omega |\nabla\psi_1|^2}{\displaystyle\int_\Omega |\psi_1|^2} = \frac{\displaystyle\int_\Omega \big|\nabla|\psi_1|\big|^2}{\displaystyle\int_\Omega |\psi_1|^2}\,,$$

where ψ_1 denotes *a* real-valued eigenfunction of the Dirichlet Laplacian in $L^2(\Omega)$ corresponding to $\lambda_1^D(\Omega)$. It follows that $|\psi_1|$ is an eigenfunction also, so the eigenfunction corresponding to the lowest eigenvalue can be chosen to be *non-negative*.

Let ψ_1^* denote the symmetric-decreasing rearrangement of the non-negative 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 2.1. □

2.7.3 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

$$\begin{cases} -\Delta\psi = \lambda\psi & \text{in} \quad \Omega\,, \\ \dfrac{\partial\psi}{\partial n} + \alpha\,\psi = 0 & \text{on} \quad \partial\Omega\,, \end{cases} \tag{2.29}$$

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 sesquilinear forms as in Section 0.5, the problem (2.29) can be again properly interpreted as a spectral problem for a self-adjoint operator $-\Delta_\alpha^\Omega$ (called *Robin Laplacian*) 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 (2.29) by $\bar\psi$ and integrate by parts using the boundary condition of (2.29)):

$$\lambda_1^\alpha(\Omega) = \inf_{\substack{\psi\in W^{1,2}(\Omega)\\ \psi\neq 0}} \frac{\displaystyle\int_\Omega |\nabla\psi|^2 + \alpha\int_{\partial\Omega}|\psi|^2}{\displaystyle\int_\Omega |\psi|^2}\,. \tag{2.30}$$

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 2.5) to repulsive boundary conditions. The proof (much harder than in the Dirichlet case) is due to Bossel [5] in dimension two and due to Danners [8] in all dimensions.

Theorem 2.6 (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 2.1.

Corollary 2.2 (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.

2.7.4 Bareket's conjecture

Let us now look at attractive Robin boundary conditions, *i.e.* $\alpha < 0$ in (2.29). 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 (2.30)), now it makes sense to maximise it. Bareket stated this expectation explicitly in 1977 [3].

Conjecture 2.1 (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 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. $|B| = |\Omega| = \text{const}$*).*

Since we state this spectral isochoric inequality as a conjecture, it might be expected that something goes wrong. Indeed, in collaboration with Freitas [13], we disproved the conjecture by showing that there exists another domain, which is better than the ball, at least if $|\alpha|$ is large.

Theorem 2.7 (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 $\alpha \leq \alpha_0$,*

$$\lambda_1^\alpha(B_R) < \lambda_1^\alpha(A_{R_1,R_2})\,, \tag{2.31}$$

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:

$$\begin{aligned} \lambda_1^\alpha(B_R) &= -\alpha^2 + \frac{d-1}{R}\,\alpha + o(\alpha)\,, \\ \lambda_1^\alpha(A_{R_1,R_2}) &= -\alpha^2 + \frac{d-1}{R_2}\,\alpha + o(\alpha)\,, \end{aligned}$$

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 (2.31) for all sufficiently large $|\alpha|$. ☐

Theorem 2.7 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 [2]) that the ball is the maximiser within the class of *simply connected* domains (*i.e.*, Bareket's Conjecture 2.1 holds for such domains).

The isoperimetric constraint seems to be much simpler, at least in low dimensions.

Theorem 2.8 (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 minimum 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 [2]. It is believed (and supported by numerical experiments, see [2]) 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 [6].

For the optimisation of the lowest Robin eigenvalue in the *exterior* of compact sets, see [19, 20].

Chapter 3

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 3.1 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 3.1. 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.

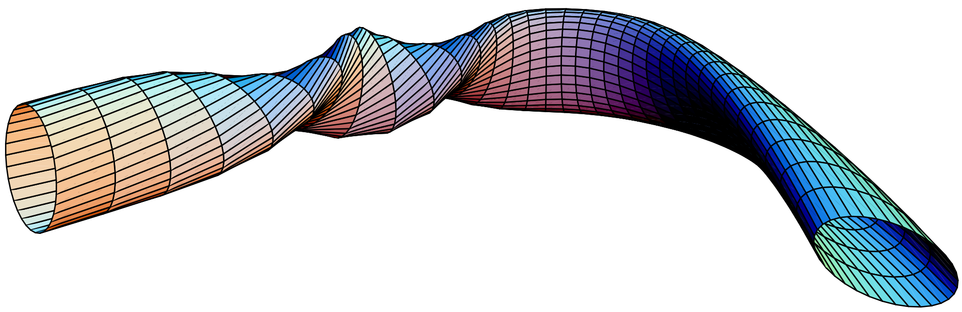


Figure 3.1: An example of a tube of elliptical cross-section. The geometric deformations of twisting and bending are demonstrated on the left and right part of the picture, respectively.

3.1 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 3.1 (General location of the essential spectrum)**.** *Let $\Omega \subset \mathbb{R}^d$ be an arbitrary open set. Set*

$$R_{\max} := \sup\left\{R \,:\, \Omega \textit{ contains a sequence of disjoint balls of radius } R\right\}$$

(by convention, we set $R_{\max} := 0$ if there is no such a sequence.) There exists a dimensional constant c_d such that

$$\inf \sigma_{\rm ess}(-\Delta_D^\Omega) \leq \frac{c_d}{R_{\max}^2} \tag{3.1}$$

(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 (3.1) 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* (2.8)) 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 2.4), we get

$$\lambda_n^D(\Omega) \le \frac{c_d}{R^2}$$

for *all* $n \in \mathbb{N}^*$. Consequently (*cf* (2.18)),

$$\inf \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = \lim_{n\to\infty} \lambda_n^D(\Omega) \le \frac{c_d}{R^2}\,.$$

Since the argument holds for all $R \in (0, R_{\max})$, we conclude with the stated inequality. □

As a consequence of Theorem 3.1, we get the following implications:

$$\begin{array}{lcr}
\Omega \text{ is quasi-conical} & \Longrightarrow & \inf \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = 0\,, \\
\Omega \text{ is quasi-cylindrical} & \Longrightarrow & \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) \ne \varnothing\,, \\
\Omega \text{ is quasi-bounded} & \Longleftarrow & \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = \varnothing\,.
\end{array}$$

The first implication (in fact, much more) has been established previously, see Theorem 1.1. The last implication says that the quasi-boundedness is a *necessary* condition for the discreteness of the spectrum of the Dirichlet Laplacian (by Theorem 2.1, 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 3.1. *Let $\Omega \subset \mathbb{R}^d$ be any quasi-cylindrical domain. Then*

$$\sigma_{\mathrm{ess}}(-\Delta_D^\Omega) \ne \varnothing\,.$$

Proof. Although the result follows directly from the quantitative Theorem 1.1, we provide an alternative proof, which does not use (2.18). Let us assume, by contradiction, that the spectrum of $-\Delta_D^\Omega$ is purely discrete. Then, proceeding as in the proof of Theorem 1.1, we get

$$\lim_{n\to\infty} \lambda_n^D(\Omega) \le \frac{c_d}{R^2}\,.$$

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 $\{\psi_n\}_{n\in\mathbb{N}^*}$, we have the decomposition

$$\begin{aligned}\forall\psi\in\operatorname{dom}(-\Delta_D^\Omega)\,,\qquad (\psi,-\Delta_D^\Omega\psi) &= \sum_{n,m=1}^\infty \big((\psi_n,\psi)\psi_n,(\psi_m,-\Delta\psi)\psi_m\big)\\ &= \sum_{n,m=1}^\infty \big((\psi_n,\psi)\psi_n,(\nabla\psi_m,\nabla\psi)\psi_m\big)\\ &= \sum_{n,m=1}^\infty \big((\psi_n,\psi)\psi_n,\lambda_m(\psi_m,\psi)\psi_m\big)\\ &= \sum_{n=1}^\infty \lambda_n\,|(\psi_n,\psi)|^2\\ &\le \lambda_\infty \sum_{n=1}^\infty |(\psi_n,\psi)|^2\\ &= \lambda_\infty\,\|\psi\|^2\,.\end{aligned}$$

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

$$\begin{aligned}(\varphi_N,-\Delta_D^\Omega\varphi_N) &= N^2\int_{\operatorname{supp}\varphi_N}|\nabla\varphi(Nx)|^2\,\mathrm{d}x = N^2N^{-d}\int_{\operatorname{supp}\varphi}|\nabla\varphi(y)|^2\,\mathrm{d}y\,,\\ \|\varphi_N\|^2 &= \int_{\operatorname{supp}\varphi_N}|\varphi(Nx)|^2\,\mathrm{d}x = N^{-d}\int_{\operatorname{supp}\varphi}|\varphi(y)|^2\,\mathrm{d}y\,.\end{aligned}$$

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_∞. □

3.2 Ground-state variational formula

We also need a highly useful tool, which is an extension of the variational characterisation (2.17) of the lowest eigenvalue of an operator with purely discrete spectrum to the general case.

Theorem 3.2. *Let H be a non-negative self-adjoint operator in $\mathcal{H}$ and let h denote its associated sesquilinear form. Then*

$$\inf\sigma(H)=\inf_{\substack{\psi\in\operatorname{dom}h\\ \psi\neq 0}}\frac{h[\psi]}{\|\psi\|^2}\,. \tag{3.2}$$

Proof. Let us abbreviate

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

$\boxed{\lambda_1\ge\tilde\lambda_1}$ 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

$$\tilde\lambda_1\le h[\psi_n]=(\psi_n,H\psi_n)=(\psi_n,H\psi_n-\lambda_1\psi_n)+\lambda_1\le\|H\psi_n-\lambda_1\psi_n\|+\lambda_1\,.$$

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.*,

$$\forall n \in \mathbb{N}, \quad \|\psi_n\| = 1 \qquad \text{and} \qquad \lim_{n\to\infty} h[\psi_n] = \tilde{\lambda}_1 \,. \tag{3.3}$$

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 (3.3). On the other hand, since (3.3) 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

$$\lim_{n\to\infty} \|u_n\| = \frac{1}{\sqrt{\tilde{\lambda}_1 + 1}} \,. \tag{3.4}$$

• $\underline{\|Hu_n - \tilde{\lambda}_1 u_n\|.}$ 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 (3.3) and (3.4). □

3.3 Straight tubes

The special class of quasi-cylindrical domains we shall consider are obtained as a "local" perturbation of the *straight tube*

$$\Omega_0 := \mathbb{R} \times \omega \,, \tag{3.5}$$

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

$$-\Delta_D^{\Omega_0} \cong -\Delta_D^{\mathbb{R}} \otimes I_\omega + I_{\mathbb{R}} \otimes -\Delta_D^{\omega} \qquad \text{in} \qquad L^2(\Omega_0) \cong L^2(\mathbb{R}) \times L^2(\omega)\,, \tag{3.6}$$

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 1.1)

$$\sigma(-\Delta_D^{\mathbb{R}}) = \sigma_{\mathrm{ess}}(-\Delta_D^{\mathbb{R}}) = [0,\infty)\,.$$

On the other hand, since ω is bounded, its Dirichlet spectrum is purely discrete (see Theorem 2.1)

$$\sigma(-\Delta_D^{\omega}) = \sigma_{\mathrm{disc}}(-\Delta_D^{\omega}) =: \{E_1 \le E_2 \le \dots\}_{k=1}^{\infty}\,.$$

Since the spectrum of the operator on the right-hand side of (3.6) 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 3.3. *Let $\omega \subset \mathbb{R}^{d-1}$ be an arbitrary bounded open domain. Then*

$$\sigma(-\Delta_D^{\Omega_0}) = \sigma_{\mathrm{ess}}(-\Delta_D^{\Omega_0}) = [E_1,\infty)\,, \tag{3.7}$$

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 (3.6).

$\boxed{\sigma(-\Delta_D^{\Omega_0}) \subset [E_1,\infty)}$ 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 (3.2) implies

$$\forall \phi \in W_0^{1,2}(\omega)\,, \qquad \int_\omega |\nabla\phi(y)|^2\,\mathrm{d}y \ge E_1 \int_\omega |\phi(y)|^2\,\mathrm{d}y\,.$$

Consequently, using in addition Fubini's theorem, we have

$$\begin{aligned}
\forall \psi \in \operatorname{dom} h\,, \qquad h[\psi] &= \int_{\Omega_0} \left(|\partial_x\psi(x,y)|^2 + |\nabla_y\psi(x,y)|^2\right)\,\mathrm{d}x\,\mathrm{d}y \\
&\ge \int_{\mathbb{R}}\int_\omega |\nabla_y\psi(x,y)|^2\,\mathrm{d}y\,\mathrm{d}x \\
&\ge E_1 \int_{\mathbb{R}}\int_\omega |\psi(x,y)|^2\,\mathrm{d}y\,\mathrm{d}x \\
&= E_1\,\|\psi\|^2\,.
\end{aligned}$$

By Theorem 3.2, it follows that $\inf\sigma(-\Delta_D^{\Omega_0}) \ge E_1$.

$\boxed{\sigma(-\Delta_D^{\Omega_0}) \supset [E_1,\infty)}$ 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 φ_n is as in the proof of Theorem 1.1, namely

$$\varphi_n(x) := n^{-1/2}\,\varphi\left(\frac{x-n}{n}\right)$$

with $\varphi \in C_0^2(\mathbb{R})$ 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 4c). The space

$$L_0^2(\Omega_0) := \{\psi \in L^2(\Omega_0) :\ \exists N>0,\ \operatorname{supp}\psi \subset [-N,N]\times\overline{\omega}\} \tag{3.8}$$

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* (1.4))

$$\inf\operatorname{supp}\varphi_n = n + n\,\inf\operatorname{supp}\varphi\,. \tag{3.9}$$

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 (3.7) suggests that we deal with a reasonable model for semiconductor waveguide nanostructure (the ionisation energy E_1 is strictly positive).

3.4 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 3.1. 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

$$\Omega \setminus Q = \Omega_0 \setminus Q\,. \tag{3.10}$$

Obviously, the unbounded parts of Ω and Ω_0 are the same, so the following theorem is very expected.

Theorem 3.4. *Let $\Omega \subset \mathbb{R}^d$ be a local deformation of the straight tube Ω_0. Then*

$$\sigma_{\mathrm{ess}}(-\Delta_D^{\Omega}) = \sigma_{\mathrm{ess}}(-\Delta_D^{\Omega_0}) = [E_1,\infty)\,. \tag{3.11}$$

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 3.3. Indeed, the singular sequence $\{\psi_n\}_{n\in\mathbb{N}^*}$ is "localised at infinity" (*cf* (3.9)), so it works just the same for Ω due to (3.10).

$\boxed{\sigma_{\mathrm{ess}}(-\Delta_D^\Omega) \subset [E_1, \infty)}$ 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 Remark 2.5), one has

$$\inf \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = \lim_{k\to\infty} \lambda_k(\Omega)\,, \tag{3.12}$$

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 3.1, 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

$$\mathcal{W}(\Omega_\iota) := \{\psi \restriction \Omega_\iota :\ \psi \in W_0^{1,2}(\Omega)\}\,, \qquad \iota \in \{\mathrm{left}, \mathrm{centre}, \mathrm{right}\}\,,$$

and set

$$\mathcal{D}(\Omega) := \mathcal{W}(\Omega_{\mathrm{left}}) \oplus \mathcal{W}(\Omega_{\mathrm{centre}}) \oplus \mathcal{W}(\Omega_{\mathrm{right}})\,. \tag{3.13}$$

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)

$$\forall k \in \mathbb{N}^*\,, \qquad \lambda_k(\Omega) \geq \lambda_k^N(\Omega)\,. \tag{3.14}$$

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 (3.13) of the space $\mathcal{D}(\Omega)$, we clearly have

$$\{\lambda_k^N(\Omega)\}_{k=1}^\infty = \{\lambda_k^N(\Omega_{\mathrm{left}})\}_{k=1}^\infty \cup \{\lambda_k^N(\Omega_{\mathrm{centre}})\}_{k=1}^\infty \cup \{\lambda_k^N(\Omega_{\mathrm{right}})\}_{k=1}^\infty\,, \tag{3.15}$$

where

$$\lambda_k^N(\Omega_\iota) := \inf_{\substack{\mathcal{L}_k \subset \mathcal{W}(\Omega_\iota) \\ \dim \mathcal{L}_k = k}} \sup_{\substack{\psi \in \mathcal{L}_k \\ \psi \neq 0}} \frac{\displaystyle\int_{\Omega_\iota} |\nabla\psi|^2}{\displaystyle\int_{\Omega_\iota} |\psi|^2}\,, \qquad \iota \in \{\mathrm{left}, \mathrm{centre}, \mathrm{right}\}\,.$$

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 (3.15) 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

$$\lim_{k\to\infty} \lambda_k^N(\Omega) = E_1 . \tag{3.16}$$

Combining (3.12), (3.14) and (3.16), 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.

3.5 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 (2.6) and (2.7), we have

$$E_1 = \left(\frac{\pi}{a}\right)^2 \qquad \text{and} \qquad \mathcal{J}_1(y) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{\pi}{a}y\right) \tag{3.17}$$

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 3.2. Given any continuous function $\theta : \mathbb{R} \to \mathbb{R}$ satisfying $\theta > -a$, we define a *deformed tube* by setting

$$\Omega := \left\{(x,y) \in \mathbb{R}^d : \ x \in \mathbb{R} \ \wedge \ 0 < y < a + \theta(x)\right\} .$$

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).

3.6 Bound states due to protrusions

In this section we investigate the effect of protrusions. The following theorem is originally due to [7].

Theorem 3.5. *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, for every $0 < \varepsilon \leq 1$, the scaled function $\theta_\varepsilon := \varepsilon\theta$ satisfies the hypotheses of the theorem. Moreover, $\operatorname{supp}\theta_\varepsilon = \operatorname{supp}\theta$ and $\theta_\varepsilon \leq \theta$. The latter implies $\Omega \supset \Omega_\varepsilon$. 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* (2.14)), Theorem 3.2 implies (*cf* Proposition 2.5)

$$\inf \sigma(-\Delta_D^\Omega) \leq \inf \sigma(-\Delta_D^{\Omega_\varepsilon}) \,.$$

Hence, it is enough to prove the theorem for the function θ_ε.

The proof is similar to that of Theorem 1.3. 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 3.2, it is enough to find a test function $\psi \in W_0^{1,2}(\Omega_\varepsilon)$ such that $Q_\varepsilon[\psi] < 0$. We set

$$\psi_n(x,y) := \varphi_n(x)\,\sin\left(\frac{\pi}{a+\theta_\varepsilon(x)}\,y\right) \qquad \text{with} \qquad \varphi_n(x) := \varphi\left(\frac{x}{n}\right) ,$$

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 (3.17). 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

$$\begin{aligned}
Q_\varepsilon^{(2)}[\psi_n] &= \int_{\mathbb{R}} \int_0^{a+\theta_\varepsilon(x)} \left[\left(\frac{\pi}{a+\theta_\varepsilon(x)}\right)^2 - \left(\frac{\pi}{a}\right)^2\right] |\psi_n(x,y)|^2 \,\mathrm{d}y\,\mathrm{d}x \\
&= \int_{\operatorname{supp}\theta} \int_0^{a+\theta_\varepsilon(x)} \left[\left(\frac{\pi}{a+\theta_\varepsilon(x)}\right)^2 - \left(\frac{\pi}{a}\right)^2\right] \sin^2\left(\frac{\pi}{a+\theta_\varepsilon(x)}\,y\right) \mathrm{d}y\,\mathrm{d}x \\
&= \int_{\operatorname{supp}\theta} \left[\left(\frac{\pi}{a+\theta_\varepsilon(x)}\right)^2 - \left(\frac{\pi}{a}\right)^2\right] \frac{a+\theta_\varepsilon(x)}{2}\,\mathrm{d}x \,,
\end{aligned}$$

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 $0 < \varepsilon < 1$,

$$Q_\varepsilon^{(2)}[\psi_n] = \frac{\pi^2}{2a^2} \int_{\operatorname{supp}\theta} \frac{-2a\,\varepsilon\,\theta(x) - \varepsilon^2\,\theta(x)^2}{a+\theta_\varepsilon(x)}\,\mathrm{d}x \leq -\frac{\pi^2\varepsilon}{a(a+\max\theta)} \int_{\operatorname{supp}\theta} \theta(x)\,\mathrm{d}x =: -c_1\varepsilon$$

where c_1 is a positive constant independent of both n and ε.

$\boxed{Q_\varepsilon^{(1)}}$ For the first form, we have

$$\begin{aligned}
Q_\varepsilon^{(1)}[\psi_n] &= \int_{\mathbb{R}}\int_0^{a+\theta_\varepsilon(x)} \left|\frac{1}{n}\varphi'\left(\frac{x}{n}\right)\sin\left(\frac{\pi}{a+\theta_\varepsilon(x)}\,y\right) - \varphi\left(\frac{x}{n}\right)\frac{\pi\,y\,\theta_\varepsilon'(x)}{[a+\theta_\varepsilon(x)]^2}\cos\left(\frac{\pi}{a+\theta_\varepsilon(x)}\,y\right)\right|^2 \mathrm{d}y\,\mathrm{d}x \\
&\leq 2\int_{\mathbb{R}}\int_0^{a+\theta_\varepsilon(x)} \left[\frac{1}{n^2}\varphi'\left(\frac{x}{n}\right)^2\sin^2\left(\frac{\pi}{a+\theta_\varepsilon(x)}\,y\right) + \varphi\left(\frac{x}{n}\right)^2\frac{\pi^2\,\theta_\varepsilon'(x)^2}{[a+\theta_\varepsilon(x)]^2}\cos^2\left(\frac{\pi}{a+\theta_\varepsilon(x)}\,y\right)\right]\mathrm{d}y\,\mathrm{d}x \\
&= \int_{\mathbb{R}}\left[\frac{1}{n^2}\varphi'\left(\frac{x}{n}\right)^2[a+\theta_\varepsilon(x)] + \varphi\left(\frac{x}{n}\right)^2\frac{\pi^2\,\theta_\varepsilon'(x)^2}{a+\theta_\varepsilon(x)}\right]\mathrm{d}x \\
&\leq \frac{1+\max\theta}{n}\int_{\mathbb{R}}|\varphi'(x)|^2\,\mathrm{d}x + \varepsilon^2\,\frac{\pi^2}{a}\int_{\mathbb{R}}|\theta'(x)|^2\,\mathrm{d}x \\
&=: \frac{c_2}{n} + c_3\varepsilon^2\,,
\end{aligned}$$

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 3.4, 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).

3.7 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 3.6. *Let $\theta \in C^0(\mathbb{R})$ be such that $\theta > -a$. Then*

$$\forall\phi \in W_0^{1,2}(\Omega), \qquad \int_\Omega |\nabla\psi|^2 - E_1\int_\Omega|\psi|^2 \geq \int_\Omega\left[\left(\frac{\pi}{a+\theta(x)}\right)^2 - \left(\frac{\pi}{a}\right)^2\right]|\psi(x,y)|^2\,\mathrm{d}x\,\mathrm{d}y\,. \tag{3.18}$$

Proof. Given any bounded open interval $I \subset \mathbb{R}$, recall (*cf* Section 2.2) that $(\pi/|I|)^2$ is the lowest eigenvalue of the Dirichlet Laplacian in $L^2(I)$. As a consequence of the variational formula (3.2), we thus get the inequality

$$\forall\phi \in W_0^{1,2}(I), \qquad \int_I |\phi'|^2 \geq \left(\frac{\pi}{|I|}\right)^2\int_I|\phi|^2\,. \tag{3.19}$$

By means of Fubini's theorem, we therefore obtain

$$\begin{aligned}
\forall\psi \in W_0^{1,2}(\Omega)\,, \qquad \int_\Omega |\nabla\psi|^2 &= \int_{\mathbb{R}} \int_0^{a+\theta(x)} \left(|\partial_x\psi(x,y)|^2 + |\partial_y\psi(x,y)|^2\right) \mathrm{d}y\,\mathrm{d}x \\
&\geq \int_{\mathbb{R}} \int_0^{a+\theta(x)} |\partial_y\psi(x,y)|^2 \,\mathrm{d}y\,\mathrm{d}x \\
&\geq \int_{\mathbb{R}} \left(\frac{\pi}{a+\theta(x)}\right)^2 \int_0^{a+\theta(x)} |\psi(x,y)|^2 \,\mathrm{d}y\,\mathrm{d}x \\
&= \int_\Omega \left(\frac{\pi}{a+\theta(x)}\right)^2 |\psi(x,y)|^2 \,\mathrm{d}x\,\mathrm{d}y\,.
\end{aligned}$$

It remains to recall the definition (3.17) of E_1. □

Notice that the square bracket of (3.18) 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 3.2. *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 (3.18) is equivalent to the Hardy-type inequality

$$-\Delta_D^\Omega - E_1 I \geq \left(\frac{\pi}{a+\theta}\right)^2 - \left(\frac{\pi}{a}\right)^2 \tag{3.20}$$

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 3.4 implies that the essential spectrum equals the interval $[E_1, \infty)$ and Corollary 3.2 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 (3.20) is non-negative and non-trivial. It is important to notice that such a scenario does not happen for the straight strip.

Proposition 3.1. *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 1.3 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 3.3. *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 3.4, we obtain that

$$\inf \sigma_{\text{ess}}(-\Delta_D^\Omega) \geq \min\{\lambda_{\text{left}}, \lambda_{\text{right}}\}\,, \tag{3.21}$$

where

$$\lambda_\iota := \inf_{\substack{\psi \in \mathcal{W}(\Omega_\iota) \\ \psi \neq 0}} \frac{\displaystyle\int_{\Omega_\iota} |\nabla\psi|^2}{\displaystyle\int_{\Omega_\iota} |\psi|^2}\,, \qquad \iota \in \{\text{left}, \text{right}\}\,, \qquad \begin{aligned} \Omega_{\text{left}} &:= [(-\infty, -R) \times \mathbb{R}] \cap \Omega\,, \\ \Omega_{\text{right}} &:= [(+R, +\infty) \times \mathbb{R}] \cap \Omega\,. \end{aligned}$$

Proceeding as in the proof of Theorem 3.6, we get

$$\begin{aligned} \forall \psi \in \mathcal{W}(\Omega_{\text{right}})\,, \qquad \int_{\Omega_{\text{right}}} |\nabla\psi|^2 &\geq \int_{\Omega_{\text{right}}} \left(\frac{\pi}{a + \theta(x)}\right)^2 |\psi(x,y)|^2 \, \mathrm{d}x \, \mathrm{d}y \\ &\geq \left(\frac{\pi}{a + \inf\limits_{(R,\infty)} \theta}\right)^2 \int_{\Omega_{\text{right}}} |\psi|^2\,, \end{aligned}$$

and similarly for Ω_{left}. Consequently,

$$\lambda_{\text{left}} \geq \left(\frac{\pi}{a + \inf\limits_{(-\infty,-R)} \theta}\right)^2 \qquad \text{and} \qquad \lambda_{\text{right}} \geq \left(\frac{\pi}{a + \inf\limits_{(R,\infty)} \theta}\right)^2.$$

Because of our hypothesis, both λ_{left} and λ_{right} tend to ∞ as $R \to \infty$. Since the left-hand side of (3.21) is independent of R and the right-hand side can made arbitrarily large by taking R large, it follows that $\inf \sigma_{\text{ess}}(-\Delta_D^\Omega) = \infty$. □

3.8 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 3.1. 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 [18] 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).
- $\chi_S(x) := \begin{cases} 1 & \text{if} \quad x \in S\,, \\ 0 & \text{otherwise}\,, \end{cases}$ (characteristic function of a set S), where $S \subset \mathbb{R}^d$.