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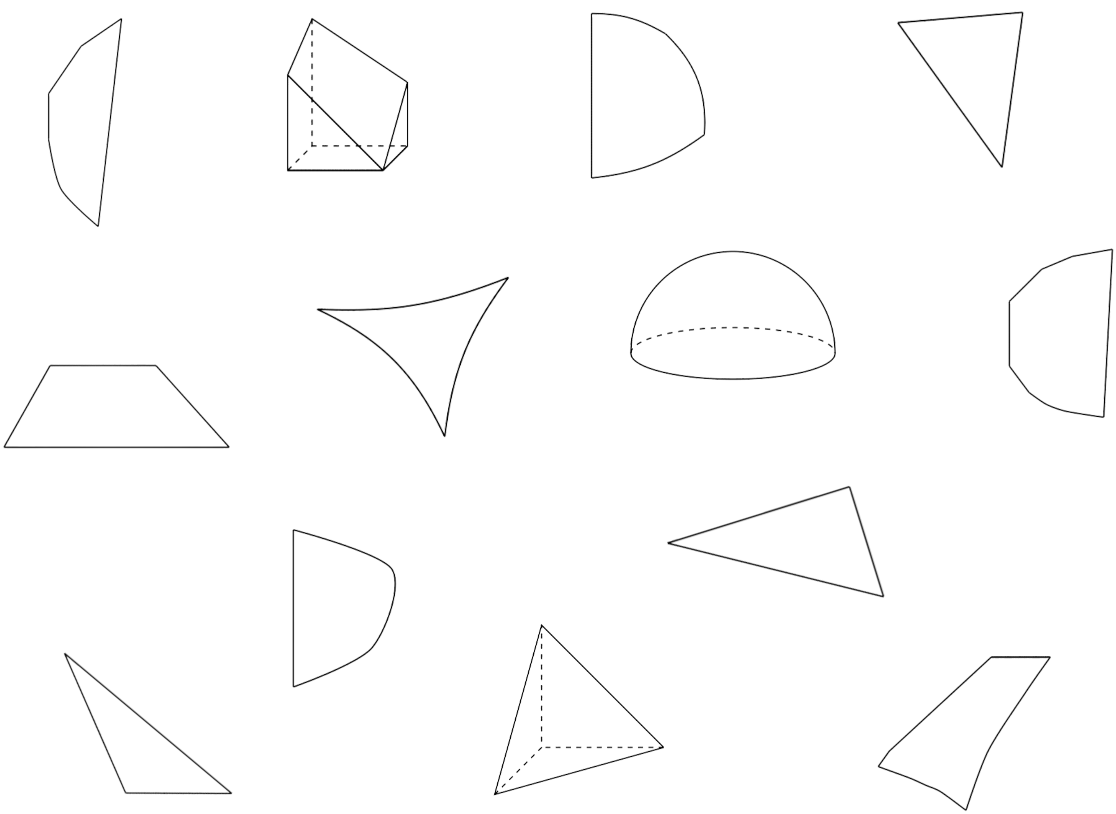
Eigenvalues and eigenfunctions of Laplacians and Schrödinger operators with mixed boundary conditions

Nausica Aldeghi



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Nausica Aldeghi

Academic dissertation for the Degree of Doctor of Philosophy in Mathematics at Stockholm University to be publicly defended on Tuesday 24 September 2024 at 13.00 in Hörsal 4, Hus 2, Albano, Albanovägen 18.

Abstract

This thesis consists of three papers, all concerned with the eigenvalue problem for the Schrödinger operator $-\Delta+V$, and in particular the Laplacian $-\Delta$, on bounded, connected, Lipschitz domains with mixed boundary conditions, where a Dirichlet boundary condition is imposed on a subset of the boundary and a Neumann boundary condition on its complement. Given different such choices of boundary conditions on the same domain, we compare the resulting mixed Dirichlet-Neumann eigenvalues by establishing inequalities between them, and prove a variant of the hot spots conjecture for the lowest mixed Dirichlet-Neumann eigenfunction of the Laplacian. Our approach is purely variational and relies on both classical and novel variational principles; the geometric features of the underlying domain, such as convexity or curvature of the boundary, play a crucial role in our results.

In Paper I we consider the Laplacian on planar, convex domains and compare the lowest eigenvalues corresponding to different choices of mixed boundary conditions in the case in which the boundary contains a straight line segment. The proof relies on estimating the Rayleigh quotient of the derivative of a certain eigenfunction in the unique direction normal to this segment; as a result the established inequalities depend on the geometry of the boundary with respect to this direction, as well as on the convexity of the domain.

In Paper II we also compare the lowest mixed eigenvalues of the Laplacian on simply connected planar domains, but instead rely on a novel variational principle where the minimizers are gradients of eigenfunctions. To the best of our knowledge, this variational principle has not appeared in the literature before. This allows to replace the convexity assumption with a more general assumption regulating the normal directions to the boundary, and to drop the assumption that the boundary contains a straight line segment. Using this novel variational principle we also prove a version of the hot spots conjecture for mixed Dirichlet-Neumann boundary conditions.

In Paper III we extend the eigenvalue inequalities of Paper I to Schrödinger operators on both planar and higher-dimensional domains by generalizing the variational approach therein established; in this case we require the boundary to contain a subset of a hyperplane. The inequalities rely again on the convexity of the domain and on the geometry of both the boundary and the potential V with respect to the unique direction normal to this hyperplane. Further, we prove an inequality between higher order mixed Dirichlet-Neumann eigenvalues and pure Dirichlet eigenvalues of Schrödinger operators.

Keywords: *Spectral theory of differential operators, Laplacian, Schrödinger operator, Eigenvalue inequalities, Mixed boundary conditions, Hot spots conjecture.*

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Sammanfattning

Denna avhandling består av tre artiklar, alla rörande egenvärdesproblemet för Schrödinger-operatorn $-\Delta + V$, och i synnerhet Laplaceoperatorn $-\Delta$, på begränsade, sammanhängande, Lipschitz-områden med blandade randvillkor, där ett Dirichlet-randvillkor ställs på en delmängd av randen och ett Neumann-randvillkor på komplementet. Givet olika sådana val av randvillkor på samma område jämför vi de resulterande blandade Dirichlet-Neumann egenvärdena genom att etablera olikheter mellan dem och vi bevisar en variant av "hot spots-förmodan för den lägsta blandade Dirichlet-Neumann-egenfunktionen av Laplaceoperatorn. Vår metod är helt variationell och bygger både på klassiska och nya variationsprinciper; de geometriska egenskaperna hos det underliggande området, såsom konvexitet eller krökning av randen, spelar en avgörande roll i våra resultat.

I Artikel I undersöker vi Laplaceoperatorn på konvexa områden i planet och jämför de lägsta egenvärdena motsvarande olika val av blandade randvillkor i det fall då randen innehåller ett rakt linjesegment. Beviset bygger på att vi uppskattar Rayleigh-kvoten av derivatan av en viss egenfunktion i den unika riktningen ortogonal till detta segment. Följaktligen beror de etablerade olikheterna på randens geometri i förhållande till denna riktning samt på områdets konvexitet.

I Artikel II jämför vi också de lägsta blandade egenvärdena för Laplaceoperatorn på enkelt sammanhängande områden i planet men bygger istället på en ny variationsprincip där de minimerande funktionerna är gradienter av egenfunktioner. Såvitt vi vet har denna variationsprincip inte förekommit i litteraturen tidigare. Detta möjliggör att vi kan ersätta konvexitetsantagandet med ett mer generellt antagande som reglerar normalriktningarna till randen och att vi kan släppa antagandet att randen innehåller ett rakt linjesegment. Genom att använda denna nya variationsprincip bevisar vi även en version av "hot spots-förmodan för blandade Dirichlet-Neumann randvillkor.

I Artikel III utvidgar vi egenvärdesolikheterna i artikel I till Schrödinger-operatorer på både områden i planet och i högre dimensioner genom att generalisera den variationella metoden som etablerats i den; i detta fall kräver vi att randen innehåller en delmängd av ett hyperplan. Olikheterna beror återigen på områdets konvexitet och på geometrin hos både randen och potentialen V i förhållande till den unika riktningen normal till detta hyperplan. Vidare bevisar vi en olikhet mellan högre ordningens blandade Dirichlet-Neumann-egenvärden och rena Dirichlet-egenvärden för Schrödinger-operatorer.

Odi et amo. Quare id faciam, fortasse requiris.
Nescio, sed fieri sentio et excrucior.

Catullus 85

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I am really happy to be writing these acknowledgements. For a long time it seemed to me as though this day would never come. I am very proud for persevering, but of course I also owe this achievement to the people who have supported me during these five long years.

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List of papers

The following papers, referred to in the text by their Roman numerals, are included in this thesis.

Paper I: **Inequalities between the lowest eigenvalues of Laplacians with mixed boundary conditions**
Nausica Aldeghi, Jonathan Rohleder
Journal of Mathematical Analysis and Applications 524 (2023), no. 1, Paper No. 127078.

Paper II: **On the first eigenvalue and eigenfunction of the Laplacian with mixed boundary conditions**
Nausica Aldeghi, Jonathan Rohleder
Preprint: arXiv:2403.17717, submitted.

Paper III: **Inequalities for eigenvalues of Schrödinger operators with mixed boundary conditions**
Nausica Aldeghi
Preprint, submitted.

Author's contribution. Paper I and Paper II are collaborative works between N. Aldeghi and J. Rohleder; equal contribution from both authors.

Contents

Introduction

I would like to start with a very informal introduction to my research. It is dedicated to my family and friends who have been asking me about my job for years, and who were always very puzzled when I started talking about drums.

Think of a simple round drum that can be played with hands, sticks or a pedal. Now, say we would like to describe mathematically the nature of the sounds produced by the drum when struck. A drum is made of a box with a circular opening over which a membrane, the drumhead, is stretched. Let's forget about the specifics of the box and only focus on the membrane and its shape; we can describe the opening over which the membrane rests as a round domain in the (x, y)-plane called Ω. When struck, the membrane starts vibrating; we can describe this mathematically by a function f depending on both space and time which takes its values in every point of Ω and tells us how much this point is displaced as the membrane vibrates. When we do not play the drum, the displacement f identically equals zero, and it is always zero on the boundary of the membrane, which we call $\partial\Omega$, as the membrane is clamped there and does not move; we write $f|_{\partial\Omega} = 0$ and say that f satisfies a *Dirichlet boundary condition* on $\partial\Omega$. Then, we need to describe how the membrane vibrates, that is, the values of the displacement f over time. The physics of the vibration satisfies an equation, know as the *wave equation*, which governs the behaviour of f in space and time; together with the Dirichlet boundary condition $f|_{\partial\Omega} = 0$ and initial conditions specifying the value of f and its time derivative at the initial time this equation completely describes the vibration of the drum when struck.

Now, the sounds produced by the drum are composed by tones of various frequencies, and these frequencies can be computed in terms of the solutions λ to the time-independent system

$$\begin{cases} -\Delta u = \lambda u, \\ u|_{\partial\Omega} = 0, \end{cases} \tag{0.1}$$

where $-\Delta = -\partial_x^2 - \partial_y^2$ is the (negative) Laplacian. This system is obtained as the part of the wave equation which depends on space only; this process is known as separation of variables and u is a function on Ω obtained from f using this process. We solve the system for both u and λ and call these numbers λ *eigenvalues*; we arrange them increasingly in a sequence $\lambda_1, \lambda_2, \ldots$ we call the *spectrum* associated to Ω. The eigenvalues thus describe the sounds that the drum shaped like Ω can create and depend in a subtle way on the geometry of Ω. This dependency is the main subject of *spectral geometry*. Marc Kac's famous question from 1966 "Can one hear the shape of a drum?", wondering if two drums which have the same spectrum, i.e. sound the same, have the same shape, is widely regarded to have initiated the field and has been motivating a lot of research since.

This thesis contributes to the field in the following direction. Imagine that the membrane of our drum is only partially clamped to the frame, say on a subset Γ of $\partial\Omega$, while the remainder has some freedom of movement except along the direction ν that is orthogonal to the boundary. We can obtain the sounds that this drum would make by modifying the boundary condition in (0.1) and reducing it to the subset Γ where the membrane is clamped, and by introducing on the remainder $\Gamma^c = \partial\Omega \setminus \Gamma$ a new condition, called the *Neumann boundary condition*, which expresses the allowed range of movement of the membrane as follows,

$$\begin{cases} -\Delta u = \lambda u, \\ u|_{\Gamma} = 0, \\ \partial_\nu u|_{\Gamma^c} = 0, \end{cases} \tag{0.2}$$

where ν is the outer unit normal vector defined on $\partial\Omega$ and ∂_ν is the derivative with respect to this direction; the condition $\partial_\nu u|_{\Gamma^c} = 0$ means that on Γ^c the membrane cannot move along the direction ν. We call this combination of boundary conditions *mixed Dirichlet-Neumann boundary conditions*. A question naturally arises: how is the spectrum influenced by these mixed boundary conditions? In other words, how does the sound that the drum make depend on the choice of the subsets Γ and Γ^c? We know that enlarging the Dirichlet part leads to higher eigenvalues, that is, the system (0.2) produces lower eigenvalues than the ones produced by the same system where Γ is replaced by a larger set Γ' which contains Γ, cf. Corollary 2.12. However, not so much is known about how the spectrum depends on the length of Γ and Γ' if these subsets do not intersect.

One of the aims of this thesis is to investigate this dependency: we focus on the lowest eigenvalue, which limits the fundamental tone that the drum can produce, compare two different configurations of mixed Dirichlet-Neumann boundary conditions on the same drum and provide sufficient conditions on the shape of Ω and on the choice of Γ and Γ' ensuring that one configuration produces a lower eigenvalue than the other one. We also study equation (0.2) under the addition of a linear term Vu to the Laplacian; this produces the (time-independent) *Schrödinger operator* $-\Delta + V$, which naturally appears in physics in the setting of quantum mechanics, V is called *potential*. We do not limit our analysis to planar domains Ω but also study higher-dimensional domains; we also study the behaviour of the solutions of u of (0.2) for the lowest eigenvalue in connection with the famous *"hot spots" conjecture* which is tied to role the Laplacian plays in models for heat diffusion.

The remainder of this introduction is composed of three sections in which we progressively construct the mathematical background needed for the rigorous formulation of the mixed Dirichlet-Neumann problem (0.2) and the study of its eigenvalues and eigenfunctions. We start in Section 1 with an introduction to the theory of self-adjoint operators on Hilbert spaces, their spectra and their representation via sesquilinear forms; in Section 2 we use this theory to define (0.2) for the Laplacian and Schrödinger operator and describe their spectra. In both sections we provide proofs for the key results, as well as references for more details for the interested readers. Section 3 is devoted to more recent research topics; there we review inequalities for mixed Dirichlet-Neumann eigenvalues as well as the hot spots conjecture.

1 Preliminaries: self-adjoint operators and quadratic forms on Hilbert spaces

In this preliminary section we present some fundamental facts and definitions which lay the foundation for the main part of this thesis. In Section 1.1 we quickly go over some basics on not necessarily bounded linear operators on Hilbert spaces, while in Section 1.2 we focus on self-adjoint operators and briefly review some results on their spectra. In Section 1.3 we recall some results on semibounded sesquilinear forms and their representations via selfadjoint operators; this representation will play an important role in Papers I - III. In particular, we prove the variational principle of Theorem 1.4 which is instrumental for the proofs of most of our results. In Section 1.4 we gather some technical facts on Lipschitz domains and Sobolev spaces.

For Sections 1.1 – 1.3 we mainly follow [Schmudgen, Part I] and [Kato, Chapter VI]; these facts can be found in many standard textbooks on functional analysis, for instance [BlanchardBruning, ReedSimon, Teschl]. In Section 1.4 we mainly follow [McLean]; see also [AkhiezerGlazman, EdmundsEvans, Evans, McLean] for more details.

1.1 Linear operators on Hilbert spaces

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be complex Hilbert spaces with scalar products $(\cdot,\cdot)_1, (\cdot,\cdot)_2$ and corresponding norms $\|\cdot\|_1, \|\cdot\|_2$ respectively; we assume the Hilbert spaces to be separable and adopt the convention that the scalar products are linear in the first argument and antilinear in the second. A (not necessarily bounded) *operator* T from $\mathcal{H}_1$ into $\mathcal{H}_2$ is a linear map defined on a linear subspace of $\mathcal{H}_1$, called the *domain* of T and denoted by dom T, into $\mathcal{H}_2$; we will also write $T : \text{dom } T \subset \mathcal{H}_1 \to \mathcal{H}_2$. We say that T is *densely defined* if dom T is dense in $\mathcal{H}_1$, and that T is *bounded* if there exists a constant $c > 0$ such that $\|Tx\|_2 \leq c\|x\|_1$ for all $x \in \text{dom } T$.

We call *range* the subset of $\mathcal{H}_2$ defined as $\text{ran } T = \{Tx : x \in \text{dom } T\}$, *kernel* of T the subset of $\mathcal{H}_1$ defined as $\ker T = \{x \in \text{dom } T : Tx = 0\}$, and *graph* of T the subset of $\mathcal{H}_1 \times \mathcal{H}_2$ defined as $\{(x, Tx) : x \in \text{dom } T\}$; they are linear subspaces of $\mathcal{H}_2$, $\mathcal{H}_1$ and $\mathcal{H}_1 \times \mathcal{H}_2$ respectively; we will sometimes write $T : \text{dom } T \subset \mathcal{H}_1 \to \text{ran } T \subset \mathcal{H}_2$. We say that T is *closed* if its graph is a closed subset of $\mathcal{H}_1 \times \mathcal{H}_2$. If $\ker T = \{0\}$, the *inverse operator* T^{-1} is the linear operator from $\mathcal{H}_2$ into $\mathcal{H}_1$ defined on $\text{dom } T^{-1} = \text{ran } T$ by $T^{-1}(Tx) = x$ for $x \in \text{dom } T$ and $T(T^{-1}x) = x$ for $x \in \text{ran } T$. We say that T is *compact* if T maps bounded sets in $\mathcal{H}_1$ into precompact sets in $\mathcal{H}_2$ or, equivalently, if for each bounded sequence $(x_n)_n \subset \mathcal{H}_1$, $(Tx_n)_n$ has a convergent subsequence in $\mathcal{H}_2$.

Let now $\mathcal{H}$ be a complex Hilbert space with scalar product $(\cdot,\cdot)$ and corresponding norm $\|\cdot\|$. Given a closed operator T on $\mathcal{H}$, i.e. from $\mathcal{H}$ into itself, with $\ker T = \{0\}$, we consider for $\lambda \in \mathbb{C}$ the operator $(T-\lambda)^{-1}$ on $\mathcal{H}$ and define the *resolvent set* of T as

$$\rho(T) = \{\lambda \in \mathbb{C} : (T-\lambda)^{-1} \text{ is bounded and everywhere defined on } \mathcal{H}\}.$$

We call *spectrum* of T the set

$$\sigma(T) = \mathbb{C} \setminus \rho(T).$$

The set $\rho(T)$ is an open subset of $\mathbb{C}$ and therefore $\sigma(T)$ is closed, see e.g. [Schmudgen, Proposition 2.6]. For $\lambda \in \rho(T)$ we call the operator $(T-\lambda)^{-1}$ on $\mathcal{H}$ the *resolvent* of T at λ and denote it by $R_\lambda(T) = (T-\lambda)^{-1}$.

By the open mapping theorem, $T-\lambda$ has a bounded inverse if it is bijective. The spectrum can then be subdivided according to how $T-\lambda$ violates the bijectivity condition; we define in particular the *point spectrum* of T as

$$\sigma_P(T) = \{\lambda \in \mathbb{C} : \ker(T-\lambda) \neq \{0\}\}.$$

For an unbounded operator, $\sigma(T) \setminus \sigma_P(T)$ may be non-empty and can be further partitioned; we single out the point spectrum as it makes up the whole spectrum for the class of operators that we consider, as detailed in the following subsection. We call $\lambda \in \sigma_P(T)$ an *eigenvalue* of T, the dimension of $\ker(T-\lambda)$ its *multiplicity*, and any non-zero element of $\ker(T-\lambda)$ an *eigenvector* of T corresponding to the eigenvalue λ. We say that an eigenvalue λ of T is *simple* if $\dim(\ker(T-\lambda)) = 1$, i.e. if it corresponds to one eigenvector only up to multiples. Note that λ is an eigenvalue of T if and only if

$$Tx = \lambda x \tag{1.1}$$

holds for some $x \in \text{dom } T \setminus \{0\}$. The spectrum of T is said to be *purely discrete* if $\sigma(T)$ only consists of isolated eigenvalues with finite multiplicities. This is true if the resolvent operator $(T-\lambda)^{-1}$ is compact for one, and thus for all, $\lambda \in \rho(T)$, see for instance [Schmudgen, Proposition 2.11].

1.2 The spectrum of a self-adjoint operator

Let A be a densely defined operator on $\mathcal{H}$ and set

$$\text{dom } A^\star = \{v \in \mathcal{H} : \exists\, w \in \mathcal{H} \text{ s.t. } (Au, v) = (u, w)\ \forall\, u \in \text{dom } A\}.$$

Since dom A is dense in $\mathcal{H}$, an element $w \in \mathcal{H}$ satisfying $(Au, v) = (u, w)$ for all $u \in \text{dom } A$ is uniquely determined by v. Thus, by setting

$$A^\star v = w, \quad v \in \text{dom } A^\star,$$

we obtain a well-defined operator $A^\star$ on $\mathcal{H}$; we call $A^\star$ the *adjoint* of A. Note that $A^\star$ is always a closed operator in $\mathcal{H}$, and that $(Au, v) = (u, A^\star v)$ holds for all $u \in \text{dom } A$ and $v \in \text{dom } A^\star$. The operator A is called *symmetric* if $(Au, v) = (u, Av)$ holds for all $u, v \in \text{dom } A$ or if, equivalently, $(Au, u) \in \mathbb{R}$ for all $u \in \text{dom } A$, or if dom $A \subseteq$ dom $A^\star$ and $Au = A^\star u$ for $u \in \text{dom } A$. Further, A is called *self-adjoint* if $A = A^\star$ holds. Every self-adjoint operator is symmetric, but the converse implication is not always true.

If A is a self-adjoint operator on $\mathcal{H}$, then its spectrum $\sigma(A)$ is contained in $\mathbb{R}$. Further, we say that a self-adjoint operator A is *semibounded below* by $\mu \in \mathbb{R}$ if

$$(Au, u) \geq \mu \|u\|^2, \quad u \in \text{dom } A; \tag{1.2}$$

note that μ is not unique since $(Au,u) \geq \mu\|u\|^2$ implies $(Au,u) \geq \tilde{\mu}\|u\|^2$ for all $\tilde{\mu} \in \mathbb{R}$ such that $\tilde{\mu} \leq \mu$. We call *lower bound* of A the largest number μ with the property (1.2); if μ is a lower bound of A the spectrum of A is bounded below by μ, that is, $\sigma(A) \subset [\mu, +\infty)$. Note that if λ_1 is the lowest eigenvalue of A, then by (1.1) $\mu\|u\|^2 \leq (Au,u) = \lambda_1(u,u) = \lambda_1\|u\|^2$ for the eigenvector u of A corresponding to λ_1, that is, $\mu \leq \lambda_1$.

We stated above that an operator with compact resolvent has purely discrete spectrum. A self-adjoint operator with compact resolvent has particularly good spectral properties as detailed in the following result, see e.g. [Schmudgen, Proposition 5.12].

Theorem 1.1. *Let $\mathcal{H}$ be infinite-dimensional and let A be a self-adjoint operator with compact resolvent on $\mathcal{H}$. Then the spectrum of A consists of a sequence $(\lambda_k)_k$ of real eigenvalues with finite multiplicities such that $\lim_{k\to\infty} |\lambda_k| = +\infty$, and the corresponding eigenvectors form an orthonormal basis of $\mathcal{H}$. Further, if A is semibounded below, then $\lim_{k\to\infty} \lambda_k = +\infty$.*

The spectrum of a self-adjoint operator which is semibounded below by some $\mu \in \mathbb{R}$ and has compact resolvent then consists of a sequence of eigenvalues which can be arranged non-decreasingly and counted according to their multiplicities as follows

$$\mu \leq \lambda_1 < \lambda_2 \leq \lambda_3 \leq \ldots;$$

note that the lowest eigenvalue is indexed by 1. We adopt this notation throughout this thesis.

Remark 1.2. Theorem 1.1 requires the self-adjoint operator to have compact resolvent. As detailed in the proof of Theorem 1.4 below, this is true whenever the domain of the operator is compactly embedded in the Hilbert space $\mathcal{H}$.

1.3 Sesquilinear forms and the min-max principle

Let $\mathcal{H}$ be again a complex Hilbert space with scalar product $(\cdot,\cdot)$ and corresponding norm $\|\cdot\|$. A mapping $\mathfrak{a}[\cdot,\cdot] : \mathrm{dom}\ \mathfrak{a} \times \mathrm{dom}\ \mathfrak{a} \to \mathbb{C}$ where $\mathrm{dom}\ \mathfrak{a} \subset \mathcal{H}$ is a linear subspace of $\mathcal{H}$ is called a *sesquilinear form* (or *form*) on $\mathcal{H}$ if it is linear in the first entry and anti-linear in the second. We call $\mathrm{dom}\ \mathfrak{a}$ the *domain* of $\mathfrak{a}$, and say that $\mathfrak{a}$ is *densely defined* if $\mathrm{dom}\ \mathfrak{a}$ is dense in $\mathcal{H}$. We call *quadratic form* associated to the form $\mathfrak{a}$ the map $\mathfrak{a}[\cdot] : \mathrm{dom}\ \mathfrak{a} \to \mathbb{C}$ defined by $\mathfrak{a}[u] \coloneqq \mathfrak{a}[u,u]$ for all $u \in \mathrm{dom}\ \mathfrak{a}$. A form $\mathfrak{a}$ is called *symmetric* if

$$\mathfrak{a}[u,v] = \overline{\mathfrak{a}[v,u]}, \quad u,v \in \mathrm{dom}\ \mathfrak{a},$$

or if, equivalently, $\mathfrak{a}[u]$ is real for all $u \in \mathrm{dom}\ \mathfrak{a}$. We say that a form $\mathfrak{a}$ is *semibounded below* (or *semibounded*) by $\mu \in \mathbb{R}$ if

$$\mathfrak{a}[u] \geq \mu\|u\|^2, \quad u \in \mathrm{dom}\ \mathfrak{a}, \tag{1.3}$$

If $\mu = 0$, we say that $\mathfrak{a}$ is *non-negative.* If $\mathfrak{a}$ is semibounded below by μ for some $\mu \in \mathbb{R}$, then $\mathfrak{a}$ is symmetric, and

$$(u,v)_{\mathfrak{a}} \coloneqq \mathfrak{a}[u,v] + (1-\mu)(u,v), \quad u,v \in \mathrm{dom}\ \mathfrak{a} \tag{1.4}$$

defines a scalar product on dom $\mathfrak{a}$; we denote by $\|\cdot\|_{\mathfrak{a}}$ the norm induced by $(\cdot,\cdot)_{\mathfrak{a}}$ on dom $\mathfrak{a}$. As with the analogous notion introduced above for operators, the choice of μ is not unique since $\mathfrak{a}[u] \geq \mu\|u\|^2$ implies $\mathfrak{a}[u] \geq \tilde{\mu}\|u\|^2$ for all $\tilde{\mu} \in \mathbb{R}$ such that $\tilde{\mu} \leq \mu$. However, replacing μ with $\tilde{\mu}$ in (1.4) yields a norm which is equivalent to $\|\cdot\|_{\mathfrak{a}}$ on dom $\mathfrak{a}$. We call *lower bound* of $\mathfrak{a}$ the largest number μ with the property (1.3). The notions of boundedness from above, upper bound, non-positiveness can be defined similarly, but we will only be concerned with forms semibounded below. Further, we say that a semibounded sesquilinear form $\mathfrak{a}$ on $\mathcal{H}$ is *closed* if (dom $\mathfrak{a}, (\cdot,\cdot)_{\mathfrak{a}}$) is a Hilbert space. A linear subspace $\mathcal{D}$ of dom $\mathfrak{a}$ is called a *core* of $\mathfrak{a}$ if it is dense in (dom $\mathfrak{a}, (\cdot,\cdot)_{\mathfrak{a}}$).

A closed semibounded form corresponds to a unique self-adjoint operator according to the following representation theorem. This statement is perhaps the most important in the theory of sesquilinear forms and self-adjoint operators; it can be found in [Kato, Chapter VI, Theorem 2.1] in the more general setting of sectorial forms.

Theorem 1.3. *Let $\mathfrak{a}$ be a densely defined, symmetric, semibounded below by some $\mu \in \mathbb{R}$, closed sesquilinear form in $\mathcal{H}$. Then there exists a unique self-adjoint operator A in $\mathcal{H}$ with* dom $A \subset$ dom $\mathfrak{a}$ *such that* dom A *is a core of* $\mathfrak{a}$ *and*

$$(Au, v) = \mathfrak{a}[u, v], \quad u \in \text{dom } A, v \in \text{dom } \mathfrak{a}, \tag{1.5}$$

and the operator is semibounded below by μ. Moreover, $u \in$ dom $\mathfrak{a}$ *belongs to* dom A *if and only if there exists $w \in H$ such that $\mathfrak{a}[u, v] = (w, v)$ holds for all v belonging to a core of $\mathfrak{a}$, in this case $Au = w$.*

Note that given a self-adjoint, semibounded operator A the form closure of the map $u \mapsto (Au, v)$ defines a closed, semibounded form on $\mathcal{H}$; Theorem 1.3 thus actually establishes a one-to-one correspondence between self-adjoint operators and closed forms. Also, in its bounded version this statement is equivalent to Riesz's representation theorem.

Besides its independent significance, Theorem 1.3 lays the foundation for the following classic result, know as the *(Courant – Fischer – Weyl) min-max principle* or *variational principle*; we mainly refer to it as min-max principle. It allows to compute the eigenvalues of a self-adjoint operator with purely discrete spectrum through its corresponding sesquilinear form $\mathfrak{a}$ as min-max of the quantity

$$R[u] = \frac{\mathfrak{a}[u]}{\|u\|^2},$$

know as *Rayleigh quotient* of $\mathfrak{a}$ at u.

Theorem 1.4 (Min-max principle)**.** *Let $\mathfrak{a}$ be a densely defined, closed, semibounded sesquilinear form in $\mathcal{H}$ and A be the corresponding self-adjoint, semibounded operator of Theorem 1.3. If, in addition,* dom $\mathfrak{a}$ *is compactly embedded into $\mathcal{H}$ then the spectrum of A is purely discrete, i.e. it consists of isolated eigenvalues with finite multiplicities. Upon enumerating these eigenvalues non-decreasingly according to their multiplicities,*

$$\eta_1 \leq \eta_2 \leq \dots,$$

the min-max principle

$$\eta_j = \min_{\substack{F \subset \mathrm{dom}\, \mathfrak{a} \\ \dim F = j}} \max_{u \in F \setminus \{0\}} \frac{\mathfrak{a}[u]}{\|u\|^2} \tag{1.6}$$

holds. In particular, the lowest eigenvalue η_1 *of* A *is given by*

$$\eta_1 = \min_{u \in \mathrm{dom}\, \mathfrak{a} \setminus \{0\}} \frac{\mathfrak{a}[u]}{\|u\|^2}, \tag{1.7}$$

and $u \in \mathrm{dom}\, \mathfrak{a}$ *is an eigenvector of* A *corresponding to* η_1 *if and only if* u *minimizes* (1.7)*.*

The min-max principle, in particular in its form (1.7), is crucial for the proofs of the main results in Papers I-III. For this reason, despite it being a classical result, we provide its proof, based on [BlanchardBruning, Theorem 6.1.2].

Proof. The operator A is self-adjoint, hence closed, that is, its graph is closed and so is the graph of $(A-\lambda)^{-1}$ for any $\lambda \in \rho(A)$. By the closed graph theorem, $(A-\lambda)^{-1} : \mathrm{ran}\,(A-\lambda) = \mathcal{H} \to \mathrm{dom}\,(A-\lambda) = \mathrm{dom}\, A \subset \mathcal{H}$ is bounded as it is closed and everywhere defined; here $\mathrm{dom}\, A$ is equipped with the norm $\|\cdot\|_{\mathfrak{a}}$ of $\mathrm{dom}\, \mathfrak{a}$ induced by (1.4). Now, the embedding i of $\mathrm{dom}\, A$ into $\mathcal{H}$ is compact since $\mathrm{dom}\, A \subset \mathrm{dom}\, \mathfrak{a}$ by Theorem 1.3. Thus, the resolvent $R_\lambda(A) = i(A-\lambda)^{-1} : \mathcal{H} \to \mathcal{H}$ is compact in $\mathcal{H}$. Theorem 1.1 then yields that A has a purely discrete, real spectrum accumulating at $+\infty$, and its eigenvectors form an orthonormal basis of $\mathcal{H}$.

Let now $(u_k)_k$ be an orthonormal basis of A such that $Au_k = \eta_k u_k$ for all $k \in \mathbb{N}$; its existence is guaranteed by Theorem 1.1. We wish to estimate the Rayleigh quotient

$$R[v] = \frac{\mathfrak{a}[v]}{\|v\|^2}, \quad v \in \mathrm{dom}\, \mathfrak{a},$$

by expanding the vectors $v \in \mathcal{H}$ in terms of this basis of eigenvectors with respect to the norm of $\mathcal{H}$. For each $v \in \mathrm{dom}\, \mathfrak{a}$ we have

$$v = \sum_{k=1}^{\infty} c_k u_k$$

for the complex coefficients $c_k = (v, u_k)$ such that $\|v\|^2 = \sum_{k=1}^{\infty} |c_k|^2$ is finite; the series converges in $(\mathcal{H}, \|\cdot\|_{\mathfrak{a}})$ and thus also in $\mathcal{H}$. Using (1.5) we compute

$$\mathfrak{a}[v] = (Av, v) = \sum_{k=1}^{\infty} (c_k A u_k, c_k u_k) = \sum_{k=1}^{\infty} (c_k \eta_k u_k, c_k u_k) = \sum_{k=1}^{\infty} \eta_k |c_k|^2$$

and thus

$$R[v] = \frac{\sum_{k=1}^{\infty} \eta_k |c_k|^2}{\sum_{k=1}^{\infty} |c_k|^2}.$$

Now, let $V_j = \operatorname{span}\{u_1, \dots, u_j\}$ denote the subspace of dom $\mathfrak{a}$ generated by the first j eigenvectors of A (by construction, dom $A \subset$ dom $\mathfrak{a}$). Since the eigenvalues are enumerated non-decreasingly, we have

$$\max_{v \in V_j} R[v] = \max_{(c_1,\dots,c_j)\in\mathbb{C}^d\setminus\{0\}} \frac{\sum_{k=1}^{\infty} \eta_k |c_k|^2}{\sum_{k=1}^{\infty} |c_k|^2} = \eta_j = R[v_j]; \tag{1.8}$$

it remains to show that $\max_{v\in F} R[v] \geq \eta_j$ for every other subspace F in the family of all j-dimensional subspaces of dom $\mathfrak{a}$. Let $F \neq V_j$ be such a subspace: then $F \cap V_j^{\perp} \neq \{0\}$ and it follows that

$$\max_{v\in F\setminus\{0\}} R[v] \geq \max_{v\in F\cap V_j^{\perp}\setminus\{0\}} R[v] = \max_{v=\sum\limits_{n\geq j+1} c_n v_n \in F\setminus\{0\}} \frac{\sum_{n\geq j+1} \eta_n c_n^2}{\sum_{n\geq j+1} c_n^2} \geq \eta_{j+1} \geq \eta_j$$

since any $v \in V_j^{\perp}$ can be written $v = \sum_{n\geq j+1} c_n v_n$. Thus,

$$\eta_j = \inf \max_{v\in F\setminus\{0\}} R[v]$$

which together with (1.8) proves (1.6); identity (1.7) follows immediately. As for the last statement, we first note that if u is an eigenvector of A corresponding to η_1 then it is non-zero and $R[u] = \eta_1$, that is, u minimizes (1.7). For the converse implication, assume that $u \in \operatorname{dom} \mathfrak{a} \setminus \{0\}$ minimizes (1.7), i.e., $a[u,u] = \eta_1 \|u\|^2$ holds. Our aim is to prove that

$$\mathfrak{a}[u,v] = \eta_1(u,v), \quad v \in \operatorname{dom} A; \tag{1.9}$$

$Au = \eta_1 u$ then follows from Theorem 1.3. Since u is a minimizer of the Rayleigh quotient, for all $v \in \mathcal{H}$ we have

$$0 = \frac{\mathrm{d}}{\mathrm{d}t} \frac{a[u+tv, u+tv]}{(u+tv, u+tv)}\bigg|_{t=0} = \frac{2\operatorname{Re} a[v,u] - 2\eta_1 \operatorname{Re}(v,u)}{\|u\|^2},$$

where we used the linearity of the form $\mathfrak{a}$ and of the inner product of $\mathcal{H}$ together with $a[u,u] = \eta_1\|u\|^2$. The same identity holds with Im instead of Re if v is replaced by iv, hence (1.9) holds. □

Remark 1.5. The min-max principle often appears in the literature with an operator-based Rayleigh quotient, that is,

$$R[u] = \frac{(Au,u)}{\|u\|^2}$$

for some self-adjoint, semibounded below operator A with purely discrete spectrum,
cf. [BlanchardBruning, Theorem 6.1.2] or [Teschl, Theorem 4.10]. Here, we chose to state it via a form-based Rayleigh quotient since this is how it appears in Papers I, II and III, see Section 2.1 below. We wish to point out that it might be easier to work with a form-based min-max principle since dom $A \subset$ dom $\mathfrak{a}$ holds when $\mathfrak{a}$ and A correspond in the sense of Theorem 1.3.

1.4 Lipschitz domains and Sobolev spaces

In this section we define Sobolev spaces on Lipschitz domains and on their boundaries and present some related technical facts.

Let $\Omega \subset \mathbb{R}^d$, $d \geq 1$, be an open set. Throughout this thesis we will write $x = (x_1, \dots, x_d)^\top$ for $x \in \mathbb{R}^d$. In order to handle the boundary of Ω and define function spaces on it we need additional assumptions on the set. Following [McLean, Definition 3.28], we say that $\Omega \subset \mathbb{R}^d$ is a *Lipschitz hypograph* if there exists a Lipschitz function $\xi : \mathbb{R}^{d-1} \to \mathbb{R}$ such that

$$\Omega = \{x = (x_1, \dots, x_d)^\top \in \mathbb{R}^d : x_d < \xi(x_1, \dots, x_{d-1})\}.$$

We then define Lipschitz domains as follows.

Definition 1.6. We say that $\Omega \subset \mathbb{R}^d$ is a *Lipschitz domain* if its boundary $\partial\Omega$ is compact and if there exist finite families $(W_j)_j$ and $(\Omega_j)_j$ of subsets of $\mathbb{R}^d$ such that

(i) each W_j is open and $\partial\Omega \subseteq \cup_j W_j$;

(ii) each Ω_j can be transformed into a Lipschitz hypograph by a rigid motion, i.e. a rotation plus a translation;

(iii) $W_j \cap \Omega = W_j \cap \Omega_j$ for all j.

We remark that a Lipschitz domain is not necessarily bounded nor connected; only its boundary is compact. Here and in the following we will assume in addition that $\Omega \subset \mathbb{R}^d$ is a bounded, connected Lipschitz domain. By Rademacher's theorem, for almost all $x \in \partial\Omega$ there exists a uniquely defined exterior unit normal vector $\nu(x)$; we equip the boundary $\partial\Omega$ with the standard surface measure, which we denote by σ. We denote by $L^2(\Omega)$ the Hilbert space of equivalence classes of square-integrable, complex-valued functions on Ω, equipped with the scalar product

$$(u, v)_{L^2(\Omega)} = \int_\Omega u\overline{v}, \quad u, v \in L^2(\Omega),$$

and the associated norm $\|\cdot\|_{L^2(\Omega)}$. We denote by $H^s(\Omega)$, $s > 0$, the L^2-based Sobolev space of order s on Ω; in Section 2 we will in particular make use of the scalar product

$$(u, v)_{H^1(\Omega)} = \int_\Omega (u\overline{v} + \nabla u \cdot \nabla \overline{v}), \quad u, v \in H^1(\Omega),$$

and of the associated norm $\|\cdot\|_{H^1(\Omega)}$. On the boundary we will consider the Sobolev space $H^{1/2}(\partial\Omega)$ and its dual space $H^{-1/2}(\partial\Omega)$; see for instance [McLean, Chapter 3] for the definition of fractional Sobolev spaces. Note that by [McLean, Theorem 3.37] there exists a unique bounded, everywhere defined, surjective trace map from $H^1(\Omega)$ onto $H^{1/2}(\partial\Omega)$ which continuously extends the mapping

$$C^\infty(\overline{\Omega}) \ni \varphi \mapsto \varphi|_{\partial\Omega};$$

we write $\varphi|_{\partial\Omega}$ for the trace of $\varphi \in H^1(\Omega)$ on $\partial\Omega$. Moreover, for $u \in H^1(\Omega)$ satisfying $\Delta u \in L^2(\Omega)$ in the distributional sense we define the normal derivative $\partial_\nu u|_{\partial\Omega}$ of u at $\partial\Omega$ to be the unique element in $H^{-1/2}(\partial\Omega)$ which satisfies the first Green identity (see for instance [McLean, Lemma 4.3])

$$\int_\Omega \nabla u \cdot \nabla \overline{v}\, \mathrm{d}x + \int_\Omega (\Delta u)\overline{v}\, \mathrm{d}x = (\partial_\nu u|_{\partial\Omega}, v|_{\partial\Omega})_{\partial\Omega}, \quad v \in H^1(\Omega); \tag{1.10}$$

here $(\cdot,\cdot)_{\partial\Omega}$ denotes the sesquilinear duality between $H^{1/2}(\partial\Omega)$ and its dual space $H^{-1/2}(\partial\Omega)$ defined as in [McLean, Theorem 3.14]. For sufficiently regular u, e.g., $u \in H^2(\Omega)$, the weakly defined normal derivative $\partial_\nu u|_{\partial\Omega}$ coincides with $\nu \cdot \nabla u|_{\partial\Omega}$ almost everywhere on $\partial\Omega$; in this case the duality in (1.10) may be replaced by the boundary integral of $\nu \cdot \nabla u|_{\partial\Omega}\overline{v}|_{\partial\Omega}$.

For any non-empty, relatively open set $\Sigma \subset \partial\Omega$ we denote by $H^1_{0,\Sigma}(\Omega)$ the Sobolev space

$$H^1_{0,\Sigma}(\Omega) = \left\{\varphi \in H^1(\Omega) : \varphi|_\Sigma = 0\right\},$$

where $\varphi|_\Sigma$ denotes the restriction of the trace $\varphi|_{\partial\Omega}$ to Σ; if $\Sigma = \partial\Omega$ we use the notation

$$H^1_0(\Omega) := H^1_{0,\partial\Omega}(\Omega) = \left\{\varphi \in H^1(\Omega) : \varphi|_{\partial\Omega} = 0\right\}.$$

Further, we say that $\psi \in H^{-1/2}(\partial\Omega)$ vanishes on Σ, and write $\psi|_\Sigma = 0$, if

$$(\psi, \varphi|_{\partial\Omega})_{\partial\Omega} = 0$$

holds for all $\varphi \in H^1_{0,\partial\Omega\setminus\overline{\Sigma}}(\Omega)$. Note that by continuity of the trace map $H^1_{0,\Sigma}(\Omega)$ is a closed subspace of $H^1(\Omega)$ for any $\Sigma \subset \partial\Omega$. We conclude with the following embedding statement due to Rellich, see for instance [McLean, Theorem 3.27] for a proof.

Theorem 1.7. *Let $\Omega \subset \mathbb{R}^d$ be an open, bounded, Lipschitz domain. Then the embedding of $H^1(\Omega)$ into $L^2(\Omega)$ is compact.*

2 The spectrum of Schrödinger operators with mixed boundary conditions

In this section we come to the main objects of this thesis, the eigenvalues of the mixed Dirichlet-Neumann problem for the (time-independent) Schrödinger equation. As informally mentioned at the start of this introduction, they can be obtained as solutions of the system (0.2); we now rigorously formulate the problem as an eigenvalue equation for the associated Schrödinger operator $-\Delta + V$. Showing that the system (0.2) can be solved for real λ is equivalent to showing that this operator admits non-empty, real point spectrum; in fact stronger statements on the spectrum will be shown. The mixed Dirichlet-Neumann boundary conditions will be reflected by choosing an appropriate domain for the operator.

In Section 2.1 we use the classical theory of semibounded forms representing self-adjoint operators reviewed in Section 1 to define the Schrödinger operator subject to mixed Dirichlet-Neumann boundary conditions and to prove that it admits a discrete sequence of real eigenvalues bounded below, each of which can be expressed with the min-max principle of Theorem 1.4. Further, we prove that these eigenvalues make up the whole spectrum, briefly discuss regularity of the eigenfunctions, and derive the same properties for the pure Dirichlet and Neumann problems. In Section 2.2 we put to use Theorem 1.4 to prove two preliminary results on eigenvalue inequalities between pure and mixed eigenvalues.

The mixed Dirichlet-Neumann Schrödinger operator will be defined as self-adjoint realization of the differential expression defined as follows; the (negative) Laplacian $-\Delta$ can be recovered as a special case of the Schrödinger operator by setting $V = 0$.

Definition 2.1. Let $\Omega \subset \mathbb{R}^d$ be a bounded, connected Lipschitz domain, see Definition 1.6, and let $V : \Omega \to \mathbb{R}$ be a measurable, bounded function. We define $\mathcal{S}$ on Ω as the second order partial differential expression of the form

$$\mathcal{S} = -\Delta + V = -\sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2} + V.$$

For a more detailed exposition on the Laplacian we refer to [Schmudgen, Section 10.6], for the Schrödinger operator and the choice of a potential see [Kato, Chapter V, Section 5] or [Schmudgen, Section 8.3], for further reading on their spectra see [Schmudgen, Chapter 12]; see also [AkhiezerGlazman, EdmundsEvans, ReedSimon].

2.1 Schrödinger operators and Laplacians with mixed boundary conditions

In this subsection we put to use the more abstract background developed in Section 1 to define Laplacians and Schrödinger operators with mixed Dirichlet-Neumann boundary conditions and derive their spectral properties. The results of this subsection are essentially known, but for the convenience of the reader we provide proofs.

In order to formulate the mixed Dirichlet-Neumann problem for the Schrödinger operator we make the following assumption on Ω.

Hypothesis 2.2. *The set $\Omega \subset \mathbb{R}^d$ is a bounded, connected Lipschitz domain, see Definition 1.6, and $\Gamma, \Gamma^c \subset \partial\Omega$ are relatively open subsets of the boundary such that*

$$\Gamma \cap \Gamma^c = \emptyset \quad \text{and} \quad \overline{\Gamma} \cup \overline{\Gamma^c} = \partial\Omega.$$

The function $V : \Omega \to \mathbb{R}$ is measurable and bounded.

An example of a planar domain satisfying Hypothesis 2.2 is shown in Figure 1.

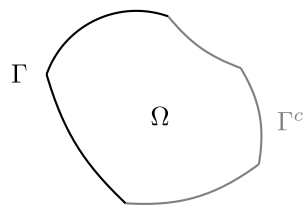

Figure 1: For this domain $\Omega \subset \mathbb{R}^2$, both Γ and Γ^c are non-empty.

Assuming that Hypothesis 2.2 holds, we define a sequilinear form $\mathfrak{a}$ on $L^2(\Omega)$ by

$$\mathfrak{a}[u, v] = \int_\Omega \left(\nabla u \cdot \overline{\nabla v} + V u \overline{v}\right)$$

with domain

$$\text{dom } \mathfrak{a} = H^1_{0,\Gamma}(\Omega) = \left\{u \in H^1(\Omega) : u|_\Gamma = 0\right\},$$

defined in the sense of Section 1.4. The following lemma ensures that Theorem 1.3 can be applied to the form $\mathfrak{a}$.

Lemma 2.3. *Let Hypothesis 2.2 be satisfied. Then the sesquilinear form $\mathfrak{a}$ is symmetric, semibounded below by $\mu = \inf_{x \in \Omega} V(x)$, and closed, and* dom $\mathfrak{a}$ *is dense in $L^2(\Omega)$. Further, the norms $\|\cdot\|_{\mathfrak{a}}$ and $\|\cdot\|_{H^1(\Omega)}$ are equivalent on* dom $\mathfrak{a}$.

Proof. First, dom $\mathfrak{a}$ is dense in $L^2(\Omega)$ since $C_0^\infty(\Omega) \subset \text{dom } \mathfrak{a}$. For $u \in \text{dom } \mathfrak{a}$ we have

$$\mathfrak{a}[u] = \int_\Omega \left(|\nabla u|^2 + V|u|^2\right) \geq \|\nabla u\|^2_{L^2(\Omega)} + \inf_{x \in \Omega} V(x) \|u\|^2_{L^2(\Omega)} \geq \mu \|u\|^2_{L^2(\Omega)} \quad (2.1)$$

where μ is the infimum of V, that is, $\mathfrak{a}$ is symmetric and semibounded below by $\mu = \inf_{x \in \Omega} V(x)$. Hence

$$(u, v)_{\mathfrak{a}} = \mathfrak{a}[u, v] + (1 - \mu) \int_\Omega u \overline{v}$$

defines a scalar product on dom $\mathfrak{a}$. To see that $\mathfrak{a}$ is closed, we need to show that the space (dom $\mathfrak{a}, \|\cdot\|_{\mathfrak{a}}$) is complete. First, note that (2.1) immediately yields

$$\|u\|_{\mathfrak{a}}^2 \geq \int_\Omega |\nabla u|^2 + \mu \int_\Omega |u|^2 + (1-\mu) \int_\Omega |u|^2 = \|u\|_{H^1(\Omega)}^2 \tag{2.2}$$

for $u \in$ dom $\mathfrak{a}$. Further, for $u, v \in$ dom $\mathfrak{a}$ we have

$$\begin{aligned} |\mathfrak{a}[u,v]| &\leq \sum_{j=1}^n \int_\Omega \left|\frac{\partial u}{\partial x_j}\right| \left|\frac{\partial v}{\partial x_j}\right| + M \int_\Omega |u||v| \\ &\leq \sum_{j=1}^n \left\|\frac{\partial u}{\partial x_j}\right\|_{L^2(\Omega)} \left\|\frac{\partial v}{\partial x_j}\right\|_{L^2(\Omega)} + M\|u\|_{L^2(\Omega)}\|v\|_{L^2(\Omega)} \end{aligned}$$

where M is an upper bound for $|V|$. Hence, there exists $c > 0$ such that

$$|a[u,v]| \leq c\|u\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)}, \quad u, v \in H^1(\Omega),$$

from which we can deduce $\|u\|_{\mathfrak{a}}^2 \leq C\|u\|_{H^1(\Omega)}^2$ for some $C > 0$. This together with (2.2) yields that the norms $\|\cdot\|_{\mathfrak{a}}$ and $\|\cdot\|_{H^1(\Omega)}$ are equivalent on dom $\mathfrak{a}$, which is a closed subspace of $H^1(\Omega)$ by the continuity of the trace map. Hence, (dom $\mathfrak{a}, \|\cdot\|_{\mathfrak{a}}$) is complete and $\mathfrak{a}$ is closed. □

We define the *Schrödinger operator with mixed Dirichlet-Neumann boundary conditions* associated with $\mathcal{S}$ in $L^2(\Omega)$ as

$$(-\Delta_\Gamma + V)u = \mathcal{S}u \tag{2.3}$$

with domain

$$\operatorname{dom}(-\Delta_\Gamma + V) = \{u \in H^1_{0,\Gamma}(\Omega) : \mathcal{S}u \in L^2(\Omega),\, \partial_\nu u|_{\Gamma^c} = 0\} \tag{2.4}$$

where V acts as a multiplication operator and the normal derivative is well-defined in the sense of Section 1.4. Note that since V is by assumption bounded, $\mathcal{S}u$ having integrable square is equivalent to Δu having integrable square. In the absence of a potential, i.e. $V = 0$, the Schrödinger operator reduces to the *(negative) Laplacian with mixed Dirichlet-Neumann boundary conditions* in $L^2(\Omega)$ as

$$-\Delta_\Gamma u = -\Delta u$$

with domain

$$\operatorname{dom}(-\Delta_\Gamma) = \{u \in H^1_{0,\Gamma}(\Omega) : \Delta u \in L^2(\Omega),\, \partial_\nu u|_{\Gamma^c} = 0\}.$$

Both operators can be shown to be self-adjoint and have good spectral properties, as follows.

Theorem 2.4. *Let Hypothesis 2.2 be satisfied. Then the operator $-\Delta_\Gamma + V$ is self-adjoint and semibounded below in $L^2(\Omega)$, and its spectrum is purely discrete and accumulates to $+\infty$.*

Proof. By Theorem 1.3, Lemma 2.3 immediately yields that there exists a unique self-adjoint operator A in $L^2(\Omega)$ with $\operatorname{dom} A \subset \operatorname{dom} \mathfrak{a} = H^1_{0,\Gamma}(\Omega)$ and

$$\mathfrak{a}[u,v] = (Au, v), \quad u \in \operatorname{dom} A, v \in \operatorname{dom} \mathfrak{a},$$

and that A is semibounded below by $\mu = \inf_{x\in\Omega} V(x)$. We now prove that $A = -\Delta_\Gamma + V$. Let $u \in \operatorname{dom} A$; for all $v \in C_0^\infty(\Omega) \subset \operatorname{dom} \mathfrak{a}$ we use integration by parts (1.10) to compute

$$\begin{aligned}(Au, v) = \mathfrak{a}[u,v] &= \int_\Omega \Big(\sum_{j=1}^d \frac{\partial u}{\partial x_j} \frac{\partial \overline{v}}{\partial x_j} + V u \overline{v} \Big) = \int_\Omega \Big(- \sum_{j=1}^d \frac{\partial^2 u}{\partial x_j^2} \overline{v} + V u \overline{v} \Big) \\ &= (\mathcal{S}u, v).\end{aligned}$$

In particular, $Au = \mathcal{S}u$ in the distributional sense and since A is an operator on $L^2(\Omega)$ we get that $\mathcal{S}u \in L^2(\Omega)$. Now, let $v \in \operatorname{dom} \mathfrak{a} = H^1_{0,\Gamma}(\Omega)$. We repeat the same computation and get

$$\begin{aligned}(Au, v) = \mathfrak{a}[u,v] &= \int_\Omega \Big(\sum_{j=1}^d \frac{\partial u}{\partial x_j} \frac{\partial \overline{v}}{\partial x_j} + V u \overline{v} \Big) \\ &= \int_\Omega \Big(\sum_{j=1}^d - \frac{\partial^2 u}{\partial x_j^2} \overline{v} + V u \overline{v} \Big) + \Big(\sum_{j=1}^d \Big(\partial_\nu \frac{\partial u}{\partial x_j} \Big)\Big|_{\partial\Omega}, v|_{\partial\Omega} \Big)_{\partial\Omega} \\ &= (\mathcal{S}u, v) + (\partial_\nu u|_{\partial\Omega}, v|_{\partial\Omega})_{\partial\Omega};\end{aligned}$$

in particular, since $v|_{\partial\Omega}$ vanishes on Γ, $Au = \mathcal{S}u$ holds in the distributional sense if and only if $\partial_\nu u|_{\partial\Omega}$ vanishes on Γ^c. Thus, we have $u \in H^1_{0,\Gamma}(\Omega)$ with $\mathcal{S}u \in L^2(\Omega)$ and $\partial_\nu u|_{\Gamma^c} = 0$, that is, $u \in \operatorname{dom}(-\Delta_\Gamma + V)$. Conversely, let $u \in \operatorname{dom}(-\Delta_\Gamma + V) \subset \operatorname{dom} \mathfrak{a}$. Then for each $v \in \operatorname{dom} \mathfrak{a} = H^1_{0,\Gamma}(\Omega)$ we have

$$(-\Delta_\Gamma u + V u, v) = (\mathcal{S}u, v) = \mathfrak{a}[u,v]$$

by the above computation. Theorem 1.3 then yields that $u \in \operatorname{dom} A$ and $Au = -\Delta_\Gamma u + Vu$. Thus, $-\Delta_\Gamma + V = A$ and $-\Delta_\Gamma + V$ is self-adjoint and semibounded below in $L^2(\Omega)$.

Since Ω is bounded, by Theorem 1.7 the embedding of $H^1_{0,\Gamma}(\Omega)$ in $L^2(\Omega)$ is compact as such is the embedding of $H^1(\Omega)$ in $L^2(\Omega)$ and $H^1_{0,\Gamma}(\Omega) \subseteq H^1(\Omega)$. An argument similar to the one performed at the start of the proof of Theorem 1.4 then yields that the resolvent of $-\Delta_\Gamma + V$ is compact in $L^2(\Omega)$, and the statement on the spectrum follows by Theorem 1.1. □

We proved that the spectrum of the Schrödinger operator $-\Delta_\Gamma + V$ under Hypothesis 2.2 consists of the sequence of eigenvalues counted according to their multiplicities

$$\lambda_1^\Gamma(V) < \lambda_2^\Gamma(V) \le \lambda_3^\Gamma(V) \le \dots;$$

this sequence is bounded below by the infimum of the potential V and the lowest eigenvalue is simple with a corresponding eigenfunction that can be chosen to be strictly positive inside Ω, see Lemma 2.6 and Remark 2.7 below. Note that the eigenvalues are indexed by the subset of the boundary Γ subject to a Dirichlet boundary condition.

By applying Theorem 1.4 we immediately get the following result.

Theorem 2.5. *Let Hypothesis 2.2 be satisfied. Then the eigenvalues of the Schrödinger operator with mixed Dirichlet-Neumann boundary conditions can be computed as*

$$\lambda_k^\Gamma(V) = \min_{\substack{L\subset H^1_{0,\Gamma}(\Omega)\\ \dim L=k}} \max_{u\in L\setminus\{0\}} \frac{\int_\Omega |\nabla u|^2 + V|u|^2}{\int_\Omega |u|^2}, \qquad k\in\mathbb{N}; \tag{2.5}$$

in particular

$$\lambda_1^\Gamma(V) = \min_{u\in H^1_{0,\Gamma}(\Omega)} \frac{\int_\Omega |\nabla u|^2 + V|u|^2}{\int_\Omega |u|^2}, \tag{2.6}$$

and $u \in H^1_{0,\Gamma}(\Omega)$ is an eigenfunction of $-\Delta_\Gamma + V$ if and only if it minimizes (2.6)*.*

We write $\lambda_k^\Gamma = \lambda_k^\Gamma(0)$ for the eigenvalues of the Laplacian $-\Delta_\Gamma$. Note that in this case (2.1) yields $\mathfrak{a}[u,u] \geq 0$, that is, the corresponding quadratic form $\mathfrak{a}$ is non-negative and thus so is the operator. The eigenvalues are then bounded below by 0; we can prove that the inequality is strict, along with some additional properties, as follows.

Lemma 2.6. *Let Hypothesis 2.2 be satisfied and assume that Γ is non-empty. Then $\lambda_1^\Gamma > 0$, λ_1^Γ is simple, and the eigenfunction corresponding to λ_1^Γ can be taken positive in Ω.*

Proof. By Theorem 2.5,

$$\lambda_1^\Gamma = \min_{u\in H^1_{0,\Gamma}(\Omega)} \frac{\int_\Omega |\nabla u|^2}{\int_\Omega |u|^2} = \frac{\int_\Omega |\nabla u_1|^2}{\int_\Omega |u_1|^2}.$$

where $u_1 \in H^1_{0,\Gamma}(\Omega)$ is an eigenfunction corresponding to λ_1^Γ. Assume by contradiction that $\lambda_1^\Gamma = 0$. Then $|\nabla u_1| = 0$ holds almost everywhere, i.e. u_1 is constant, which combined with the Dirichlet boundary condition $u_1|_\Gamma = 0$ implies $u_1 = 0$ identically on Ω, a contradiction. Now, assume by contradiction that u_1 changes sign within Ω. Then $|u_1|$ is also a minimizer of the Rayleigh quotient and is therefore also an eigenfunction of $-\Delta_\Gamma$ corresponding to λ_1^Γ by Theorem 2.5. Thus, $\Delta|u_1| = -\lambda_1^\Gamma|u_1| < 0$, and the minimum principle for superharmonic functions implies that u_1 cannot vanish inside Ω, a contradiction. Finally, if there were two eigenfunctions corresponding to λ_1^Γ it would be possible to consider a linear combination of them that changes sign, which is not possible. □

Remark 2.7. The same arguments of Lemma 2.6 yields that the lowest eigenvalue $\lambda_1^\Gamma(V)$ of the Schrödinger operator has multiplicity one and that the corresponding eigenfunction can be chosen positive in Ω; indeed if u_1 minimizes

(1.7) then its modulus $|u_1|$ is a minimizer as well. Further, note that using a simple variational argument based on (1.7) it is possible to prove that as soon as Γ is non-empty the lower bound of the infimum of V is strict, that is, $\lambda_1^\Gamma(V) > \inf_{x\in\Omega} V(x)$; we refer for instance to Lemma 2.1 in Paper III for the proof.

The eigenvalues of the Laplacian $-\Delta_\Gamma$ can then be enumerated as follows

$$0 < \lambda_1^\Gamma < \lambda_2^\Gamma \le \lambda_3^\Gamma \le \dots;$$

note that the argument proving that $\lambda_1^\Gamma > 0$ does not hold if Γ is empty, that is, λ_1^Γ is strictly positive as soon as Γ is non-empty.

The differential expression $\mathcal{S}$ introduced in Definition 2.1 admits two other important classes of self-adjoint realizations in $L^2(\Omega)$, each corresponding to a different choice of pure boundary conditions which can be obtained as extremal cases of Hypothesis 2.2. First, if $\Gamma = \partial\Omega$, the *Schrödinger operator with (pure) Dirichlet boundary conditions*, corresponding to the boundary condition $u|_{\partial\Omega} = 0$, defined as

$$(-\Delta_D + V)u = \mathcal{S}u, \qquad \operatorname{dom}(-\Delta_D + V) = \{u \in H_0^1(\Omega) : \mathcal{S}u \in L^2(\Omega)\};$$

second, if $\Gamma = \emptyset$, the *Schrödinger operator with (pure) Neumann boundary conditions*, corresponding to the boundary condition $\partial_\nu u|_{\partial\Omega} = 0$, defined as

$$(-\Delta_N + V)u = \mathcal{S}u, \qquad \operatorname{dom}(-\Delta_N + V) = \{u \in H^1(\Omega) : \mathcal{S}u \in L^2(\Omega), \partial_\nu u|_{\partial\Omega} = 0\}.$$

As a special case of Theorem 2.4 and Theorem 2.5 we get that these operators are self-adjoint with purely discrete spectrum and that their eigenvalues enjoy the min-max principle.

Corollary 2.8. *Let Hypothesis 2.2 be satisfied. The operators $-\Delta_D + V$ and $-\Delta_N + V$ are self-adjoint, semibounded below by $\inf_{x\in\Omega} V(x)$, and each of their spectra consists of a purely discrete sequence of eigenvalues, which we denote, enumerated increasingly according to their multiplicities, by $\lambda_k(V)$ and $\mu_k(V)$ respectively; they can be computed as*

$$\begin{aligned} \lambda_k(V) &= \min_{\substack{L \subset H_0^1(\Omega) \\ \dim L = k}} \max_{u \in L \setminus \{0\}} \frac{\int_\Omega |\nabla u|^2 + V|u|^2}{\int_\Omega |u|^2}, \\ \mu_k(V) &= \min_{\substack{L \subset H^1(\Omega) \\ \dim L = k}} \max_{u \in L \setminus \{0\}} \frac{\int_\Omega |\nabla u|^2 + V|u|^2}{\int_\Omega |u|^2}, \end{aligned} \tag{2.7}$$

for $k \in \mathbb{N}$. The associated sequences of eigenfunctions form orthonormal bases of $L^2(\Omega)$.

The *Dirichlet Laplacian* $-\Delta_D$ and *Neumann Laplacian* $-\Delta_N$ are defined by setting $V = 0$ and enjoy the same properties as the corresponding Schrödinger operators, with the difference that as above the absence of a potential allows for stronger spectral properties. We write $\lambda_k(0) = \lambda_k$ and $\mu_k(0) = \mu_k$ for the Dirichlet Laplacian and Neumann Laplacian eigenvalues respectively. As observed above, as a consequence of (2.1) all these eigenvalues are non-negative; in particular, since $\Gamma = \partial\Omega$ is non-empty, Lemma 2.6 holds and thus the lowest Dirichlet Laplacian eigenvalue λ_1 is strictly positive and simple:

$$0 < \lambda_1 < \lambda_2 \leq \lambda_3 \leq \dots .$$

As for the Neumann Laplacian, the Neumann boundary condition allows the first eigenvalue to be zero, making μ_2 the first relevant eigenvalue:

$$0 = \mu_1 < \mu_2 \leq \mu_3 \leq \dots .$$

We conclude this section with two remarks concerning more technical aspects of the mixed Dirichlet-Neumann problem for the Schrödinger operator.

Remark 2.9. In Definition 2.1 we require the potential V to be bounded, and this property facilitates the proofs of Lemma 2.3 and Theorem 2.4. In fact, the boundedness condition could be relaxed as it is possible to prove that the Schrödinger operator admits purely discrete spectrum also under more general assumptions, for instance if the subset of Ω on which V is positive and bounded by some constant M has finite Lebesgue measure for all $M > 0$, see [Simon09, Theorem 1]. We refer the reader to [Simon09] and to the survey [Mazya07, Section 16] for a review of more general sufficient conditions for a discrete spectrum.

Remark 2.10. We now address the question of the regularity of $\mathrm{dom}\,(-\Delta_\Gamma + V)$ on the bounded, connected Lipschitz domains Ω under our consideration; note that even though thus far we have required the boundary of Ω to be Lipschitz, in Papers I - III we make the additional assumption that $\partial\Omega$ is piecewise C^∞-smooth. Since the proofs of our main results in Papers I - III rely on taking gradients of pure or mixed eigenfunctions as test functions for the variational principles, we need these gradients to belong to $H^1(\Omega)$ and thus the functions in $\mathrm{dom}\,(-\Delta_\Gamma + V)$ to belong to $H^2(\Omega)$. In the pure Dirichlet or Neumann case, H^2-regularity holds if $\partial\Omega$ has no inward-pointing angles, see for instance [AGMT10, Proposition 4.8]; for more details we refer to e.g. [Evans, Chapter 6], [McLean, Chapter 4], or the survey [KondratevOleinik83].

The mixed case, however, is somewhat delicate. First of all, the problem can be highly singular if for instance the subset of the boundary where the transition between Dirichlet and Neumann boundary conditions takes place, i.e. $\overline{\Gamma} \cap \overline{\Gamma^c}$ in the notation of Hypothesis 2.2, is situated in the interior of a smooth subset of the boundary; see [Brown94] or [OttBrown13] for more details. We will therefore always assume that the transition happens at the singular points of the domain Ω, that is, at the intersections of the smooth subsets of which $\partial\Omega$ is composed. The general criterion for H^2-regularity is that it holds if additional assumptions are imposed on each singular point at which the transition in boundary conditions takes place; in practice, however, it is quite challenging to exactly formulate these assumptions. We refer the reader to Proposition 4.1 in Paper I, and Proposition 2.3 and Proposition 2.4 in Paper III for examples of sufficient conditions for H^2-regularity in the planar and higher-dimensional case respectively; for further reading on regularity of mixed problem we refer to [Grisvard85], [Grisvard92], [Dauge] or in particular [Dauge92]. Finally, we point out that these conditions for H^2-regularity are only sufficient as can be quickly verified by computing the eigenfunctions for the mixed Dirichlet-Neumann problem on a rectangular or cubic domain.

2.2 Some elementary eigenvalue inequalities

The min-max principles of Theorem 2.5 and Corollary 2.8 are extremely powerful tools and constitute the foundation to the proofs of the main results in Paper I-III. We point out that in Paper II we prove a joint, novel variational principle for the eigenvalues of the mixed Dirichlet-Neumann Laplacian $-\Delta_\Gamma$ and its "dual" $-\Delta_{\Gamma^c}$ with a Dirichlet boundary condition on Γ^c and Neumann on Γ, see Theorem 3.9 and Theorem 3.13 in Paper II.

We begin to illustrate the potency of the min-max principles by proving some preliminary inequalities between pure and mixed eigenvalues of the Schrödinger operator; these eigenvalue inequalities pave the way for the results contained in this thesis, as will be illustrated in Section 3.1, and can be obtained as corollaries to Theorem 2.5 and Corollary 2.8. The first result follows immediately from the inclusion of spaces $H_0^1(\Omega) \subset H_{0,\Gamma}^1(\Omega) \subset H^1(\Omega)$.

Corollary 2.11. *Let Hypothesis 2.2 be satisfied. Then,*

$$\mu_k(V) \leq \lambda_k^\Gamma(V) \leq \lambda_k(V)$$

holds for all $k \in \mathbb{N}$.

The following strict monotonicity principle describes the behaviour of the eigenvalues of the mixed Dirichlet-Neumann problem when the Dirichlet part of the boundary is increased.

Corollary 2.12. *Let Hypothesis 2.2 be satisfied. Assume that $\Gamma \subset \Gamma' \subset \partial\Omega$ are non-empty, relatively open sets such that $\Gamma' \setminus \Gamma$ has a non-trivial interior. Then*

$$\lambda_k^\Gamma(V) < \lambda_k^{\Gamma'}(V)$$

holds for all $k \in \mathbb{N}$.

The proof is based on the following unique continuation principle; it can be proved similarly to [Rohleder14, Lemma 3.1].

Lemma 2.13. *Let Ω be a bounded, connected Lipschitz domain and let $V : \Omega \to \mathbb{R}$ be measurable and bounded. Let $\lambda \in \mathbb{R}$ and $u \in H^1(\Omega)$ be such that $-\Delta u + Vu = \lambda u$. If $\Sigma \subset \partial\Omega$ is a relatively open, nonempty set such that $u|_\Sigma = 0$ and $\partial_\nu u|_\Sigma = 0$ then $u = 0$ identically on Ω.*

Proof of Corollary 2.12. Let $k \in \mathbb{N}$ and consider the eigenvalue $\lambda_k^{\Gamma'}(V)$. By the min-max principle (2.6) there exists a subspace $L \subset H_{0,\Gamma'}^1(\Omega)$ with $\dim L = k$ such that

$$\int_\Omega |\nabla u|^2 + V|u|^2 \leq \lambda_k^{\Gamma'}(V) \int_\Omega |u|^2, \quad u \in L. \tag{2.8}$$

Now, let $v \in \ker(-\Delta_\Gamma + V - \lambda_k^{\Gamma'}(V))$. For all $u \in L$ we have $u + v \in H^1_{0,\Gamma}(\Omega)$ since $H^1_{0,\Gamma'}(\Omega) \subset H^1_{0,\Gamma}(\Omega)$, and

$$\begin{aligned}\int_\Omega (|\nabla(u+v)|^2 + V|u+v|^2) &= \int_\Omega (|\nabla u|^2 + V|u|^2) + 2\,\mathrm{Re}\int_\Omega \left(\nabla v \cdot \overline{\nabla u} + V u \overline{v}\right) \\ &\quad + \int_\Omega (|\nabla v|^2 + V|v|^2) \\ &\le \lambda_k^{\Gamma'}(V) \int_\Omega |u|^2 + 2\lambda_k^{\Gamma'}(V)\,\mathrm{Re}\int_\Omega v\overline{u} + \lambda_k^{\Gamma'}(V)\int_\Omega |v|^2 \\ &= \lambda_k^{\Gamma'}(V) \int_\Omega |u+v|^2,\end{aligned} \tag{2.9}$$

where we have used (2.8) on the first summand and Green's identity (1.10) on the second and third; note that both resulting boundary integrals vanish as $u|_\Gamma = 0 = v|_\Gamma$ and $\partial_\nu v|_{\Gamma^c} = 0$. We now wish to estimate $\dim(L + \ker(-\Delta_\Gamma + V - \lambda_k^{\Gamma'}(V)))$. First, $L \cap \ker(-\Delta_\Gamma + V - \lambda_k^{\Gamma'}(V)) = \{0\}$ follows from Lemma 2.13 when choosing Σ to be the interior of $\Gamma' \setminus \Gamma$. Thus

$$\dim\left(L + \ker(-\Delta_\Gamma + V - \lambda_k^{\Gamma'}(V))\right) = k + r$$

where we denote $r = \dim(\ker(-\Delta_\Gamma + V - \lambda_k^{\Gamma'}(V)))$. This, combined with (2.9) and the min-max principle (2.6), yields

$$\lambda_k^\Gamma(V) \le \lambda_{k+r}^\Gamma(V) \le \lambda_k^{\Gamma'}(V). \tag{2.10}$$

The second inequality in (2.10) implies that $-\Delta_\Gamma + V$ has at least $k+r$ eigenvalues in $(-\infty, \lambda_k^{\Gamma'}(V)]$, hence at least k in $(-\infty, \lambda_k^{\Gamma'}(V)]$, from which $\lambda_k^\Gamma(V) < \lambda_k^{\Gamma'}(V)$. $\square$

3 Eigenvalue inequalities for Laplacians and Schrödinger operators with mixed boundary conditions, and a variant of the “hot spots” conjecture

The stage is now set to discuss more recent research topics, including the contents of this thesis, involving the eigenvalues and eigenfunctions of the Schrödinger operator with mixed Dirichlet-Neumann boundary conditions defined by (2.3) and (2.4) under Hypothesis 2.2, which for the convenience of the reader we repeat here.

Hypothesis. *The set $\Omega \subset \mathbb{R}^d$ is a bounded, connected Lipschitz domain, and $\Gamma, \Gamma^c \subset \partial\Omega$ are relatively open subsets of the boundary such that*

$$\Gamma \cap \Gamma^c = \emptyset \quad \text{and} \quad \overline{\Gamma} \cup \overline{\Gamma^c} = \partial\Omega.$$

The function $V : \Omega \to \mathbb{R}$ is measurable and bounded.

Throughout this section we assume that this hypothesis is satisfied; we will often make additional assumptions on Ω such as convexity or additional regularity of the boundary $\partial\Omega$. We recall that the eigenvalues and eigenfunctions of the Schrödinger operator with mixed Dirichlet-Neumann boundary conditions solve

$$\begin{cases} -\Delta u + Vu = \lambda u & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma, \\ \partial_\nu u = 0 & \text{on } \Gamma^c, \end{cases}$$

where the boundary conditions are to be understood in the sense of Section 1.4. If Γ and Γ^c are both non-empty we denote the eigenvalues by $\lambda_k^\Gamma(V)$, $k \in \mathbb{N}$; in the extremal case in which $\Gamma = \partial\Omega$ the problem simplifies to (pure) Dirichlet boundary conditions with eigenvalues λ_k, $k \in \mathbb{N}$, while the case $\Gamma = \emptyset$ corresponds to (pure) Neumann boundary conditions with eigenvalues μ_k, $k \in \mathbb{N}$. If $V = 0$, the Schrödinger operator simplifies to the (negative) Laplacian; we use the same notation for its eigenvalues but drop the dependency on V.

In Section 3.1 we review existing research on eigenvalue inequalities for the Schrödinger operator with Dirichlet, Neumann or mixed Dirichlet-Neumann boundary conditions, while Section 3.2 is devoted to the hot spots conjecture for Neumann and mixed Dirichlet-Neumann eigenfunctions. In both sections we briefly mention the results contained in this thesis to contextualize them, but refer the reader to the summaries of the included papers for a more detailed overview.

The eigenvalues of the mixed Dirichlet-Neumann problem for the Laplacian have also been studied from a variety of points of view; to mention a few, the limiting behaviour if the Dirichlet or Neumann portion shrinks [FNO22, FNO21], isospectrality [Herbrich11], Faber–Krahn type inequalities [AnoopKumar23], stability under domain perturbations [Cardone23].

3.1 Eigenvalue inequalities for Laplacians and Schrödinger operators with mixed boundary conditions

The mixed Dirichlet-Neumann problem for the Schrödinger operator can be naturally thought of as "in between" the pure Neumann and the pure Dirichlet problem, in the sense that as observed in Corollary 2.11 its eigenvalues satisfy

$$\mu_k(V) \leq \lambda_k^\Gamma(V) \leq \lambda_k(V), \quad k \in \mathbb{N}. \tag{3.1}$$

Further, if $\Gamma' \subseteq \Gamma \subset \partial\Omega$, we showed in Corollary 2.12 that

$$\lambda_k^{\Gamma'}(V) \leq \lambda_k^\Gamma(V), \quad k \in \mathbb{N}, \tag{3.2}$$

holds where the inequality is strict if $\Gamma \setminus \Gamma'$ has a non-trivial interior. These inequalities prompt the following questions.

(i) Can the indices appearing in the inequalities (3.1) be shifted? That is, is it possible to prove $\mu_{k+n}(V) \leq \lambda_k(V)$, $\lambda_{k+n}^\Gamma(V) \leq \lambda_k(V)$, or $\mu_{k+n}(V) \leq \lambda_k^\Gamma(V)$ for some $k, n \in \mathbb{N}$?

(ii) Can the subsets appearing in the inequality (3.2) be chosen not to satisfy an inclusion? That is, is it possible to prove that $\lambda_k^{\Gamma'} \leq \lambda_k^\Gamma$ holds for some disjoint $\Gamma, \Gamma' \subset \partial\Omega$?

One cannot answer these questions without looking at the geometric features of the underlying domain: the number n often depends on its dimension, on its convexity, on a geometric feature of the portions of boundary Γ and Γ^c or on certain properties of the potential, if present; usually, to prove an inequality of the type (3.2) one needs specific geometrical assumptions on both sets Γ and Γ' to make up for the lack of an inclusion. In this thesis we advance the existing answers to both questions, and our answers affirm the strong dependence of the eigenvalue inequalities to the mentioned features of the underlying domain; we refer to the summaries of the included papers for more details.

The first eigenvalue inequalities of the type $\mu_{k+n}(V) \leq \lambda_k(V)$ related to the question (i) date back to the 1950s and since then have been the object of considerable attention, we review them in Section 3.1.1; on the other hand, eigenvalue inequalities for mixed eigenvalues constitute a relatively recent line of research and, to the best of our knowledge, there exist only a handful of contributions besides the ones contained in Papers I - III. We review inequalities between mixed and non-mixed eigenvalues in Section 3.1.1, and devote Section 3.1.2 to inequalities between mixed eigenvalues in the line of question (ii). We emphasize that the vast majority of the available inequalities concern eigenvalues of the Laplacian, while inequalities for the eigenvalues of the Schrödinger operator are less represented. For this reason we first review inequalities for the eigenvalues of the Laplacian and address the Schrödinger operator and the end of each section.

3.1.1 Question (i) - index shifts

The trivial inequality $\mu_1 \leq \lambda_1$ was first improved by Polya [Polya52], who in 1952 proved that $\mu_2 < \lambda_1$ holds in the two-dimensional case. Szegő [Szego54], Payne

[Payne55], Aviles [Aviles86] obtained further results in this direction; in 1986 Levine and Weinberger [LevineWeinberger86] proved, amongst other estimates,

$$\mu_{k+d} < \lambda_k, \quad k \in \mathbb{N}, \tag{3.3}$$

for bounded, convex d-dimensional domains with C^2-boundary; they also pointed out that the non-strict inequality holds by approximation on any bounded, convex d-dimensional domain. The inequality (3.3) is in some sense final and cannot be further improved as, for instance, on a two-dimensional disk $\mu_4 > \lambda_1$ holds, cf. [Rohleder23, Example 4.6].

The proofs of Levine and Weinberger rely on the sign of the curvature of the boundary, which is fixed if the domain is convex (see for instance Paper I or Paper III for more details), and cannot therefore be extended to non-convex domains. Whether inequality (3.3) holds for non-convex domains remains an open question, see Conjecture 3.2.42 in [LMP23]. A major advancement was made in 1991 by Friedlander [Friedlander91] who proved that

$$\mu_{k+1} \leq \lambda_k, \quad k \in \mathbb{N}, \tag{3.4}$$

holds for bounded d-dimensional domains with C^1-boundary (see also [ArendtMazzeo12] for a different proof); in 2004 Filonov [Filonov04] showed the same strict inequality for more general d-dimensional domains. While Filonov's result remains the most general for non necessarily convex domains, we also mention the recent [Rohleder23] where $\mu_{k+2} \leq \lambda_k$ is established for bounded, simply connected, Lipschitz two-dimensional domains.

A sparse quantity of results of the type $\lambda^{\Gamma}_{k+n} \leq \lambda_k$ and $\mu_{k+n} \leq \lambda^{\Gamma}_k$ appears in the literature. The first instance of such result is due to Lotoreichik and Rohleder [LotoreichikRohleder17], who sharpened (3.4) by proving

$$\mu_{k+1} \leq \lambda^{\Gamma}_k, \quad k \in \mathbb{N}, \tag{3.5}$$

on any bounded d-dimensional Lipschitz domain and under the condition that the Neumann part Γ^c is "small" enough in the sense that there exists a non-trivial vector tangential to almost all points of Γ^c. They also proved

$$\lambda^{\Gamma}_{k+l} \leq \lambda_k, \quad k \in \mathbb{N}, \tag{3.6}$$

in case there exist l independent vectors which are tangential to all of Γ. Under additional assumptions on the choice of Γ and Γ^c these inequalities can be made strict. To the best of our knowledge, no other results of this type are available for eigenvalues of the Laplacian.

Besides the very first contributions by Polya and Szegő, which due to the planar setting made use of conformal mappings, all the eigenvalue inequalities reviewed above are essentially proved in two distinct ways:

(i) either by expressing the difference of the eigenvalue counting functions by the number of negative eigenvalues of the corresponding parameter-dependent Dirichlet-to-Neumann map operator [Friedlander91, ArendtMazzeo12];

(ii) or by using a purely variational approach and estimating the Rayleigh quotients (2.6) - (2.7) by making appropriate choices of test functions [Payne55, LevineWeinberger86, Aviles86, Filonov04, LotoreichikRohleder17, Rohleder23].

The variational approach has proven to be easier to handle; cf. [Filonov04] which even generalizes [Friedlander91] with a much shorter proof. The test functions used in order to estimate the corresponding Rayleigh quotients are either of the form $e^{i\omega \cdot x}$ for some appropriate vector ω [Filonov04] or are suitable linear combinations of partial derivatives of certain eigenfunctions [Payne55, LevineWeinberger86, Aviles86, LotoreichikRohleder17, Rohleder23]. The geometric features of the domain, such as convexity or curvature of certain portions of the boundary, contribute heavily both in the choice of the test function and in the computations leading to the estimate for the corresponding Rayleigh quotients. As will be detailed in the summaries of the included papers, all of the results on eigenvalue inequalities contained in this thesis are proved using variational techniques.

Finally, we point out that all mentioned estimates extend to Schrödinger operators with constant potentials since adding a constant simply shifts all eigenvalues by that constant; in order to establish inequalities for the eigenvalues of Schrödinger operators with non-constant potentials in general one needs to ensure that the potential is sufficiently close to a constant in some sense to be specified. The only result that fits in our precise setting is the inequality

$$\mu_{k+r}(V) \leq \lambda_k(V), \quad k \in \mathbb{N}, \tag{3.7}$$

for bounded, convex d-dimensional domains contained in [Rohleder21Schr]; $r \in \mathbb{N}$ is the number of directions that V does not depend on. Some improvements of the inequality can be obtained if the potential enjoys some additional convexity properties. In Paper III we prove an inequality between mixed and Dirichlet eigenvalues of the Schrödinger operator which can be regarded as a unification of (3.6) and (3.7).

Although in slightly different settings, other inequalities for eigenvalues of the Schrödinger operator can be found in [BRS18], which compares mixed Robin-Dirichlet eigenvalues on unbounded domains and Dirichlet eigenvalues corresponding to different potentials; we also point out [Rohleder14] dealing with Robin eigenvalues of more general elliptic operators. Further, eigenvalue inequalities of the type (3.4) have been the object of interest in other situations: Robin boundary conditions [GesztesyMitrea09, Levine88], the Laplacian on the Heisenberg group [FrankLaptev10, Hansson08] or on manifolds [AshbaughLevine97, Mazzeo91, IliasShouman20, Wang18], the Stokes operator [DenisElst22, Kelliher10], polyharmonic operators [Provenzano19, Lotoreichik24] and in the isoperimetric setting [Cox19, Siudeja10].

3.1.2 Question (ii) - inequalities of the type $\lambda_k^\Gamma \leq \lambda_k^{\Gamma'}$

Inequalities between mixed Dirichlet-Neumann eigenvalues λ_k^Γ and $\lambda_k^{\Gamma'}$ corresponding to different choices of the subsets Γ and Γ' of the boundary constitute a fairly recent and emerging research topic. Expanding the part of the boundary subject to a Dirichlet boundary condition leads to an increase of the corresponding eigenvalue if Γ and Γ' satisfy an inclusion, as shown by (3.1) and (3.2). A dependency on length is also suggested by the fact that if $\lambda_k^{\Gamma} = \lambda_k^{\Gamma^c}$ holds for all $k \in \mathbb{N}$ on planar domains, then Γ and Γ^c have the same length, see [JLNP04, Proposition 3.3.1]; we also refer to [LPP06] for more necessary conditions for isospectrality. However, in general λ_k^{Γ} does not depend monotonously on the length of Γ, that is, choosing Γ' with a smaller length than Γ but such that Γ and Γ' do not satisfy an inclusion does not always guarantee that $\lambda_k^{\Gamma'}$ is smaller than λ_k^{Γ}; a counterexample for the lowest eigenvalues based on numerical computations on a polygon can be found in [Siudeja16, Remark 3.3]. The current understanding of the validity inequalities of the type $\lambda_k^{\Gamma} \leq \lambda_k^{\Gamma'}$ if Γ and Γ' do not satisfy an inclusion is limited even for very elementary classes of domains; it should also be noted that, to the best of our knowledge, all available inequalities concern the lowest eigenvalues.

Arbitrary triangles are the simplest planar domains for which mixed eigenvalues cannot be computed explicitly. In 2016 Siudeja conjectured, cf. Conjecture 1.2 in [Siudeja16], that mixed Dirichlet-Neumann eigenvalues of the Laplacian on an arbitrary triangle can be fully ordered, as follows.

Conjecture 3.1. *Let S, M, L denote the sides of a triangle ordered non-decreasingly by their lenghts. For an arbitrary triangle,*

$$\lambda_1^S < \lambda_1^M < \lambda_1^L < \lambda_1^{S\cup M}$$

as long as the appropriate sides have different lengths.

Siudeja proved the full conjecture, cf. Theorem 1.1 in [Siudeja16], only for right triangles whose smallest angle satisfies $\pi/6 < \alpha < \pi/4$, see Figure 2, and parts of the conjecture for arbitrary triangles, that is,

$$\min(\lambda_1^S, \lambda_1^M, \lambda_1^L) < \mu_2 \leq \lambda_1^{S\cup M} < \lambda_1^{S\cup L} < \lambda_1^{L\cup M} \tag{3.8}$$

for an arbitrary triangle as long as the appropriate sides have different lengths; μ_2 is the first non-zero Neumann eigenvalue. The inequalities in [Siudeja16] are

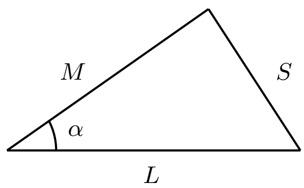

Figure 2: For this right triangle, Conjecture 3.1 is verified as its smallest angle α measures between $\pi/6$ and $\pi/4$.

proved using a very broad spectrum of techniques including the variational approach, polarization, nodal domain considerations, and the unknown trial function method. We point out that Chen, Gui and Yao recently claimed a full proof of Conjecture 3.1, cf. Theorem 7.3 in [CGY23]; their proof makes use of variational techniques relying on the monotonicity of certain eigenfunctions.

A result for domains more general than triangles is due to Rohleder [Rohleder21]: $\lambda_1^{\Gamma^c} \leq \lambda_1^{\Gamma}$ holds on polygons if Γ^c consists of a single side whose adjacent angles are smaller than $\pi/2$; an application of this result to triangles affirms parts of (3.8) without requiring that the sides have different lenghts. In [Rohleder21] Rohleder also proved

$$\max\{\lambda_1^S, \lambda_1^M\} \leq \lambda_1^L \tag{3.9}$$

for right triangles. The proofs in [Rohleder21] are purely variational, based on (2.6), and take inspiration from Levine–Weinberger [LevineWeinberger86] in choosing a test function as an appropriate directional derivative of the eigenfunction corresponding to λ_1^{Γ}; the geometric condition on the angles guarantees regularity of the chosen test function in the sense of Remark 2.10. In Papers I and III we extend and generalize this variational approach to prove inequalities of the type $\lambda_1^{\Gamma'}(V) < \lambda_1^{\Gamma}(V)$ on planar and higher-dimensional domains with piecewise smooth boundary. An application of these results will allow to prove a non-strict version of (3.9) for obtuse and right triangles. Paper II also deals with inequalities of the type $\lambda_1^{\Gamma^c} < \lambda_1^{\Gamma}$ with a variational approach, although the proofs, instead of relying on the variational principle (2.6), are based on the novel variational principles therein established.

Finally, we would like to mention that eigenvalues of mixed boundary conditions and inequalities for them have attracted interest due to their application in the study of e.g. the hot spots conjecture, as detailed in the following section, isospectral domains [GWW93], or the study of nodal set of Neumann eigenfunctions [BerardHeffler21, BBF17].

3.2 The mixed formulation of the "hot spots" conjecture

The "hot spots" conjecture in its strongest form says that the eigenfunction corresponding to the smallest positive eigenvalue of the Laplacian on a bounded domain with Neumann boundary conditions, μ_2 in the notation introduced in Section 2, attains its maximum and minimum only on the boundary of the domain. J. Rauch first proposed the conjecture in 1974 and was lead to its formulation by observing that the long time behaviour of the hottest and coldest spots in an insulated body with "generic" initial heat distribution is to diverge from each other as much as they can, that is, converge to the boundary; we refer to [Kawohl85, Section II.5] for more details. It has also been conjectured that conditioned Brownian motion on any convex domain also has the hot spots property in the sense that the Neumann boundary condition can be interpreted as a reflection condition for the Brownian motion, see for instance [BanuelosMendez06] for more details. Note that the eigenfunction might not be unique, that is, μ_2 is not necessarily a simple eigenvalue; it was shown in [BassBurdzy00] that μ_2 is simple under various conditions on the underlying domain.

The conjecture is true for simple shapes on which the eigenfunctions in question can be computed explicitly, such as balls, cubes, equilateral triangles or right isosceles triangles, but has been shown to be false for certain planar bounded domans with holes, cf. the counterexamples contained in [Burdzy05], [BurdzyWerner99] and the numerical study [Kleefeld21]. It is now widely believed that the conjecture holds for all bounded planar convex domains; however, even this remains open.

The conjecture remained completely open until 1999 when Bañuelos and Burdzy [BanuelosBurdzy99] proved that it is true for obtuse triangles and sufficiently long convex domains with symmetries. At the moment, there exists a number of few non-trivial results for planar domains: to cite only a few, Atar and Burdzy [AtarBurdzy04] showed it for so-called lip-domains, i.e. domains enclosed by the graphs of two Lipschitz continuous functions with Lipschitz constants at most one, and the most recent result is a proof for arbitrary triangles due to Judge and Mondal [JudgeMondal20, JudgeMondal22]. We also note that an earlier partial result by Siudeja [Siudeja15] for acute triangles with one angle smaller or equal to $\pi/6$ is linked to the aforementioned paper by the same author [Siudeja16]. Some of the earlier proofs are of probabilistic nature, based on reflected Brownian motion [AtarBurdzy04, BanuelosBurdzy99], but the latest developments mostly rely on tracing critical points of eigenfunctions under perturbations of the domain [JudgeMondal20, Siudeja15]. We also point out that the recent preprint [Rohleder23HotSpots] proposes a new approach to the hot spots conjecture by providing a completely analytic proof of the conjecture, based on variational principles, on lip domains.

The mixed Dirichlet-Neumann eigenvalue problem for the Laplacian holds its own significant and it is therefore natural to reformulate the hot spots conjecture in terms of it. The question was first raised in 2004 by Bañuelos and Pang [BanuelosPang04] and properly formulated in [BanuelosPangPascu04] as follows.

Question. *What conditions must be imposed on Γ and its complement Γ^c to ensure that the ground state eigenfunction u_1 associated to λ_1^Γ attains its maximum only on the boundary?*

Intuitively, one should expect that the maximum is situated on the Neumann part of the boundary Γ^c, and that the property should hold if the Dirichlet part Γ is "not too large" in an appropriate sense taking into account the geometry of Ω. Until a very recent spike in interest, this version of the hot spots conjecture has not appeared much in the literature since its formulation; the handful of existing results all concern planar domains with part of the boundary being a straight line segment. We point out that the assumption that Γ and Γ^c are connected cannot be removed as shown by the counterexample sketched in [Hatcher24, Remark 1.4].

The preliminary result [BanuelosPang04, Theorem 3.1] shows that u_1 takes its maximum only on Γ^c if Ω is simply connected, Γ is a straight line segment and Γ^c is a curve, see also [BanuelosBurdzy99, Theorem 4.3] and [Pascu02] for earlier versions of the same result. In [BanuelosPangPascu04], Corollary 1.2 extends this observation to convex domains where Γ or Γ^c is an arc of a circle, and the angles at which Γ and Γ^c meet are less than $\pi/2$. Very recently, Hatcher [Hatcher24] showed that u_1 takes its maximum only on Γ^c if Ω is a so-called graph domain, i.e. a bounded domain which is bounded by a straight line segment and by a piecewise smooth function, if Γ^c coincides with the straight line segment; Hatcher also showed that the hot spots property is satisfied if Ω is a triangle and Γ^c consists of either one or two sides of it. Even more recently, [LiYao24] studied more general semilinear problems and proved the same statement if Γ^c consists of two sides of a triangle; we point out that the aforementioned [CGY23] on mixed eigenvalues of triangles relies on results obtained in [LiYao24].

To the best of our knowledge, the most recent contribution is contained in Paper II, where we show that a certain class of planar domains whose boundary consists of the union of smooth curves has the hot spots property; we do so with a purely variational approach which, as the eigenvalue inequalities established in Paper II, is based on a novel variational principle.

Summaries of included papers

Throughout this section we assume $\Omega \subset \mathbb{R}^d$ to be a bounded, connected, Lipschitz domain.

Paper I

In this paper we consider the Laplacian on planar, convex domains Ω with piecewise smooth boundary and prove the inequality

$$\lambda_1^{\Gamma'} < \lambda_1^{\Gamma}$$

for its lowest mixed Dirichlet-Neumann eigenvalues corresponding to two different choices of disjoint subsets of the boundary Γ and Γ': either $\overline{\Gamma} \cup \overline{\Gamma'} = \partial\Omega$, or $\partial\Omega \setminus (\overline{\Gamma} \cup \overline{\Gamma'})$ having non-trivial interior. In both cases we assume Γ' to be a straight line segment, but allow the remainder of the boundary to be curved, and assume the angles adjacent to Γ to be strictly smaller than $\pi/2$. If $\partial\Omega \setminus (\overline{\Gamma} \cup \overline{\Gamma'})$ has non-trivial interior, we impose a condition regulating its curvature with respect to Γ'. An application of these results to triangles affirms parts of Siudeja's aforementioned conjecture, cf. Corollary 3.2 and Corollary 3.4 in the paper.

The proofs are variational, based on the fact that the min-max principle (2.6) together with the estimate

$$\frac{\int_\Omega |\nabla v|^2}{\int_\Omega |v|^2} \leq \lambda_1^{\Gamma}$$

for the Rayleigh quotient of some test function $v \in H^1_{0,\Gamma'}(\Omega)$ immediately yields $\lambda_1^{\Gamma'} \leq \lambda_1^{\Gamma}$; the inequality is then proved to be strict with contradiction arguments based on the unique continuation principle of Lemma 2.13. Inspired by [LevineWeinberger86], the chosen test function is the directional derivative $\partial_b u$ of the eigenfunction u corresponding to λ_1^{Γ} in the unique direction b normal to Γ'; the assumption on the angles adjacent to Γ guarantees its regularity in the sense of Remark 2.10. In order to estimate the Rayleigh quotient of $\partial_b u$ we prove a curvature-based integral identity for the second partial derivatives of Sobolev functions, Lemma 4.3 in the paper; the estimate relies on the fact that the sign of the curvature is fixed if the domain is convex, as well as on the curvature of $\partial\Omega \setminus (\overline{\Gamma} \cup \overline{\Gamma'})$.

Paper II

This paper also concerns the Laplacian on planar domains Ω with piecewise smooth boundary. In particular, we focus on a class of domains whose boundary need not contain a straight line segment nor be convex, but which satisfy Hypothesis 2.2 under the additional assumption that the normals to Γ^c belong to the closed third quadrant of the plane and the normals to Γ belong to the closed second or fourth quadrant. We prove that a variant of the hot spots conjecture holds for the lowest mixed Dirichlet-Neumann eigenfunction of the Laplacian associated to the eigenvalue $\lambda_1^{\Gamma^c}$ corresponding to a Dirichlet boundary condition on Γ^c and Neumann on Γ; if Γ does not contain any axioparallel segment we identify the point of Γ where the eigenfunction takes its maximum. Simultaneously, we prove the eigenvalue inequality

$$\lambda_1^{\Gamma^c} < \lambda_1^{\Gamma}$$

for the lowest mixed Dirichlet-Neumann eigenvalues of the Laplacian.

In order to prove these results we establish two novel variational principles for the union of the eigenvalues of the mixed Laplacians $-\Delta_\Gamma$ and $-\Delta_{\Gamma^c}$ where the minimizers are gradients of the corresponding mixed eigenfunctions. The first variational principle, Theorem 3.9 in the paper, holds for Lipschitz domains, while the second, Theorem 3.13, requires the boundary to be piecewise C^∞-smooth. The proofs include a variety of techniques, but ultimately hinge on a variant of the classical Helmholtz decomposition of $L^2(\Omega;\mathbb{C}^2)$ which is tailor-made for the treatment of mixed boundary conditions and of which we provide a straightforward proof. The proof of the variant of the hot spots conjecture is based on the variational principle of Theorem 3.13 and establishes monotonicity of the eigenfunction associated to $\lambda_1^{\Gamma^c}$ using an argument similar to the one of Courant's nodal domain theorem of taking component-wise absolute values of minimizers; the assumption on the normals to Γ and Γ^c ensures that these absolute values are also minimizers. A contradiction argument based on the monotonicity of this eigenfunction establishes the eigenvalue inequality.

Paper III

In this paper we generalize the eigenvalue inequalities established in Paper I to the Schrödinger operator on both planar and higher-dimensional domains. Namely, we prove

$$\lambda_1^{\Gamma'}(V) \leq \lambda_1^{\Gamma}(V)$$

for the Schrödinger operator on planar convex domains if Γ' is a straight line segment and if $\overline{\Gamma} \cup \overline{\Gamma'} = \partial\Omega$ or if $\partial\Omega \setminus (\overline{\Gamma} \cup \overline{\Gamma'})$ has non-trivial interior, and for convex d-dimensional domains, $d \geq 3$, if Γ' is the subset of an hyperplane and $\overline{\Gamma} \cup \overline{\Gamma'} = \partial\Omega$; in the planar case we prove that the inequality is always strict. The proofs are again based on estimating the Rayleigh quotient of the directional derivative of the eigenfunction corresponding to $\lambda_1^{\Gamma}(V)$ in the unique direction normal to Γ' and therefore rely on regulating the curvature of certain parts of the boundary or the geometry of the potential V with respect to this direction.

Further, we prove $\lambda^{\Gamma}_{k+m}(V) \leq \lambda_k(V)$, $k \in \mathbb{N}$, between mixed Dirichlet-Neumann eigenvalues and pure Dirichlet eigenvalues of the Schrödinger operator on bounded, convex, polyhedral d-dimensional domains, $d \geq 2$, if the potential is constant on some directions. The number $m \in \mathbb{N}$ is determined by these directions which are in addition tangential to the Dirichlet part Γ of the boundary. The proof is purely variational; it relies on (2.5) and the choice of a test function as an appropriate linear combination of pure Dirichlet eigenfunctions and their partial derivatives.

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