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BACHELOR THESIS

Quantitative study of Hardy inequalities in twisted waveguides

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I would like to thank my supervisor Mgr. David Krejčiřík, Ph.D. for introducing me to spectral theory, I also appreciate his kind support, valuable guidance and carefuly corrections which enabled me to write this thesis.

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Prohlášení

Prohlašuji, že jsem svou bakalářskou práci vypracovala samostatně a použila jsem pouze podklady uvedené v přiloženém seznamu.

Declaration

I declare that I wrote my bachelor thesis independently and exclusively with the use of cited bibliography.

Praha, September 1, 2010

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Název práce:
Kvantitativní vyšetření Hardyho nerovností ve zkroucených vlnovodech

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Abstrakt: Uvažujeme spektrální problém pro laplacián na nekonečném pásku v rovině s Dirichletovými a Neumannovými hraničními podmínkami. Je známo, že "zkroucená" kombinace hraničních podmínek vede k existenci nerovností Hardyho typu. Naším cílem je určit konstanty vystupující v těchto nerovnostech. Analytické horní odhady jsou odvozeny pomocí variačních metod a přesné hodnoty odhadnuty numerickým výpočtem.

Klíčová slova: kvantový vlnovod, laplacián, Dirichletovy a Neumannovy hraniční podmínky, zkroucení, Hardyho nerovnost

Title:
Quantitative study of Hardy inequalities in twisted waveguides

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Abstract: We consider the spectral problem for the Laplacian in an infinite planar strip with Dirichlet and Neumann boundary conditions. It is known that a "twisted" combination of the boundary conditions leads to the existence of Hardy-type inequalities. Our goal is to determine the constants appearing in the inequalities. Analytical upper bounds are derived by variational methods and exact values are estimated by a numerical computation.

Key words: quantum waveguide, Laplacian, Dirichlet and Neumann boundary conditions, twist, Hardy inequality

Contents

1 Introduction

Remarkable progress of the nanostructure production has been made in the last decades. It enabled one to exhibit quantum phenomena in the nanostructure devices because their typical length in a direction is comparable to the atom size. An example is given by a nanowire for which the electron transport can be modelled by a quasi-free particle with an effective mass m^* in an infinitely stretched tubular region Ω in $\mathbb{R}^3$. These nanostructures are called *quantum waveguides* [6]. The Hamiltonian of the free particle can be identified with the operator

$$H = -\frac{\hbar^2}{2m^*}\Delta \tag{1}$$

in the Hilbert space $L^2(\Omega)$, where $\hbar$ is the reduced Planck constant. Hereafter, we set $\frac{\hbar^2}{2m^*} = 1$.

Of course, to be self-adjoint, the operator (1) has to be provided with suitable *boundary conditions* imposed on $\partial\Omega$, which are determined by properties of the particle wavefunction ψ on the boundary interface. The most common boundary conditions used in literature are "hard walls", modelling a material of high chemical potential outside the nanostructure. Mathematically, they are implemented by imposing the *Dirichlet boundary condition*, i.e.

$$\psi = 0 \qquad \text{on} \qquad \partial\Omega$$

for every ψ from the operator domain of (1). The Dirichlet boundary condition can be considered as a limit case of the *Robin boundary conditions*

$$\frac{\partial\psi}{\partial n} + \alpha\psi = 0 \qquad \text{on} \qquad \partial\Omega,$$

which take into account more general types of interfaces. Here α is a given real number and n is the outward unit normal vector to $\partial\Omega$. Another special case of the Robin boundary condition is the *Neumann boundary condition*

$$\frac{\partial\psi}{\partial n} = 0 \qquad \text{on} \qquad \partial\Omega.$$

The connection between geometrical properties of the waveguide and its physical characteristics has been thoroughly studied. It was shown by P. Exner and P. Šeba in 1989 [9] that the bending of the waveguide acts as an effective attractive perturbation and thus leads to the presence of eigenvalues of the Hamiltonian below the essential spectrum, i.e. to *bound states*. Consequently, the Schrödinger equation exhibits stationary solutions and the transport properties of the waveguide become worse.

There exists a huge amount of results on the existence and the properties of bound states generated by geometric deformations of a straight waveguide (cf survey articles [6], [16] or [17]). On the other hand, a natural question arises about what the experimentalist should do to stabilize the transport in the waveguide against its possible perturbations.

From this perspective, a breakthrough result is a paper by J. Dittrich and J. Kříž [5]. The authors have shown that the bound states can be eliminated by replacing the Dirichlet boundary condition on one connected component of the boundary of a two-dimensional curved waveguide by the Neumann boundary condition.

T. Ekholm and H. Kovařík [7] showed that the bound states can be also eliminated by adding a local magnetic field. This result is inspired by the paper of A. Laptev and T. Weidl [19], who established a Hardy-type inequality for the magnetic Hamiltonian in $\mathbb{R}^2$. Indeed, a Hardy inequality is proved in [7].

More precisely, T. Ekholm and H. Kovařík considered the magnetic Hamiltonian

$$H_A := (-i\nabla + A)^2$$

in a planar straight strip subject to the Dirichlet boundary condition, where A is magnetic vector potential, and showed that the operator inequality

$$H_A - E_1 \geq \rho(.) \tag{2}$$

holds in the sense of the quadratic forms. Here, ρ is a non-negative non-trivial function and E_1 the ionisation energy of H_A, i.e. $E_1 := \inf \sigma_{\text{ess}}(H_A)$. We call this type of inequality the *Hardy inequality.* More specifically, the existence of the Hardy inequality implies the stability of the operator in the sense that no eigenvalues below the essential spectrum are generated if a small perturbation is added. We call such an operator *subcritical.*

A similar type of the Hardy inequality in the waveguide introduced under the perturbation in [5] was later proved by P. Freitas and D. Krejčiřík in [10]. T. Ekholm, H. Kovařík and D. Krejčiřík showed in [8] that the Hardy inequality is generated in 3D waveguides by purely geometric deformation of twisting; a numerical study of the Hardy inequality was performed in the thesis [21]. D. Krejčiřík demonstrated in [15] the existence of the Hardy inequality in two-dimensional strips twisted in the three-dimensional Euclidean space.

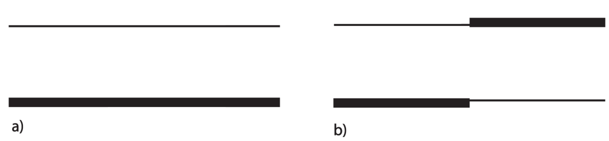

Figure 1: a) An untwisted and b) a twisted waveguide. The bold line denotes the Dirichlet and the thin line the Neumann boundary condition.

Finally, H. Kovařík and D. Krejčiřík considered in [14] a planar twisted waveguide, where the twist is represented by the switch of boundary conditions in one point. In Figure 1b there is considered such a waveguide defined in $\Omega := \mathbb{R} \times (-a, a)$. The twist makes the waveguide satisfy a Hardy inequality

$$H - E_1 \geq \rho(.), \tag{3}$$

where H is the Hamiltonian (1) defined in $L^2(\Omega)$ and E_1 is the ionization energy.

In fact, this type of waveguide was initially introduced by J. Dittrich and J. Kříž in [4], who studied the emergence of eigenvalues from the essential spectrum by overlapping the Neumann boundary conditions. Summing up, the choice of the boundary conditions is important for the criticality of the Hamiltonian.

Let us now be more precise about the model of [14], [4] which constitutes the subject of the thesis. We consider the planar twisted Dirichlet-Neumann model confined to Ω depicted in Figure 1b. First of all, we locate the spectrum of the unpertubed system (Figure 1a):

$$\sigma(H) = \sigma_{\text{ess}}(H) = [\pi^2/(4a)^2, \infty)$$

and show that the spectrum does not change while twisting the conditions.

The main results are presented in the the last part of the thesis where we introduce a more quantitative study of the Hardy inequality of the type (3) proved in [14]. More specifically, the inequality is established with two types of functions on the right-hand side:

$$\rho_g(x,y) := \frac{c_g}{1+x^2}, \qquad \rho_l(x,y) := c_l \chi_{(-a,a)^2}(x,y).$$

Here χ_A denotes the characteristic function of a set A. First, we obtain an upper estimate of the *Hardy constants* c_g, c_l. Second, we numerically compute the optimal value of c_l. That is, the value c_l^* for which the operator $H_c := H - E_1 - c\chi_{[-a,a]^2}$ becomes critical, i.e. $H_{c_l^*} - V$ possesses negative spectrum (eigenvalue) for any non-trivial non-negative V.

2 Preliminaries

2.1 Elements of spectral theory

First of all, we introduce some relevant mathematic definitions and theorems, which will be used below. Most of them are taken from [2].

Remark. We will always use the separable complex *Hilbert space* $\mathcal{H}$ with the scalar product (ψ, η), $\psi, \eta \in \mathcal{H}$ which is by convention linear in the second variable and conjugate linear in the first variable, and the norm $\|\psi\| = \sqrt{(\psi, \psi)}$.

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

Definition 1. The linear operator H on a Hilbert space $\mathcal{H}$ is called *symmetric* if and only if

$$(H\psi, \phi) = (\psi, H\phi)$$

for all elements ψ, ϕ from the domain $D(H)$.

Definition 2. Given a densely defined linear operator H on $\mathcal{H}$, by the Riesz representation theorem there is a unique operator called *adjoint* A^* defined as follows:

$$(H\psi, \phi) = (\psi, H^*\phi), \qquad \forall \psi \in D(H),\ \phi \in D(H^*)$$

such that

$$D(H^*) := \{\phi \in \mathcal{H} \mid \exists \eta \in \mathcal{H}, \forall \psi \in D(H) \quad (H\psi, \phi) = (\psi, \eta)\}.$$

Definition 3. Let H be symmetric and $D(H) = D(H^*)$. We call the operator H *self-adjoint.*

Definition 4. The *spectrum* of H on $\mathcal{H}$, denoted by $\sigma(H)$, is a set of complex numbers λ, for which the operator $H - \lambda I$ is not bijective from $D(H)$ into $\mathcal{H}$. Then one of the following alternatives occurs:

1. $H - \lambda I$ is not injective. Then there exists ψ, such that $\psi \in D(H)$, $\|\psi\| = 1$ and $H\psi = \lambda\psi$, i.e. λ is an eigenvalue of H. The *point spectrum* $\sigma_p(H)$ is defined as a set of all eigenvalues of H. The dimension of $\ker(H - \lambda I)$ is called *the multiplicity* of λ.

2. $H - \lambda I$ is not surjective and the range is dense in $\mathcal{H}$. We say, that λ belongs to the *continuous spectrum* σ_c.

3. $H - \lambda I$ is not surjective and the range is not dense in $\mathcal{H}$. The complex number λ is in the *residual spectrum* σ_r.

It can be shown that the spectrum of a self-adjoint operator is a subset of real numbers, i.e. $\sigma(H) \subset \mathbb{R}$, [[2], Cor. 7.3.6b]. At the same time, the residual spectrum is empty for any self-adjoint operator [[2], 7.3.7a]. Hence, the spectrum of a self-adjoint operator H can be decomposed into two disjoint sets $\sigma(H) = \sigma_p(H) \cup \sigma_c(H)$. For our purposes, however, it is more convenient to have another partition of the spectrum.

Definition 5. Let $\sigma_{\text{disc}}(H)$ be the *discrete spectrum* defined as a set of eigenvalues of finite multiplicity which are isolated points of the spectrum. *Essential spectrum* $\sigma_{\text{ess}}(H)$ of H is defined as

$$\sigma_{\text{ess}}(H) := \sigma(H) \backslash \sigma_{\text{disc}}(H),$$

so it consists of the eigenvalues of infinite multiplicity and the accumulation points of $\sigma(H)$.

The Weyl criterion provides a valuable tool for establishing whether a point lies in the spectrum or not. The proof could be found in [3], Lemma 4.1.2.

Theorem 2.1 (Weyl criterion)**.** *A number $\lambda \in \mathbb{R}$ lies in the spectrum of a self-adjoint operator H if and only if there exists a sequence of functions $\{\psi_n\}_{n\in\mathbb{N}}$, such that*

1. $\psi_n \in D(H), \quad \forall n \in \mathbb{N}$

2. $\|\psi_n\| = 1, \quad \forall n \in \mathbb{N}$

3. $\|H\psi_n - \lambda\psi_n\| \overset{n\to\infty}{\longrightarrow} 0.$

In this thesis we set $\mathbb{N} := \{1, 2, 3 \ldots\}$.

Definition 6. The operator H on $\mathcal{H}$ is *semi-bounded* if there exists a real number K such that

$$(\psi, H\psi) \geq K\|\psi\|^2 \qquad \forall\psi \in D(H).$$

We denote $H \geq K$.

An advantage of the partition of the spectra introduced in Definition 5 is that the discrete eigenvalues below the essential spectrum can be characterised by means of a variational technique called the minimax principle. We refer to [3], Theorem 4.5.2. for the proof.

Theorem 2.2 (Minimax principle)**.** *Let H be a semi-bounded self-adjoint operator on $\mathcal{H}$ and let $\{\lambda_m\}_{m\in\mathbb{N}}$ be a non-decreasing sequence of real numbers defined as*

$$\lambda_m := \inf \left\{ \sup_{\psi\in\mathcal{P}} \frac{(\psi, H\psi)}{\|\psi\|^2} \;\middle|\; \mathcal{P} \subseteq D(H), \quad \dim \mathcal{P} = m \right\}.$$

Then one of the following cases occurs.

1. *σ_{ess} is empty if $\lambda_m \overset{m\to\infty}{\longrightarrow} = +\infty$.*
2. *There exists $a < \infty$ such that $\lambda_m < a$, $\forall m \in \mathbb{N}$ and $\lambda_m \overset{m\to\infty}{\longrightarrow} a$. Then a is the smallest number of the essential spectrum and the part of the spectrum of H in $(-\infty, a)$ consists of the eigenvalues λ_m each repeated a number of times equal to its multiplicity.*
3. *There exists $a < \infty$ and $N < \infty$ such that $\lambda_N < a$ but $\lambda_m = a$ for all $m > N$. Then $a = \inf \sigma_{ess}$ and the part of the spectrum of H in $(-\infty, a)$ consists of the eigenvalues $\lambda_1, \ldots \lambda_N$ each repeated a number of times equal to its multiplicity.*

By considering the one-dimensional space in the minimax principle, we get:

Corollary 1 (Rayleigh-Ritz)**.** *Let H be a semi-bounded self-adjoint operator on $\mathcal{H}$. Then*

$$\inf \sigma(H) = \inf_{\psi\in D(H)\setminus\{0\}} \frac{(\psi, H\psi)}{\|\psi\|^2}$$

Remark. Instead of the domain of the Hamiltonian $D(H)$, which is not always easy to find, one can use the form domain of H in Theorem 2.2 and Corollary 1 [[3], Section 4.4].

2.2 Hamiltonians defined by quadratic forms

Let us recall the Hamiltonian (1) which act as the Laplacian in $\mathcal{H} := L^2(\Omega)$. However, it is not always obvious that the differential expression $-\Delta$ subject to boundary condition defines a self-adjoint operator H in $\mathcal{H}$. To avoid difficulties with operator domains, we introduce the Hamiltonian in a proper way as an operator associated with its quadratic form.

Definition 7. *Sesquilinear form* is a mapping $h : D(h) \times D(h) \to \mathbb{C}$ which is linear in the second and semilinear in the first argument, $D(h) \subset \mathcal{H}$ is the domain of h. The mapping $h : D(h) \to \mathbb{C}$ defined by $\psi \longmapsto h[\psi] := h(\psi, \psi)$ will be called the *quadratic form* associated with h.

Definition 8. A quadratic form h is *generated* by the operator H if $D(h) := D(H)$ and $h(\phi, \xi) := (\phi, H\xi)$. The numerical range of H is denoted by $\Theta(H)$, i.e. $\Theta(H) := \{(\psi, H\psi)|\ \psi \in D(H),\ \|\psi\| = 1\}$.

Theorem 2.3 (The representation theorem)**.** *Let h be a densely defined, closed, symmetric and semi-bouded form. There exists a self-adjoint operator H satisfying $D(H) \subset D(h)$ and $h(\phi, \xi) = (\phi, H\xi)$ for all $\phi \in D(h)$, $\xi \in D(H)$.*

The proof could be found in [2], Theorem 7.5.8. We call the operator H from Theorem 2.3 the operator *associated* with the form h.

Quadratic forms are a convenient tool for studying Schrödinger operators, because many differential operators with quite different domains have the quadratic forms with the same domain. Another advantage is that the quadratic-form framework can be used to find self-adjoint extensions of symmetric semi-bounded operators as we explain below.

Let $\dot{H}$ be a symmetric operator and H its symmetric extension. Then the inclusions hold

$$\dot{H} \subset H \subset H^* \subset \dot{H}^*,$$

because for any symmetric operator $H \subset H^*$. It is clear that H is a self-adjoint extension of $\dot{H}$, if the central inclusion becomes sharp (i.e. $H = H^*$). However, it is not that easy.

The Friedrichs extension provides a useful way how to find one special self-adjoint extension of a symmetric operator. The proof may be found in [2].

Theorem 2.4 (Friedrichs extension)**.** *Let $\dot{H}$ be symmetric semi-bounded operator, h is the closure of the quadratic form generated by $\dot{H}$ and H is the self-adjoint operator associated with the form h. Then*

1. *$\dot{H} \subset H$ and $D(H) \subset D(h)$,*
2. $\inf \Theta(H) = \inf \Theta(\dot{H})$,

while every self-adjoint operator satisfying 1. is identical with H.

Example (The free Hamiltonian in $\mathbb{R}^n$). Let us start with the *minimal operator* $\dot{H}_0$ defined by

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

We define H_0 to be the (self-adjoint) Friedrichs extension (Theorem 2.4) of $\dot{H}_0$. That means, H_0 is the operator associated with the closure h_0 of the $\dot{h}_0$ defined by

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

From the theory of Sobolev spaces we know the closure explicitly [1]:

$$D(h_0) = H_0^1(\mathbb{R}^n) = H^1(\mathbb{R}^n), \qquad h_0[\psi] = \|\nabla\psi\|^2,$$

where ∇ is to be understood in the distributional sense. By the representation theorem (Theorem 2.3) it follows that

$$D(H_0) = \{\psi \in H^1(\mathbb{R}^n) \big| \Delta\psi \in L^2(\mathbb{R}^n)\}, \qquad H_0\psi = -\Delta\psi.$$

The generalized solution $\psi \in H^1(\mathbb{R}^n)$ to the problem $-\Delta\psi = \eta \in L^2(\mathbb{R}^n)$ is known to belong to $H^2(\mathbb{R}^n)$ by standart elliptic regularity [11]. We conclude that

$$D(H_0) := H^2(\mathbb{R}^n), \qquad H_0\psi := -\Delta\psi. \tag{4}$$

In the same way, starting with the Laplacian defined in $C_0^\infty(\Omega)$, we could introduce the Hamiltonian of the particle constrained to an open subset $\Omega \subset \mathbb{R}^n$ via Dirichlet boundary conditions. To implement the Neumann boudary condititons, however, a more subtle approach has to be used. Let Q_0 be the quadratic form defined by

$$Q_0(\psi, \varphi) := \int_\Omega \overline{\nabla\psi} \cdot \nabla\varphi \, \mathrm{d}^2x$$

with the domain $D(Q_0) := \{\psi \in H^1(\Omega) \big| \psi \restriction \mathcal{D} = 0\}$. We denote as $\psi \restriction \mathcal{D}$ the trace [1] of function ψ on the part $\mathcal{D} \subset \partial\Omega$, where the Dirichlet condition is imposed. At the same time, $\mathcal{N}$ is the part where the Neumann boundary condition is imposed.

Q_0 is densely defined ($D(Q_0)$ contains $C_0^\infty(\Omega)$ which is known to be dense in $L^2(\Omega)$ [1]), symmetric ($Q_0(\psi, \varphi) = Q_0(\varphi, \psi)$), semi-bounded ($Q_0[\psi] \geq 0$) and closed ([4]) quadratic form. Hence, according to Theorem 2.3 there exists a unique self-adjoint operator associated with this form. We denote this operator $-\Delta_{DN}^\Omega$ and its domain $D(-\Delta_{DN}^\Omega)$. According to the Theorem 1 in [4], the domain of the operator $-\Delta_{DN}^\Omega$ is

$$\begin{aligned} D(-\Delta_{DN}^\Omega) &= \{\psi \in H^1(\Omega) \big| -\Delta\psi \in L^2(\Omega),\ \psi \restriction \mathcal{D} = 0,\ \frac{\partial\psi}{\partial n} \restriction \mathcal{N} = 0\}, \\ -\Delta_{DN}^\Omega\psi &= -\Delta\psi \qquad \text{for every } \psi \in D(-\Delta_{DN}^\Omega). \end{aligned} \tag{5}$$

In the situation we are interested in, i.e. the twisted Dirichlet-Neumann waveguide (27), it can be shown (cf. Lemma 2 in [4]) that the set

$$\tilde{Q}(\Omega) = \{\psi \in C^\infty(\overline{\Omega}) |\ \psi = \tilde{\psi} \restriction \Omega,\ \tilde{\psi} \in C_0^\infty(\mathbb{R}^2),\ \psi \restriction \mathcal{D} = 0\}$$

is dense in $D(Q_0)$ with respect to $H^1(\Omega)$ norm. That is, $-\Delta_{DN}^\Omega$ is actually the Friedrichs extension of the Laplacian initially defined on $\tilde{Q}(\Omega)$.

2.3 Hardy inequalities

Hardy-type inequalities are the centrepiece of this work. Let us recall some basic facts about them. They are named after G. H. Hardy, who published their simplest version in 1920 [12]. An entire book by B. Opic and A. Kufner [20] is devoted to them.

We are interested in a special case: let H be a self-adjoint bounded from below operator in $L^2(\Omega)$, $\Omega \subseteq \mathbb{R}^n$ is an arbitrary open connected set.

Definition 9. We will say, that H satisfies the *Hardy inequality*, if there exists a non-negative measurable function $\rho \neq 0$ (which means that there exists a measurable subset $M \subseteq \Omega$, such that $\int_M \rho \, \mathrm{d}x \neq 0$) such that

$$Q_H[\psi] - \inf \sigma(H)\|\psi\|^2 \geq \int_\Omega \rho|\psi|^2 \, \mathrm{d}x, \qquad \forall \psi \in D(Q_H). \tag{6}$$

Q_H denotes the quadratic form associated with H, i.e. $Q_H[\psi] := \|[H - \inf \sigma(H)]^{1/2}\psi\|^2$, where $D(Q_H) := D([H - \inf \sigma(H)]^{1/2})$ is called the form domain of H.

Recall that the norm in $L^2(\Omega)$ is defined as

$$\|\psi\|^2 = \int_\Omega |\psi|^2 dx.$$

Let us first recall classical Hardy inequalities which concern the free Hamiltonian H_0, defined in the precedent section as (4). H_0 is non-negative because from the definition follows

$$(\psi, H_0\psi) = \|\nabla\psi\|^2 \geq 0$$

for all $\psi \in D(H_0)$.

Lemma 2.5 (Classical 1D Hardy inequality)**.** *The inequality*

$$\int_0^\infty |\psi'(x)|^2 \, \mathrm{d}x \geq \frac{1}{4} \int_0^\infty \frac{|\psi(x)|^2}{x^2} \, \mathrm{d}x. \tag{7}$$

holds for all $\psi \in H_0^1((0,\infty))$.

Proof. We can consider $\psi \in C_0^\infty((0,\infty))$ in view of the density in $H_0^1((0,\infty))$ [1]. Then we have

$$\int_0^\infty \frac{|\psi(x)|^2}{x^2} \, \mathrm{d}x = \int_0^\infty \left(-\frac{1}{x}\right)' |\psi(x)|^2 \, \mathrm{d}x = \int_0^\infty \frac{1}{x} 2\, \Re[\overline{\psi(x)}\psi'(x)] \, \mathrm{d}x$$
$$\leq 2 \sqrt{\int_0^\infty \frac{|\psi(x)|^2}{x^2} \, \mathrm{d}x} \sqrt{\int_0^\infty |\psi'(x)|^2 \, \mathrm{d}x}.$$

Here the first equality comes from intergration by parts and the inequality is due to Schwarz inequality. Then the outcome is a square-root version of (2.5). □

The inequality (7) could be re-written as $-\Delta_D^{(0,\infty)} \geq \frac{1}{4x^2}$ in the sense of quadratic forms.

Notation. In general, if it is needed for the Laplacian to emphasize the set Ω we are working on, the superscript $-\Delta^{\Omega}$ will be used. The subscript is reserved for the boundary conditions which are imposed, $-\Delta_D$ denotes the Dirichlet condition on the boundary, $-\Delta_N$ the Neumann condition and $-\Delta_{DN}$ both of them.

Lemma 2.5 will be used to prove a well-known Hardy inequality for the free Hamiltonian in $\mathbb{R}^3$.

Theorem 2.6 (Classical 3D Hardy inequality)**.**

$$\int_{\mathbb{R}^3} |\nabla\psi(x)|^2 \, \mathrm{d}x \geq \frac{1}{4}\int_{\mathbb{R}^3} \frac{|\psi(x)|^2}{|x|^2} \, \mathrm{d}x, \tag{8}$$

holds true for all $\psi \in H^1(\mathbb{R}^3)$.

Proof. In the view of the density [1] of $C_0^\infty(\mathbb{R}^3)$ in $H^1(\mathbb{R}^3)$ it is enough to prove the inequality for $\psi \in C_0^\infty(\mathbb{R}^3)$. By introducing the spherical coordinates $(r,\theta) \in \mathbb{R}_+ \times S^2$ such that $\psi(x) = \tilde{\psi}(r,\theta)$ we get

$$\begin{aligned}\int_{\mathbb{R}^3} |\nabla\psi(x)|^2 \, \mathrm{d}x &= \int_{\mathbb{R}_+\times S^2} \left(\left|\frac{\partial\tilde{\psi}}{\partial r}\right|^2 + \frac{|\nabla_\theta \tilde{\psi}|^2}{r^2} \right) r^2 \, \mathrm{d}r \, \mathrm{d}\theta \\ &\geq \int_{\mathbb{R}_+\times S^2} \left|\frac{\partial\tilde{\psi}}{\partial r}\right|^2 r^2 \, \mathrm{d}r \, \mathrm{d}\theta. \end{aligned} \tag{9}$$

The inequality follows from neglecting the angular-derivative term, which is obviously non-negative. We employ a substitution $\Phi(r,\theta) = r\tilde{\psi}(r,\theta)$, such that the mapping $r \mapsto \Phi(r,\theta) \in H_0^1(\mathbb{R}_+)$ for all $\psi \in S^2$. Then

$$\left|\frac{\partial\tilde{\psi}}{\partial r}\right|^2 = \left|\frac{\partial\Phi}{\partial r}\right|^2 \frac{1}{r^2} + \frac{\Phi^2}{r^4} - 2\Re\frac{\Phi}{r^3}\frac{\partial\Phi}{\partial r}$$

Substituting into (9) and integrating by parts, we get

$$\begin{aligned}\int_{\mathbb{R}_+\times S^2} \left|\frac{\partial\tilde{\psi}}{\partial r}\right|^2 r^2 \, \mathrm{d}r \, \mathrm{d}\theta = \int_{\mathbb{R}_+\times S^2} \left|\frac{\partial\Phi}{\partial r}\right|^2 \mathrm{d}r \, \mathrm{d}\theta \geq \int_{\mathbb{R}_+\times S^2} \frac{1}{4r^2}|\Phi|^2 \, \mathrm{d}r \, \mathrm{d}\theta \\ = \frac{1}{4}\int_{\mathbb{R}^3} \frac{|\psi|^2}{|x|^2} \, \mathrm{d}x. \end{aligned}$$

The inequality follows from Lemma 2.5. □

Remark. The proof od Theorem 2.6 extends to $\mathbb{R}^n$, $n > 3$:

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

The inequality (8) could be re-written as $H_0 = -\Delta^{\mathbb{R}^3} \geq \frac{1}{4|x|^2}$ in the sense of quadratic forms.

It turns out that the existence/non-existence of the Hardy inequality is closely related to spectral properties of the free Hamiltonian under potential perturbation. Namely, the validity of (8) has a connection to the stability of the *spectral threshold* with respect to small perturbations. The local potential perturbation of the free Hamiltonian $-\Delta^{\mathbb{R}^3}$ may cause creation of the discrete values below the essential spectrum. These eigenvalues are called *bound states* in quantum mechanics and correspond to stationary solutions of the Schrödinger equation. The existence of Hardy inequality excludes the existence of such bound states as long as the perturbation is small.

Indeed, let $0 \leq V(x) \in L^\infty(\mathbb{R}^n)$ be a small perturbation in the sense that $V(x) \to 0$ as $|x| \to \infty$, $V(x)$ decays faster than $\frac{1}{|x|^2}$, then by Theorem 2.6 we get

$$-\Delta^{\mathbb{R}^3} - \epsilon V \geq \frac{1}{4|x|^2} - \epsilon V \geq 0,$$

for sufficiently small ϵ.

The spectrum of the free Hamiltonian is $\sigma(H_0) = \sigma_{\text{ess}}(H_0) = [0, \infty)$. Hence, although the existence of the Hardy inequality does not make the operator strictly positive, it can be interpreted as a kind of *repulsive perturbation* "sitting at the ground-state energy" $\inf(\sigma(H_0)) = 0$. Thus, since ϵ is small enough, no discrete values below the essential spectrum appear and the spectra of the perturbed and unperturbed operators are identical.

As a consequence of Theorem 2.6 and the remark below it, the Hardy inequality holds in $\mathbb{R}^n$ for $n \geq 3$. Lemma 2.5 proves the existence of the Hardy inequlity in $(0, \infty)$ with the Dirichlet boundary condition at 0. For the free Hamiltonian, however, dimensions 1 and 2 play a special role in the sense that there is no Hardy inequality of the type (6).

Theorem 2.7. *Let $n = 1$ or $n = 2$. Assume, that there exists some measurable function $\rho(x) \geq 0$, such that the inequality (6) holds for all $u \in H^1(\mathbb{R}^n)$, H be the Hamiltonian of the free particle in $\mathbb{R}^n$. Then $\rho \equiv 0$.*

Proof. The proof is taken from [21]. We make the proof separately for the dimensions.

$n = 1$: Let u_n be defined as

$$u_n(x) = e^{-\left|\frac{x}{n}\right|}, \tag{10}$$

$u_n \in H^1(\mathbb{R})$, then $\forall n \in \mathbb{N}$

$$\int_{\mathbb{R}} |u_n'|^2 \, \mathrm{d}x = \frac{1}{n^2} \int_{\mathbb{R}} e^{-2\left|\frac{x}{n}\right|} \, \mathrm{d}x = \frac{2}{n^2} \int_0^\infty e^{-2\frac{x}{n}} \, \mathrm{d}x = \frac{2}{n^2}\frac{n}{2} = \frac{1}{n}.$$

Assume $\rho \in L^1_{loc}$. Let K be a compact subset of $\mathbb{R}$. Assuming the validity of the Hardy inequality we have

$$\int_K |u_n|^2 \rho(x) \, \mathrm{d}x \leq \int_{\mathbb{R}} |u_n'(x)|^2 \, \mathrm{d}x = \frac{1}{n} \stackrel{n\to\infty}{\longrightarrow} 0.$$

At the same time due to the monotone convergence theorem, it follows that

$$\int_K |u_n|^2 \rho(x)\,\mathrm{d}x = \int_K e^{-2\left|\frac{x}{n}\right|}\rho(x)\,\mathrm{d}x \overset{n\to\infty}{\longrightarrow} \int_K \rho(x)\,\mathrm{d}x$$

Summing up, $\int_K \rho(x)\,\mathrm{d}x = 0$ for any compact subset $K \subset \mathbb{R}$. This implies $\rho \equiv 0$.

$n = 2$: We define the function

$$u_n(x) := \begin{cases} 1 & \text{if } |x| \leq 1, \\ (\ln n)^{-1}(\ln n - \ln|x|)_+ & \text{if } |x| > 1. \end{cases}$$

The plus sign in the subscript of the brackets denotes a positive part of the term. We compute the first derivative:

$$\nabla u_n(x) := \begin{cases} 0 & \text{if } |x| \leq 1, \\ (|x|\ln n)^{-1} & \text{if } |x| > 1. \end{cases}$$

It is clear that

$$\int_{\mathbb{R}^2} |\nabla u_n(x)|^2\,\mathrm{d}x \overset{n\to\infty}{\longrightarrow} 0.$$

Similarly as in one dimension, we get

$$\int_K |u_n(x)|^2 \rho(x)\,\mathrm{d}x \leq \int_{\mathbb{R}^2} |\nabla u_n(x)|^2\,\mathrm{d}x \overset{n\to\infty}{\longrightarrow} 0.$$

and at the same time

$$\int_K |u_n(x)|^2 \rho(x)\,\mathrm{d}x = \int_K \left|\frac{(\ln n - \ln|x|)_+}{\ln n}\right|^2 \rho(x)\,\mathrm{d}x \overset{n\to\infty}{\longrightarrow} \int_K \rho(x)\,\mathrm{d}x$$

and subsequently $\rho \equiv 0$

□

As a consequence of Theorem 2.7, in one- and two-dimensional space there does not exist any non-trivial Hardy weight. However, some kind of Hardy inequality holds under some modifications. This situation occurs when we add an external magnetic field or we restrict to a subdomain $\Omega \subset \mathbb{R}^n$ and impose some boundary conditions. In this paper we consider a planar quantum waveguide with combined Dirichlet and Neumann boundary conditions.

3 The unperturbed waveguide

In this section, we are interested in a straight waveguide with combined boundary condition. A free particle moving inside the waveguide may be described by the Laplacian in a strip $\mathbb{R} \times (-a, a)$ with the Dirichlet boundary condition on the lower line and Neumann boundary condition on the upper line, c.f. Figure 2. More precisely, we are solving the spectral problem for a self-adjoint

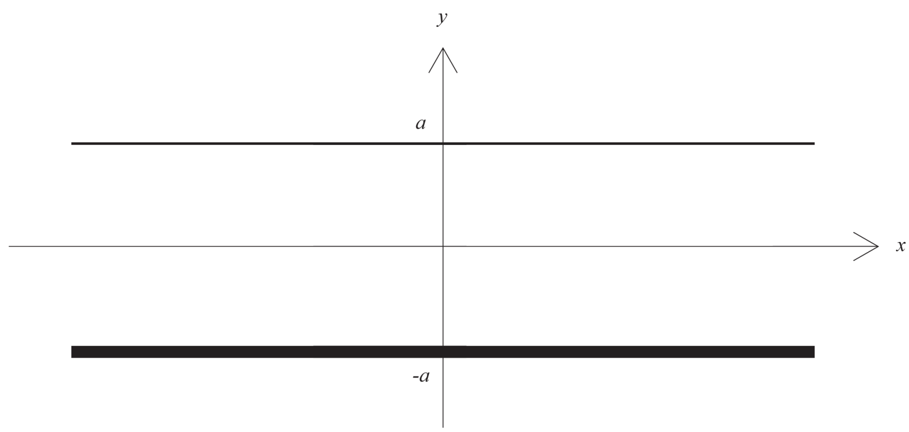

Figure 2: Waveguide with Neumann boundary condition on the upper line (thin) and Dirichlet boundary condition on the lower line (bold).

operator, denoted by $-\Delta^{\text{untwist}}$ and called Dirichlet-Neumann Laplacian here. The operator $-\Delta^{\text{untwist}}$ is according to (5) well defined by the prescription

$$\begin{aligned} -\Delta^{\text{untwist}}\phi &:= -\Delta\phi \\ D(-\Delta^{\text{untwist}}) &:= \{\phi \in H^2(\mathbb{R}\times(-a,a)) \mid \phi(x,-a)=0,\ \partial_y\phi(x,a)=0\}. \end{aligned}$$

Acting of Laplacian should be understood in the distributional sense.

The spectral problem for $-\Delta^{\text{untwist}}$ can be solved by *separation of variables*. To explain this, let us formally look for a solution of the generalized eigenvalue problem:

$$\begin{cases} -\Delta\phi = E\phi, & \text{in } \mathbb{R}\times(-a,a) \\ \phi(x,-a)=0, & \\ \partial_y\phi(x,a)=0 & \forall x\in\mathbb{R}. \end{cases} \tag{11}$$

We use Ansatz

$$\phi(x,y) = \varphi(x)\psi(y). \tag{12}$$

Then the problem (11) can be written into the form

$$-\frac{\varphi''(x)}{\varphi(x)} = \frac{\psi''(y)}{\psi(y)} + E = C, \tag{13}$$

where C is a constant and the last equality follows from the fact that the left-hand side of the first equality is dependent on x only, whereas the right-hand side is function of y. These two sides may equal only if they are constant. Thus the separation leads to the division to two one-dimensinal problems, a longitudinal and a transversal one.

3.1 Transversal Hamiltonian

We are looking for the spectrum of the transversal Hamiltonian given by

$$H_y\psi := -\Delta\psi,$$

for all $\psi \in D(H_y) := \{\psi \in H^2((-a,a)) \mid \psi(-a) = 0\ ,\ \psi'(a) = 0\}$. The self-adjointness of H_y follows as a special case from the self-adjointness of the general operator (5). Self-adjoint operators may possess in principle both the essential and the discrete spectrum. We begin with researching the latter one.

3.1.1 Point spectrum

Our goal is to solve this problem:

$$\begin{cases} -\psi''(y) = E\psi(y), & y \in (-a,a) \\ \psi(-a) = 0, \\ \psi'(a) = 0. \end{cases} \tag{14}$$

The transversal Hamiltonian is surely a non-negative operator. It follows from the minimax principle (Theorem 2.2) and from $(\psi, H_y\psi) = \|\psi'\|^2$. Multiplying (14) by $\overline{\psi}$ and integrating by parts, the energy E may be put as

$$E = \frac{\int_{-a}^{a} |\psi'|^2}{\int_{-a}^{a} |\psi|^2} \tag{15}$$

that is certainly bigger or equal to 0.

The general solution of the linear differential equation in (14) is of the form

$$\psi(y) = A\cos(\sqrt{E}y) + B\sin(\sqrt{E}y), \tag{16}$$

where $A, B \in \mathbb{C}$. Restricting the general solution by the boundary conditions in (14) we get the system

$$M\begin{pmatrix} A \\ B \end{pmatrix} = 0 \tag{17}$$

where

$$M := \begin{pmatrix} \cos(\sqrt{E}a) & -\sin(\sqrt{E}a) \\ -\sqrt{E}\sin(\sqrt{E}a) & \sqrt{E}\cos(\sqrt{E}a) \end{pmatrix}.$$

The system from (17) is a homogeneous equation, requiring $\det M = 0$ in order to get non-trivial solution we arrive at the equation:

$$\sqrt{E}\cos(2\sqrt{E}a) = 0. \tag{18}$$

One can conclude from (15), that $E \geq 0$. We show that the inequality is strict. $E \neq 0$ results from following: if $E = 0$, the right hand side of (14) vanishes and the equation $-\psi'' = 0$ immediately implies, that $\psi(y) = Ay + B$ where A, B are constant values. Only in the case $A = 0, B = 0$ the solution satisfies the Neumann-Dirichlet conditions, i.e. we only get a trivial solution of (14). This implies $E > 0$.

Hence one can conclude from (18) that

$$E_k = \left(\frac{\pi}{4a}\right)^2 (2k-1)^2, \qquad k \in \mathbb{N}. \tag{19}$$

Clearly, when k is rising the value of E_k grows: $E_1 < E_2 < \ldots$. This means that $E_1 = (\frac{\pi}{4a})^2$ is the lowest eigenvalue of the operator H_y.

3.1.2 The eigenfunctions

It follows from (17), that A, B are dependent on each other, namely

$$A = \frac{B \sin(\sqrt{E_n} a)}{\cos(\sqrt{E_n} a)}. \tag{20}$$

Then by inserting A from (20) into (16) and using the goniometrical formula $\sin(\alpha)\cos(\beta) = \frac{1}{2}[\sin(\alpha-\beta) + \sin(\alpha+\beta)]$ we get

$$\psi_n^{DN}(y) := \frac{B}{\cos(\sqrt{E_n} a)} \sin(\sqrt{E_n}(a+y)).$$

Normalizing the eigenfunctions by requiring $\|\psi_n\|^2 = 1$ we arrive at

$$\psi_n^{DN}(y) = \sqrt{\frac{1}{a}} \sin(\sqrt{E_n}(a+y)) \tag{21}$$

for $n \in \mathbb{N}$.

By imposing the reverse boundary condition, i.e. the Dirichlet boundary condition $\psi(a) = 0$ and the Neumann boundary condition $\psi'(-a) = 0$, the solution is similar for all $n \in \mathbb{N}$ to the above one:

$$\psi_n^{ND}(y) := \sqrt{\frac{1}{a}} \sin(\sqrt{E_n}(a-y)). \tag{22}$$

Lemma 3.1. *$\{\psi_n^{DN}\}_{n=1}^{\infty}$ composes a complete orthonormal set.*

Proof. The orthonormality is easy to prove by an explicit computation

$$(\psi_n^{DN}, \psi_m^{DN}) = \begin{cases} 0 & m \neq n, \\ 1 & m = n, \end{cases}$$

for all $m, n \in \mathbb{N}$. The completeness of $\{\psi_n^{DN}\}_{n=1}^{\infty}$ is a standard result of the Fourier analysis. In Theorem 208 in [13] may be found the proof, that the l-periodical system

$$\left\{ \sqrt{\frac{1}{l}}, \sqrt{\frac{2}{l}} \cos\left(\frac{2k\pi x}{l}\right), \sqrt{\frac{2}{l}} \sin\left(\frac{2k\pi x}{l}\right) \right\}_{k=0}^{\infty} \tag{23}$$

composes a complete orthonormal set in $L^2(x, x+l)$. An orthonormal set of functions $\{\psi_n\}_{n=1}^{\infty}$ is complete in $L^2(x, x+l)$ if and only if the Parseval equality [2] holds:

$$\sum_{n=1}^{\infty} |(\psi_n, \varphi)|_l^2 = \|\varphi\|_l^2, \qquad \forall \varphi \in L^2(x, x+l). \tag{24}$$

Here $(.,.)_l$, $\|.\|_l$ denote the scalar product and the norm on $L^2(0,l)$ respectively.

Let $\{\chi_n\}_{n=1}^{\infty}$ be the complete orthonormal $4d$-periodical system (23) in $L^2(0, 4d)$. We consider a function φ in $L^2(0,d)$ and its even extension with respect to d in $(0, 2d)$ and finally an odd extension of the already evenly extended function with respect to $2d$ in $(0, 4d)$. We keep the same symbol φ for the extensions.

We compute

$$\begin{aligned}\sum_{n=1}^{\infty} |(\chi_n, \varphi)_{4d}|^2 &= \sum_{n=1}^{\infty} \left| \left(\sqrt{\frac{1}{2d}} \sin \frac{n\pi x}{2d}, \varphi \right)_{4d} \right|^2 = \sum_{n=1}^{\infty} \left| 2 \left(\sqrt{\frac{1}{2d}} \sin \frac{n\pi x}{2d}, \varphi \right)_{2d} \right|^2 \\ &= \sum_{n=1,\mathrm{odd}}^{\infty} \left| 2 \left(\sqrt{\frac{1}{2d}} \sin \frac{n\pi x}{2d}, \varphi \right)_{2d} \right|^2 = \sum_{n=1,\mathrm{odd}}^{\infty} \left| 4 \left(\sqrt{\frac{1}{2d}} \sin \frac{n\pi x}{2d}, \varphi \right)_{d} \right|^2 \\ &= \sum_{n=1}^{\infty} \left| \left(\sqrt{\frac{8}{d}} \sin \frac{(2n-1)\pi x}{2d}, \varphi \right)_{d} \right|^2 . \end{aligned} \tag{25}$$

The first equality follows from the fact that φ is odd in $(0, 4d)$ and the scalar product (χ_n, φ) is nontrivial only for χ_n odd. This requirement satisfies the sinus function from (23) only. The third equality holds because φ is even in $(0, 2d)$ and the function $\sqrt{\frac{1}{2d}} \sin \frac{n\pi x}{2d}$ from (23) is odd (respectively, even) in $(0, 2d)$ if n is even (respectively, n odd).

At the same time, an easy consequence of the fact that φ is even on $(0, 2d)$ and odd on $(0, 4d)$ is

$$\|\varphi\|_{4d}^2 = 2\|\varphi\|_{2d}^2 = 4\|\varphi\|_d^2.$$

Then this together with (25) and the Parseval equality (24) for the trigonometric system (23) yields

$$\sum_{n=1}^{\infty} \left| \left(\sqrt{\frac{2}{d}} \sin \frac{(2n-1)\pi x}{2d}, \varphi \right)_{d} \right|^2 = \|\varphi\|_d^2, \qquad \forall \varphi \in L^2(0,d).$$

Hence the set $\left\{ \sum_{n=1}^{\infty} \left| \left(\sqrt{\frac{2}{d}} \sin \frac{(2n-1)\pi x}{2d}, \varphi \right)_d \right|^2 \right\}_{n=1}^{\infty}$ is complete in $L^2(0,d)$.

It remains to realize that this implies the completeness of our set $\{\psi_n^{DN}\}_{n=1}^{\infty}$ in $L^2(-a, a)$ after an obvious linear transformation (translation). □

3.1.3 Essential spectrum

Finally, we prove that the essential spectrum of transversal Hamiltonian is empty.

Proposition 3.2. *Spectrum of H_y is purely discrete.*

Proof. An important criterion for the self-adjoint operators to have empty essential spectrum can be found in [3], Theorem 4.1.5: The essential spectrum of a self-adjoint operator H is empty if and only if there exists a complete orthonormal set of eigenfunctions $\{\psi_n\}_{n=1}^{\infty}$ such that the corresponding eigenvalues $\lambda_n \to \infty$ as $n \to \infty$. We have just proven the completeness of $\{\psi_n^{DN}\}_{n=1}^{\infty}$ in Lemma 3.1 and $E_n \to \infty$ as $n \to \infty$, hence the spectrum of H_y is discrete. □

3.2 Longitudinal Hamiltonian

Let

$$H_x \psi := -\Delta \psi$$

be the longitudinal Hamiltonian on the domain $D(H_x) := H^2(\mathbb{R})$. To solve the longitudinal spectral problem associated with (13) we are therefore looking for (generalized) solution ψ of the shifted Helmholtz equation

$$-\Delta \psi(x) = \lambda \psi(x), \qquad \text{in } \mathbb{R}, \tag{26}$$

where $\lambda = E - C$.

3.2.1 Point spectrum

The first observation tells us that we might not use the same procedure as used in searching for transversal spectrum because the general function ψ which solves the equation (26)

$$\psi(x) = Ae^{i\lambda x} + Be^{-i\lambda x}$$

does not belong to $L^2(\mathbb{R})$. This implies $\sigma_p(H_x) = \varnothing$, i.e. the point spectrum is empty. In particular, $\sigma_{\text{disc}}(H_x) = \varnothing$ and the spectrum of H_x is purely essential.

3.2.2 Essential spectrum

Proposition 3.3. $\sigma(H_x) = \sigma_{ess}(H_x) = [0, \infty)$.

Proof. We split the proof into three steps:

1. $\sigma(H_x) \subseteq [0, \infty)$
   The non-negativity $(\psi, H_x\psi) = \|\psi'\|^2 \geq 0$ follows from the minimax principle (c.f. Theorem 2.2).
2. $\sigma(H_x) \supseteq [0, \infty)$
   To verify the other inclusion we define

$$\psi_n(x) := \varphi_n(x) e^{i\sqrt{\lambda} x}$$

where $\varphi_1 : \mathbb{R} \to \mathbb{R}$, such that $\varphi_1 \in C_0^\infty(\mathbb{R})$ and $\|\varphi_1\| = 1$ and

$$\varphi_n(x) = \frac{1}{\sqrt{n}} \varphi_1 \left(\frac{x}{n} \right).$$

The sequence is chosen in such a way, that also each φ_n is normalized to 1 in $L^2(\mathbb{R})$. Next we compute

$$\|\varphi_n'\|^2 = \frac{1}{n^2} \|\varphi_1'\|^2,$$
$$\|\varphi_n''\|^2 = \frac{1}{n^4} \|\varphi_1''\|^2.$$

Now we are ready to check the hypothesis of Weyl's theorem (c.f. Theorem 2.1). It is clear, that each $\psi_n \in D(H_x)$ and that $\|\psi_n(x)\| = 1$. The last requirement is also satisfied, indeed:

$$\begin{aligned}\|(H_x - \lambda)\psi_n(x)\|^2 &= \|(-\varphi_n''(x) - 2i\sqrt{\lambda}\varphi_n'(x))e^{i\sqrt{\lambda}x}\| \\ &\le \|\varphi_n''(x)\|^2 + 4\lambda\|\varphi_n'(x)\|^2 \xrightarrow{n \to \infty} 0.\end{aligned}$$

Summing up, according to Weyl's criterion every $\lambda \geq 0$ belongs to $\sigma(H_x)$.

3. $\sigma(H_x) = \sigma_{\text{ess}}(H_x)$
   We have shown $\sigma(H_x) = [0, \infty)$, from which it is clear that the spectrum is essential. Indeed, the interval contains no isolated points.

□

3.3 Hamiltonian of the planar strip

Let us recall the notation used at the beginning of this section. The Hamiltonian $-\Delta^{\text{untwist}}$ of the unpertubed planar strip can be defined as (11). We already know the spectra of the one-dimensional Hamiltonians, to which $-\Delta^{\text{untwist}}$ reduces by virtue of the separation of variables.

The spectrum of the Dirichlet-Neumann Laplacian $-\Delta^{\text{untwist}}$ in the 2D waveguide is equal to the sum of the transversal and the longitudinal one:

Proposition 3.4. *One has $\sigma(-\Delta^{untwist}) = \sigma_{ess}(-\Delta^{untwist}) = [E_1, \infty)$.*

Proof. The proof is divided into two parts:

1. $\sigma(-\Delta^{\text{untwist}}) \subseteq [E_1, \infty)$
   We estimate the quadratic form associated with the Hamiltonian:

$$\begin{aligned}Q[\psi] := (\psi, -\Delta^{\text{untwist}}\psi) = \|\nabla\psi\|^2 = \int_\Omega \left(\left| \frac{\partial \psi}{\partial x} \right|^2 + \left| \frac{\partial \psi}{\partial y} \right|^2 \right) \mathrm{d}x \, \mathrm{d}y \\ \geq \int_{\mathbb{R}} \mathrm{d}x \int_{-a}^{a} \mathrm{d}y \left| \frac{\partial \psi}{\partial y} \right|^2 \geq \int_{\mathbb{R}} \mathrm{d}x \int_{-a}^{a} \mathrm{d}y \, E_1 |\psi|^2 = E_1 \|\psi\|^2\end{aligned}$$

for all $\psi \in D(Q)$. The first inequality results from neglecting the first (non-negative) term, and the other one uses Fubini's theorem and the minimax principle, employing the knowledge of the spectrum of the transversal Hamiltonian $-\Delta_{DN}^{(-a,a)}$. By considering the domain $D(Q) = \{\psi \in H^1(\mathbb{R} \times (-a,a)) | \psi = 0 \text{ on } \mathbb{R} \times \{-a\}\}$ we claim, that $H \geq E_1$ and at the same time

$$\sigma(-\Delta^{\text{untwist}}) \subseteq [E_1, \infty).$$

2. $\sigma(-\Delta^{\text{untwist}}) \supseteq [E_1, \infty)$

   As in the one-dimensional case we give the function ψ_n and verify the hypothesis of Weyl's criterion (Theorem 2.1). We use the decomposition

$$\psi_n(x,y) := \varphi_n(x) e^{i\sqrt{\lambda}x} \psi_1^{DN}(y),$$

   where φ_n comes from (2) and ψ_1^{DN} is the eigenfunction of H_y corresponding to the lowest eigenvalue E_1. Then clearly $\|\psi_n(x,y)\|^2 = 1$ and $\psi_n \in D(-\Delta^{\text{untwist}})$. The last item of Weyl's criterion is also satisfied, indeed:

$$\begin{aligned}\|(-\Delta^{\text{untwist}} - (\lambda + E_1))\psi_n(x,y)\|^2 = \|(&-\varphi_n''(x)\psi_1^{DN}(y) - 2i\sqrt{\lambda}\varphi_n'(x)\psi_1^{DN}(y) \\ &- \varphi_n(x)\psi_1^{DN''}(y) - E_1\varphi_n(x)\psi_1^{DN}(y))e^{i\sqrt{\lambda}x}\| \\ &\leq \|\varphi_n''(x)\psi_1^{DN}(y)\|^2 + 4\lambda\|\varphi_n'(x)\psi_1^{DN}(y)\|^2 \overset{n\to\infty}{\longrightarrow} 0.\end{aligned}$$

   This implies that every $\lambda \geq E_1$ belongs to the spectrum of the Hamiltonian H. Summing up, the final spectrum consists of the sum of the spectrum of the transversal as well as the longitudinal Hamiltonian: $\sigma(-\Delta^{\text{untwist}}) = \sigma(H_x) + \sigma(H_y) = [\pi^2/(4a)^2, \infty)$.

3. $\sigma(-\Delta^{\text{untwist}}) = \sigma_{\text{ess}}(-\Delta^{\text{untwist}})$

   Again, this follows from the fact that the spectrum is composed of an interval which contains no isolated points.

□

4 The twisted waveguide

In this section we employ a planar twisted Dirichlet-Neumann waveguide. The boundary conditions are not overlapped, the twist is realised in one point, cf Figure 3. The corresponding Hamiltonian $-\Delta^{\text{twist}}$ is defined as follows

$$\begin{aligned}-\Delta^{\text{twist}}\phi :=& -\Delta\phi \\ D(-\Delta^{\text{twist}}) :=& \{\phi \in H^1(\mathbb{R} \times (-a,a)) | -\Delta\phi \in L^2(\mathbb{R} \times (-a,a)), \\ & \phi[(-\infty,0) \times \{-a\} \cup (0,\infty) \times \{a\}] = 0, \\ & \partial_y\phi[(-\infty,0) \times \{a\} \cup (0,\infty) \times \{-a\}] = 0\}. \end{aligned} \tag{27}$$

We are looking for the spectrum of the Hamiltonian:

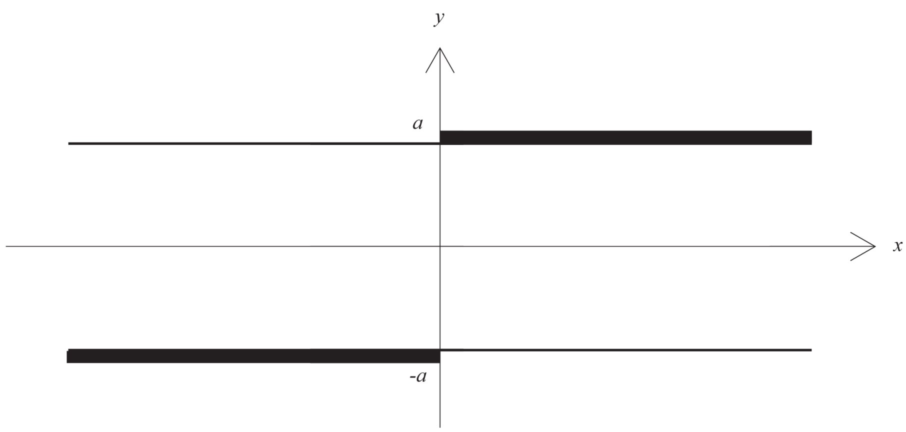

Figure 3: Twisted waveguide with a switch of Dirichlet (bold) and Neumann boundary conditions (thin).

$$\begin{cases} -\Delta\phi = E\phi, & \text{in } \mathbb{R}\times(-a,a), \\ \phi(x,-a) = 0, & x<0, \\ \phi(x,a) = 0, & x>0, \\ \partial_y\phi(x,-a) = 0, & x<0, \\ \partial_y\phi(x,a) = 0, & x>0, \end{cases} \tag{28}$$

considered as a generalized problem. We take an advantage of the knowledge of the spectrum of $-\Delta^{\mathrm{untwist}}$ and use Weyl's criterion to prove that the spectrum does not change under twisting.

Proposition 4.1. *The spectrum of the twisted Dirichlet-Neumann waveguide is* $\sigma(-\Delta^{twist}) = \sigma_{ess}(-\Delta^{twist}) = [E_1,\infty)$.

Proof. We use two inclusions to prove the equality.

1. $\sigma(-\Delta^{\mathrm{twist}}) \subset [E_1,\infty)$

   This inclusion is satisfied according to the minimax principle using the same type of arguments as in item 1 of the proof of Proposition 3.4.

2. $\sigma(-\Delta^{\mathrm{twist}}) \supset [E_1,\infty)$

   We employ Weyl's criterion (Theorem 2.1) and show that the operator $-\Delta^{\mathrm{twist}}$ satisfies all the three conditions of the theorem. Let

   $$\psi_n(x,y) := \varphi_n(x)e^{i\sqrt{\lambda}x}\psi_1^{ND}(y),$$

   be the decomposition, ψ_1^{ND} is the eigenfuction (22) corresponding to eigenvalue E_1. φ_n is given by

   $$\varphi_n(x) = \frac{1}{\sqrt{n}}\,\varphi_1\left(\frac{x}{n}-n\right),$$

where $\varphi_1 : \mathbb{R} \to \mathbb{R}$, such that $\varphi_1 \in C_0^\infty(\mathbb{R})$ and $\|\varphi_1\| = 1$. Then $(\exists n_0 \in \mathbb{N})(\forall n > n_0)(\psi_n \in D(-\Delta^{\text{twist}}))$ and $\|\psi_n\|^2 = 1$, $\forall n \in \mathbb{N}$.
The sequence φ_n is chosen in such a way that the support is shifting to infinity as $n \to \infty$:

$$\text{supp } \varphi_1 \subset [-1, 1], \qquad \text{supp } \varphi_n \subset [n(n-1), n(n+1)].$$

We compute

$$\|\varphi_n'\|^2 = \frac{1}{n^2}\|\varphi_1'\|^2,$$
$$\|\varphi_n''\|^2 = \frac{1}{n^4}\|\varphi_1''\|^2.$$

Finally,

$$\begin{aligned}\|(-\Delta^{\text{twist}} - (\lambda + E_1))\psi_n(x, y)\|^2 = &\|(-\varphi_n''(x)\psi_1^{ND}(y) - 2i\sqrt{\lambda}\varphi_n'(x)\psi_1^{ND}(y) \\ &- \varphi_n(x)(\psi_1^{ND}(y))'' - E_1\varphi_n(x)\psi_1^{ND}(y))e^{i\sqrt{\lambda}x}\| \\ \leq &\|\varphi_n''(x)\psi_1^{ND}(y)\|^2 + 4\lambda\|\varphi_n'(x)\psi_1^{ND}(y)\|^2 \overset{n\to\infty}{\longrightarrow} 0.\end{aligned}$$

Weyl's criterion is satisfied.

3. $\sigma(-\Delta^{\text{twist}}) = \sigma_{\text{ess}}(-\Delta^{\text{twist}})$
The discrete spectrum is empty. Indeed, the interval does not contain any isolated points.

□

5 Quantitative analysis of the Hardy inequalities

In the previous sections we have shown that the spectra of the Laplacian in untwisted and twisted waveguides are the same:

$$\sigma(-\Delta^\theta) = \sigma_{\text{ess}}(-\Delta^\theta) = [E_1, \infty),$$

$\theta \in \{\text{twist}, \text{untwist}\}$. However it is known from [14] that there is a fine difference between the twisted and untwisted operator, reflected in the existence of the Hardy inequality for the Laplacian in the twisted waveguide.

5.1 Upper estimates of the Hardy constant

Theorem 5.1 ([14]). *The Hardy inequality* (6) *holds in the twisted Dirichlet-Neumann waveguide in the sense of quadratic forms*

$$-\Delta^{twist} - E_1 \geq \rho_g := \frac{c_g}{1 + x^2}, \tag{29}$$

$$-\Delta^{twist} - E_1 \geq \rho_l := c_l\chi_{(-a,a)\times(-a,a)}, \tag{30}$$

where c_g, c_l are strictly positive constants, χ denotes the characteristic function.

The proof may be found in [14]. We call (29) *global* Hardy inequality because the weight on the right-hand side is supported everywhere. (30) is called *local* Hardy inequality because the weight is compactly supported.

H. Kovařík and D. Krejčiřík have also established lower bound for the constants. Indeed, c_g^{KK} defined by

$$c_g^{\mathrm{KK}} := \frac{c_l}{16c_l + 2 + 16/a^2}$$

represents a lower bound for c_g:

$$c_g^{\mathrm{KK}} \leq c_g,$$

Moreover, c_l satisfies $c_l \geq s_1 E_1$ where s_1 is the smallest root of the equation

$$\sqrt{1-s}\tanh\left(\frac{\pi\sqrt{1-s}}{2\sqrt{2}}\right) = \sqrt{1/2+s}\tan\left(\frac{\pi\sqrt{1/2+s}}{2\sqrt{2}}\right).$$

In [14] the authors also find the numerical value $s_1 \approx 0.039$.

Now we approach a problem of quantitative analysis of the Hardy inequality. Our goal is to verify the upper bound to the Hardy constant c_g.

Theorem 5.2. *We recall the notation used in* (29). *Then*

$$c_g \leq 1/2.$$

Proof. The proof is a modification of the proof in [18]. Let us consider the operator $-\Delta_{DN}^{\mathbb{R}\times(-a,a)} - E_1 - \rho_g$. We proceed by contradiction: assume that this operator is non-negative in the sense of quadratic forms and at the same time $c_g > 1/2$. Hence it is enough to find ψ a test function from $\mathcal{D}(\tilde{Q}_{c_g})$ such that

$$\tilde{Q}_{c_g}[\psi] := Q_{-\Delta}[\psi] - E_1 \int_{\mathbb{R}\times(-a,a)} |\psi(x,y)|^2 \,\mathrm{d}x\,\mathrm{d}y - \int_{\mathbb{R}\times(-a,a)} \rho_g |\psi(x,y)|^2 \,\mathrm{d}x\,\mathrm{d}y \tag{31}$$

is negative. The sequence of the wave-functions ψ_n could be expressed for every $n \in \mathbb{N}$ in the form

$$\psi_n(x,y) = \psi_1^{ND}(y)\,\varphi_n(x), \tag{32}$$

where $\psi_1^{ND}(y)$ is the eigenfunction corresponding to E_1 of the Laplacian normalized to 1 in $L^2(\mathbb{R})$. $\varphi_n(x)$ is given by

$$\varphi_n(x) = \begin{cases} \dfrac{x - b_1^n}{b_2^n - b_1^n} & \text{if } x \in [b_1^n, b_2^n), \\ \dfrac{b_3^n - x}{b_3^n - b_2^n} & \text{if } x \in [b_2^n, b_3^n), \\ 0 & \text{otherwise.} \end{cases} \tag{33}$$

The numerical sequences $\{b_i^n\}_{n\in\mathbb{N}}$, $i = 1,2,3$, are specified $\forall n \in \mathbb{N}$ in view of:

1. $b_1^n < b_2^n < b_3^n$,
2. $\frac{b_3^n}{b_2^n} \to \infty$,
3. $\frac{b_2^n}{b_1^n} \to \infty$,
4. $b_1^n \to \infty$ as $n \to \infty$.

ψ_1^{ND} is the eigenfunction corresponding to E_1 defined by (22), hence

$$\int_{-a}^{a} |\partial_y \psi_1^{ND}(y)|^2 \, \mathrm{d}y = E_1 \int_{-a}^{a} |\psi_1^{ND}(y)|^2 \, \mathrm{d}y. \tag{34}$$

By using the decomposition (32) and the equation (34), the quadratic form (31) immediately yields

$$\tilde{Q}_{c_g}[\psi_n] = \|\dot{\varphi}_n\|^2_{L^2(\mathbb{R})} - c_g \|\rho_g \varphi_n\|^2_{L^2(\mathbb{R})}.$$

With the view of clearness the specific values are written down below:

$$\|\dot{\varphi}_n\|^2_{L^2(\mathbb{R})} = \frac{1}{b_2^n - b_1^n} + \frac{1}{b_3^n - b_2^n}$$

$$\|\rho_g \varphi_n\|^2_{L^2(\mathbb{R})} = \frac{b_2^n - b_1^n + [(b_1^n)^2 - 1](\arctan b_2^n - \arctan b_1^n) - b_1^n \log \frac{1+(b_2^n)^2}{1+(b_1^n)^2}}{(b_2^n - b_1^n)^2}$$
$$- \frac{b_3^n - b_2^n + [(b_3^n)^2 - 1](\arctan b_3^n - \arctan b_2^n) - b_3^n \log \frac{1+(b_3^n)^2}{1+(b_2^n)^2}}{(b_3^n - b_2^n)^2}.$$

On the basis of the relations between particular sequences $\{b_i^n\}_{n\in\mathbb{N}}$ we get the limit

$$b_2^n \tilde{Q}_{c_g}[\psi_n] \to 1 - 2c_g$$

as n tends to infinity. Since the limit is negative when $c_g > 1/2$, we can choose n sufficiently large to make the quadratic form negative. This leads to a contradiction. □

Secondly, we consider the Hardy inequality (30) for the twisted Dirichlet-Neumann waveguide.

Theorem 5.3. $c_l \leq 4E_1$.

Proof. We begin the proof of this theorem analogously to the proof of the previous one. Let us consider the operator $-\Delta_{DN}^{\mathbb{R}\times(-a,a)} - E_1 - c_l \chi_{(-a,a)^2}$ and assume it is non-negative. Then

$$\tilde{Q}_{c_l}[\psi] := Q_{-\Delta}[\psi] - E_1 \int_{\mathbb{R}\times(-a,a)} |\psi(x,y)|^2 \, \mathrm{d}x \, \mathrm{d}y - c_l \int_{(-a,a)^2} |\psi(x,y)|^2 \, \mathrm{d}x \, \mathrm{d}y \tag{35}$$

denotes the quadratic form associated with the operator above. We employ the decomposition

$$\psi_n(x,y) = \varphi_n(x) \psi_1^{ND}(y) \tag{36}$$

where ψ_1^{ND} is the normalized eigenfuction of transversal Hamiltonian associated with the eigenvalue E_1 and φ_n is given by

$$\varphi_n(x) = \begin{cases} \dfrac{\sin(\sqrt{c_l}x)}{\sin(\sqrt{c_l}a)} & \text{in} \quad [0,a), \\ \dfrac{n-x}{n-a} & \text{in} \quad [a,n), \\ 0 & \text{otherwise} \end{cases} \tag{37}$$

Since φ_n vanishes for $x < 0$, ψ_n belongs to $D(Q_{c_l})$. Using the decomposition (36), the quadratic form turns to

$$\tilde{Q_{c_l}}[\psi_n] = \|\dot{\varphi}_n\|^2_{L^2(\mathbb{R})} - c_l \|\chi_{[-a,a]}\varphi_n\|^2_{L^2(\mathbb{R})} \,. \tag{38}$$

We get

$$\tilde{Q_{c_l}}[\psi_n] \stackrel{n\to\infty}{\longrightarrow} \sqrt{c_l}\cot(\sqrt{c_l}a)$$

from which we deduce that $\tilde{Q_{c_l}}[\varphi_n]$ can be made negative $\forall n \in \mathbb{N}$ if

$$c_l > \left(\frac{\pi}{2a}\right)^2 = 4\left(\frac{\pi}{4a}\right)^2 = 4E_1 \,.$$

This is in contradiction with the non-negativity of the quadratic form (35) and hence

$$c_l \le 4E_1.$$

□

Remark. The reason why we have chosen φ_n as in (37) is the following: we try to find a function ψ to make the quadratic form (38) *minimal* to obtain the best estimation of c_l. The part in (a,∞) is not relevant, since the derivative term tends to 0 as $n \to \infty$ anyway. More mathematicaly, we introduce the functional F

$$F[\psi] = \int_0^a (\psi')^2 - c_l \int_0^a \psi^2. \tag{39}$$

We are interested in a minimization problem of the (39) which means we are to find $\inf_\psi F[\psi]$, where a and c_l are given positive constants and the infimum is taken over all Lipschitz functions $\psi : (0,a) \to \mathbb{R}$ such that

$$\psi(0) = 0 \qquad \text{and} \qquad \psi(a) = 1\,. \tag{40}$$

We compute the first variation of F. For any Lipschitz function η such that

$$\eta(0) = 0 = \eta(a) \tag{41}$$

(so that $\psi + \varepsilon\eta$ is an admissible function, i.e., it satisfies the boundary conditions (40) for any $\varepsilon \in \mathbb{R}$) we have

$$\delta_\eta F[\psi] := \lim_{\varepsilon\to 0} \frac{F[\psi+\varepsilon\eta] - F[\psi]}{\varepsilon} = 2\int_0^a (\eta'\psi' - c_l\eta\psi) = 2\int_0^a \eta\,(-\psi'' - c_l\psi)\,. \tag{42}$$

Here the last equality follows by an integration by parts, employing (41).

The critical points of F are determined by those ψ_* for which $\delta_\eta F[\psi_*] = 0$ for any η with the above restrictions. The arbitrariness of η in (42) implies that the critical points ψ_* satisfy the boundary value problem

$$\begin{cases} -\psi'' - c_l\psi = 0 \quad \text{in} \quad (0,a)\,, \\ \qquad \psi(0) = 0\,, \\ \qquad \psi(a) = 1\,. \end{cases} \tag{43}$$

If $a^2 c_l \notin \pi\mathbb{N}$ then the (unique) solution of (43) is clearly given by

$$\psi_*(x) = \frac{\sin(\sqrt{c_l}x)}{\sin(\sqrt{c_l}a)}\,,$$

and there is no other solution.

By calculating the second variation of F, it is possible to show that the critical points of F correspond to minima of F.

The second variation of the functional F is defined by

$$\delta_\eta^2 F[\psi] := \frac{d^2}{d\varepsilon^2} F[\psi + \varepsilon\eta]\big|_{\varepsilon=0}, \tag{44}$$

where η is taken over all Lipschitz function such that $\eta(0) = \eta(a) = 0$ and $\eta(x) \neq 0$, $\forall x \in \mathbb{R}$. We suppose $\delta_\eta F[\psi_*] = 0$ and at the same time ψ_* satisfies (43). The non-negativity of $\delta_\eta^2 F[\psi_*]$ is necessary, positivity is a sufficient condition for ψ_* being minimum.

We already know from Theorem 5.3:

$$c_l \leq 4E_1 = 4\left(\frac{\pi}{4a}\right)^2 < \left(\frac{\pi}{a}\right)^2. \tag{45}$$

We compute (44):

$$\delta_\eta^2 F[\psi_*] = \lim_{\varepsilon\to 0} \frac{\delta_\eta F[\psi_* + \varepsilon\eta] - \delta_\eta F[\psi_*]}{\varepsilon} = 2\int_0^a ({\eta'}^2 - c_l\eta^2) = 2\int_0^a \eta(-\eta'' - c_l\eta)$$

It follows from the minimax principle (Theorem 2.2):

$$\left(\frac{\pi}{a}\right)^2 = \inf_{\eta\in H_0^1((0,a))} \frac{\int_0^a |\eta'(x)|^2\,\mathrm{d}x}{\int_0^a |\eta(x)|^2\,\mathrm{d}x} \leq \frac{\int_0^a |\eta'(x)|^2\,\mathrm{d}x}{\int_0^a |\eta(x)|^2\,\mathrm{d}x}, \qquad \forall \eta \in H_0^1((0,a)). \tag{46}$$

Indeed,

$$Q[\eta] := \int_0^a |\eta'(x)|^2\,\mathrm{d}x,$$

$$D(Q) := \{\eta \in H^1((0,a))|\; \eta(0) = \eta(a) = 0\} = H_0^1((0,a))$$

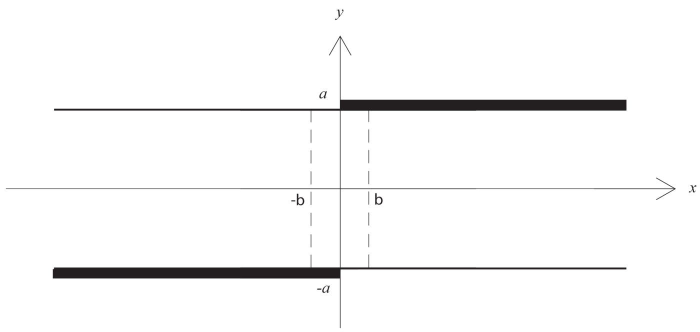

Figure 4: Twisted waveguide.

is a quadratic form associated with the Dirichlet Laplacian on $L^2(0,a)$. Using (46) and integrating by parts, we obtain

$$\begin{aligned}\frac{1}{2}\delta_\eta^2 F[\psi_*] &= \int_0^a (\eta'(x))^2\,\mathrm{d}x - \int_0^a c_l(\eta(x))^2\,\mathrm{d}x \\ &\geq \left(\frac{\pi}{a}\right)^2 \int_0^a (\eta(x))^2\,\mathrm{d}x - \int_0^a c_l(\eta(x))^2\,\mathrm{d}x = \left[\left(\frac{\pi}{a}\right)^2 - c_l\right]\|\eta\|^2,\end{aligned}$$

which is greater or equal to 0, for sure. Indeed, η is non-trivial and from (45) follows the strict positivity. Thus $F[\psi_*]$ coincides with the minimum.

5.2 Numerical results

As we already know from the previous section, the optimal Hardy constant c_l from (30) belongs to the range $0.039E_1 \leq c_l \leq 4E_1$. Our goal is to compute the optimal value of c_l numerically.

More generally, we consider the twisted waveguide, where $2a$ is the width of the waveguide and $[-b,b]\times[-a,a]$ is the area where the step-like potential $\chi_{[-b,b]\times[-a,a]}$ acts (see Fig 4). Let us denote by H_0 the Hamiltonian

$$\begin{aligned}H_0\psi &:= -\Delta\psi, \\ D(H_0) &:= \{H^1(\mathbb{R}\times(-a,a))|\ -\Delta\psi \in L^2(\mathbb{R}\times(-a,a)),\ \psi = 0 \text{ on } [(-\infty,0)\times\{-a\}] \\ &\quad \cup [(0,\infty)\times\{a\}],\ \partial_y\psi = 0 \text{ on } [(-\infty,0)\times\{a\}]\cup[(0,\infty)\times\{-a\}].\end{aligned}$$

We consider the bounded perturbation of H_0:

$$H_c := H_0 - c\chi_{[-b,b]\times[-a,a]},$$

$c \geq 0$. For c small it follows from the Hardy inequality (30) that $\inf\sigma(H_c) \geq E_1$. Hence $\sigma(H_c) = \sigma_{\mathrm{ess}}(H_c) = [E_1,\infty)$. In particular, $\sigma_{\mathrm{disc}}(H_c) = \varnothing$. We want to find the critical $c^* > 0$ such that:

1. $\forall c \leq c^*$, $\sigma_{\mathrm{disc}}(H_c) = \varnothing$
2. $\sigma_{\mathrm{disc}}(H_{c^*+0}) \neq \varnothing$,

i.e. the first eigenvalue of H_c appears at c^*.

5.2.1 Passing to undimensional units

We are looking for a solution of the equation

$$\left[-\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}-c\chi_{[-b,b]\times[-a,a]}(x,y)\right]\psi=\lambda\psi, \qquad \text{in } \mathbb{R}\times(-a,a), \tag{47}$$

$\lambda < E_1 \equiv \left(\frac{\pi}{4a}\right)^2$ subject to the appropriate boundary conditions.

It is convenient to work in undimensional units by introducing a transformation, e.g.

$$\tilde{\lambda}:=\frac{\lambda}{E_1},\ \tilde{x}:=\sqrt{E_1}x,\ \tilde{y}:=\sqrt{E_1}y,\ \tilde{c}:=\frac{c}{E_1},\ \tilde{b}:=\frac{b}{a}.$$

Then (47) is equivalent to

$$\left[-\frac{\partial^2}{\partial \tilde{x}^2}-\frac{\partial^2}{\partial \tilde{y}^2}-\tilde{c}\chi_{[-\frac{\pi}{4}\tilde{b},\frac{\pi}{4}\tilde{b}]\times[-\frac{\pi}{4},\frac{\pi}{4}]}(\tilde{x},\tilde{y})\right]\psi=\tilde{\lambda}\psi \qquad \text{in } \mathbb{R}\times\left(-\frac{\pi}{4},\frac{\pi}{4}\right).$$

In these units, $\tilde{E_n}=(2n-1)^2$, $n\in\mathbb{N}$. At the same time $0.039<\tilde{c}<4$.

It is also useful to work with the shifted equation

$$\left[-\frac{\partial^2}{\partial \tilde{x}^2}-\frac{\partial^2}{\partial \tilde{y}^2}-\tilde{c}\chi_{[-\frac{\pi}{4}\tilde{b},\frac{\pi}{4}\tilde{b}]\times[-\frac{\pi}{4},\frac{\pi}{4}]}(\tilde{x},\tilde{y})-1\right]\psi=\tilde{\tilde{\lambda}}\psi,$$

so that $\tilde{\tilde{\lambda}}:=\tilde{\lambda}-1$, i.e. the essential spectrum of the problem starts at 0. Henceforth, we eliminate the tildas.

5.2.2 Ansatz for solutions

Using the fact that the equation admits explicit solutions in the regions:

$$\begin{aligned}
\Omega_1 &:= \left(-\infty,-\frac{\pi}{4}b\right)\times\left(-\frac{\pi}{4},\frac{\pi}{4}\right),\\
\Omega_2 &:= \left(-\frac{\pi}{4}b,0\right)\times\left(-\frac{\pi}{4},\frac{\pi}{4}\right),\\
\Omega_3 &:= \left(0,\frac{\pi}{4}b\right)\times\left(-\frac{\pi}{4},\frac{\pi}{4}\right),\\
\Omega_4 &:= \left(\frac{\pi}{4}b,\infty\right)\times\left(-\frac{\pi}{4},\frac{\pi}{4}\right),
\end{aligned}$$

and the requirement on L^2-integrability in Ω_1, Ω_4, it is natural to look for the solutions in the form:

$$\psi(x,y) = \begin{cases} \sum_{n=1}^{\infty} a_n^1 e^{\sqrt{E_n-1-\lambda}\,x} \psi_n^{DN}(y), & \text{in } \Omega_1, \\ \sum_{n=1}^{\infty} (a_n^2 \sinh(p_n\,x) + b_n^2 \cosh(p_n\,x)) \psi_n^{DN}(y), & \text{in } \Omega_2, \\ \sum_{n=1}^{\infty} (a_n^3 \sinh(p_n\,x) + b_n^3 \cosh(p_n\,x)) \psi_n^{ND}(y), & \text{in } \Omega_3, \\ \sum_{n=1}^{\infty} a_n^4 e^{\sqrt{E_n-1-\lambda}\,x} \psi_n^{ND}(y), & \text{in } \Omega_4, \end{cases}$$

where $p_n := \sqrt{E_n - 1 - \lambda - c}$. Let us recall the transverse bases defined in (21), (21).

5.2.3 Passing to algebraic equations

ψ contains 7 unknowns: $a_n^1, a_n^2, b_n^2, a_n^3, b_n^3, a_n^4, \lambda$. Requiring $\psi \in D(H_c) = D(H_0)$, we arrive at 6 equations:

$$\psi(x_-, y) = \psi(x_+, y),$$
$$\partial_x \psi(x_-, y) = \partial_x \psi(x_+, y),$$

where $x \in \left\{-\frac{\pi}{4}b,\ 0,\ \frac{\pi}{4}b\right\}$, for all $y \in \left(-\frac{\pi}{4}, \frac{\pi}{4}\right)$. The last unknown is free (as usual for eigenvalue problems). We evaluate:

1. $x = -\frac{\pi}{4}$
   The C^1-continuity at $-\frac{\pi}{4}$ and the same basis ψ_n^{DN} on $(-\infty, 0)$ lead for all $y \in \left(-\frac{\pi}{4}, \frac{\pi}{4}\right)$ and for all $n \in \mathbb{N}$, to:
   (a)
   $$a_n^1 e^{-\sqrt{E_n-1-\lambda}\,\frac{\pi}{4}b} = -a_n^2 \sinh\left(p_n\,\frac{\pi}{4}b\right) + b_n^2 \cosh\left(p_n\,\frac{\pi}{4}b\right), \tag{48}$$
   (b)
   $$a_n^1 \sqrt{E_n - 1 - \lambda}\, e^{-\sqrt{E_n-1-\lambda}\,\frac{\pi}{4}b} = a_n^2 \cosh\left(p_n\,\frac{\pi}{4}b\right) p_n - b_n^2 \sinh\left(p_n\,\frac{\pi}{4}b\right) p_n. \tag{49}$$
2. $x = 0$
   The basis are not identical:
   (a)
   $$\sum_{n=1}^{\infty} b_n^2 \psi_n^{DN}(y) = \sum_{n=1}^{\infty} b_n^3 \psi_n^{ND}(y), \tag{50}$$

(b)

$$\sum_{n=1}^{\infty} a_n^2\, p_n\, \psi_n^{DN}(y) = \sum_{n=1}^{\infty} a_n^3\, p_n\, \psi_n^{ND}(y). \tag{51}$$

3. $x = \frac{\pi}{4}$
   For all $n \in \mathbb{N}$, $y \in \left(-\frac{\pi}{4}, \frac{\pi}{4}\right)$:
   (a)

$$a_n^4 e^{-\sqrt{E_n - 1 - \lambda}\, \frac{\pi}{4} b} = a_n^3 \sinh\Big(p_n\, \frac{\pi}{4} b\Big) + b_n^3 \cosh\Big(p_n\, \frac{\pi}{4} b\Big), \tag{52}$$

   (b)

$$\begin{aligned} -a_n^4 \sqrt{E_n - 1 - \lambda}\, e^{-\sqrt{E_n - 1 - \lambda}\, \frac{\pi}{4} b} = a_n^3 \cosh\Big(p_n\, \frac{\pi}{4} b\Big) p_n \\ + b_n^3 \sinh\Big(p_n\, \frac{\pi}{4} b\Big) p_n. \end{aligned} \tag{53}$$

Multiplying the equations (50), (51) by ψ_m^{DN}, integrating over $(-\frac{\pi}{4}, \frac{\pi}{4})$ and using the orthonormality $(\psi_m^{DN}, \psi_n^{DN})_{L^2\left(-\frac{\pi}{4}, \frac{\pi}{4}\right)} = \delta_{mn}$, we obtain

$$b_m^2 = \sum_{n=1}^{\infty} b_n^3\, (\psi_m^{DN}, \psi_n^{ND}) =: \sum_{n=1}^{\infty} C_{mn} b_n^3, \tag{54}$$

$$a_m^2 p_m = \sum_{n=1}^{\infty} a_n^3\, p_n\, (\psi_m^{DN}, \psi_n^{ND}) =: \sum_{n=1}^{\infty} C_{mn}\, p_n\, a_n^3. \tag{55}$$

Here $(\psi_m^{DN}, \psi_n^{ND})$ are elementary integrals to be calculated. From (52), (53) it follows:

$$a_n^3 = \frac{(-\sqrt{E_n - 1 - \lambda}\, \cosh\left(\frac{\pi}{4} b\, p_n\right) - p_n\, \sinh\left(\frac{\pi}{4} b\, p_n\right)) b_n^3}{p_n\, \cosh\left(\frac{\pi}{4} b\, p_n\right) + \sqrt{E_n - 1 - \lambda}\, \sinh\left(\frac{\pi}{4} b\, p_n\right)} =: k(n) b_n^3.$$

It is possible, to reduce all this to

$$\sum_{n=1}^{\infty} M_{mn} b_n^3 = 0, \tag{56}$$

where

$$\begin{aligned} M_{mn} := \sqrt{E_m - 1 - \lambda}\Big[\sum_{n=1}^{\infty} -k(n)\, b_n^3\, C_{mn} p_n \sinh\left(\frac{\pi}{4} b\, p_m\right) + C_{mn} p_m\, b_n^3 \cosh\left(\frac{\pi}{4} b\, p_m\right)\Big] \\ - p_m \Big[\sum_{n=1}^{\infty} k(n)\, b_n^3\, C_{mn} p_n \cosh\left(\frac{\pi}{4} b\, p_m\right) - C_{mn} p_m\, b_n^3 \sinh\left(\frac{\pi}{4} b\, p_m\right)\Big]. \end{aligned}$$

5.2.4 Numerical solution

The equation (56) is a homogeneous equation for the coefficients $\{b_n^3\}_{n=1}^{\infty}$. It admits a non-trivial solution if

$$\det (M_{mn})_{m,n=1}^{\infty} = 0. \tag{57}$$

This represents an implicit equation for λ. The numerics consists in taking $N \in \mathbb{N}$, instead of ∞, i.e.

$$\det (M_{mn})_{m,n=1}^{N} = 0. \tag{58}$$

Solving this equation, we get the curves:

$$c \longmapsto \lambda(c).$$

We investigate the influence of the width b on the spectral properties.

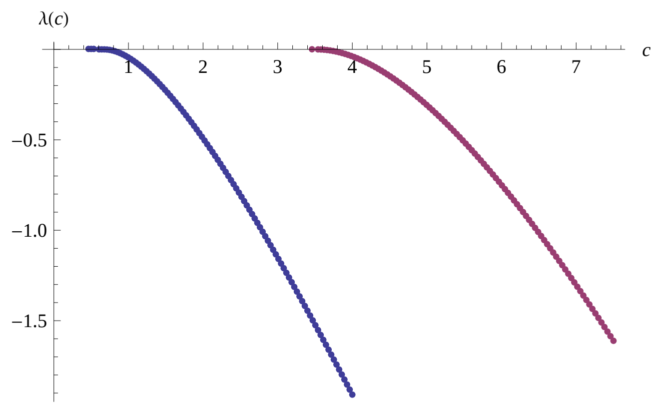

Figure 5: The plot of $\lambda(c)$ for $b = a$, $N = 5$.

Firstly, we consider $b = a$, i.e. $\tilde{b} = 1$. The plot $\lambda(c)$ may be evaluated, see Figure 5. One can see that the first eigenvalue is generated by $c^* \approx 0.8$. This gives an estimation on the value of the optimal Hardy constant in (30), i.e.

$$c_l^* \approx 0.8E_1.$$

The other curve establishes the value $c^{**} \approx 3.5$, i.e. the value by which the second eigenvalue below the essential spectrum begins to exist. Unfortunatelly, the numerical solution is quite sensitive to small values of N, so the values vary in the range ± 0.2 depending on $N \in \{1, \dots, 14\}$. At the same time, owing to our rather poor technical equipement (Intel Core^{TM}2 Duo processor $T5500$, 1.66 GHz, 667 MHz FSB, 2 MB L2 cache), the values could not be computed for greater N, hence the results are not of highest precision.

Secondly, for $b := 2a$ we obtain Figure 6. The numerical value of c^* is approximatelly 0.3 (cf. Figure 6). This implies that the first eigenvalue is generated by a smaller perturbation than in the case $b = a$.

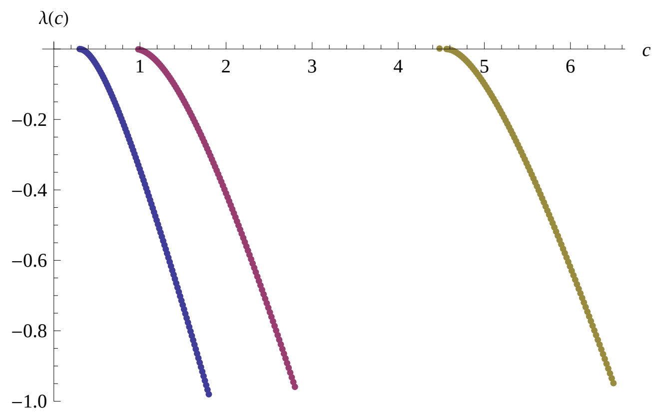

Figure 6: The plot of $\lambda(c)$ for $b = 2a$, $N = 5$.

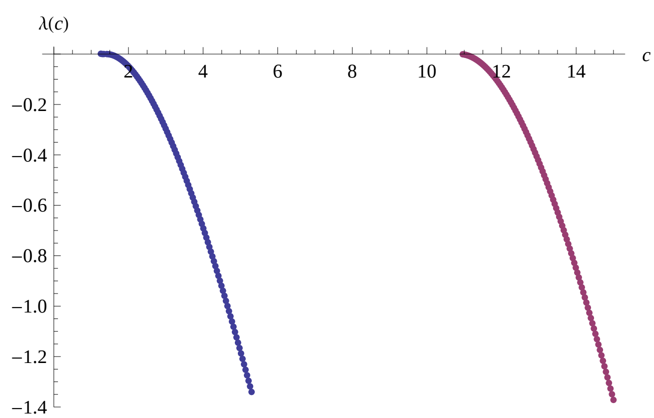

Figure 7: The plot of $\lambda(c)$ for $b = a/2$, $N = 5$.

Finally, we consider $b := \frac{a}{2}$ (Figure 7). Thus, the bound states are not generated until $c^* \approx 1.4$.

As a consequence, the wider the support of the step-like potential is, the smaller the constant c^* is.

6 Conclusion

In this thesis we were concerned with spectral properties of a planar twisted quantum waveguide with a combination of Dirichlet and Neumann conditions imposed on the boundary. First of all, we were interested in Hardy inequalities which have connection with the stability of the essential spectrum. Namely, if the Hardy inequality (6) is satisfied then no eigenvalues below the essential spectrum are generated by a small potential perturbations. Secondly, we have shown, that the essential spectrum of the straight waveguide does not change while twisting the boundary conditions.

The motivation for the present thesis was to make familiar with spectral theory and recent progress in quantum waveguides research, above all in the twisted waveguides. The main goal, i.e. the quantitative study of the Hardy inequalities, gave an upper bound and consequently an exact numerical value of the optimal Hardy constant. This completes the study of [14] where just a lower bound to the Hardy constant has been obtained.

The possible aim how to extend the thesis lies in considering higher dimensional waveguides. It would be also desirable to make the numerical computation more precise by using a better computer. Finally, it remains to investigate more thoroughly the dependence of the optimal Hardy constant on the width of the step-like weight.

Appendix A

The source code for Wolfram Mathematica

In this section we provide the source code for the numerics in Wolfram Mathematica 7.0. The function *abs* denotes the scalar product of the two transverse bases. *mmn* is the matrix M_{mn}. The function f is searching for the root of the determinant of M_{mn}. And finally, *p11* plots a curve by using a repeating for-cycle.

$$\text{abs}[\text{m\_}, \text{n\_}]{:=}\text{If}\left[m!{=}n, \frac{(-1+2n)\text{Cos}[m\pi]+(1-2m)\text{Cos}[n\pi]}{(m-n)(-1+m+n)\pi}, \frac{2\text{Cos}[n\pi]}{\pi-2n\pi} - \text{Sin}[n\pi]\right]$$

$$\text{Clear}[\text{mmn}];$$
$$\text{mmn}[\text{m\_}, \text{n\_}, \lambda\text{\_}, \text{c\_}]{:=}\Big(\Big(\sqrt{-1+(2n-1)^2-\lambda}\text{Cosh}\left[\tfrac{\text{Pi}}{4}\sqrt{-1-c+(2n-1)^2-\lambda}\right]+$$
$$\sqrt{-1-c+(2n-1)^2-\lambda}\text{Sinh}\left[\tfrac{\text{Pi}}{4}\sqrt{-1-c+(2n-1)^2-\lambda}\right]\Big)$$
$$\text{Sqrt}\left[(2n-1)^2-1-\lambda-c\right]*$$
$$\text{abs}[m,n]\text{Sinh}\left[\tfrac{\text{Pi}}{4}\sqrt{-1-c+(2m-1)^2-\lambda}\right]+$$
$$\text{abs}[m,n]\text{Cosh}\left[\tfrac{\text{Pi}}{4}\sqrt{-1-c+(2m-1)^2-\lambda}\right]*$$
$$\text{Sqrt}\left[(2m-1)^2-1-\lambda-c\right]*$$
$$\Big(\sqrt{-1-c+(2n-1)^2-\lambda}\text{Cosh}\left[\tfrac{\text{Pi}}{4}\sqrt{-1-c+(2n-1)^2-\lambda}\right]+$$
$$\sqrt{-1+(2n-1)^2-\lambda}\text{Sinh}\left[\tfrac{\text{Pi}}{4}\sqrt{-1-c+(2n-1)^2-\lambda}\right]\Big)\Big)*\text{Sqrt}\left[(2m-1)^2-1-\lambda\right]-$$
$$\Big(\Big(-\sqrt{-1+(2n-1)^2-\lambda}\text{Cosh}\left[\tfrac{\text{Pi}}{4}\sqrt{-1-c+(2n-1)^2-\lambda}\right]-\sqrt{-1-c+(2n-1)^2-\lambda}*$$
$$\text{Sinh}\left[\tfrac{\text{Pi}}{4}\sqrt{-1-c+(2n-1)^2-\lambda}\right]\Big)\text{Sqrt}\left[(2n-1)^2-1-\lambda-c\right]*\text{abs}[m,n]*$$
$$\text{Cosh}\left[\tfrac{\text{Pi}}{4}\sqrt{-1-c+(2m-1)^2-\lambda}\right]-\text{abs}[m,n]\text{Sinh}\left[\tfrac{\text{Pi}}{4}\sqrt{-1-c+(2m-1)^2-\lambda}\right]*$$
$$\text{Sqrt}\left[(2m-1)^2-1-\lambda-c\right]*$$
$$\Big(\sqrt{-1-c+(2n-1)^2-\lambda}\text{Cosh}\left[\tfrac{\text{Pi}}{4}\sqrt{-1-c+(2n-1)^2-\lambda}\right]+$$
$$\sqrt{-1+(2n-1)^2-\lambda}\text{Sinh}\left[\tfrac{\text{Pi}}{4}\sqrt{-1-c+(2n-1)^2-\lambda}\right]\Big)\Big)*$$
$$\text{Sqrt}\left[(2m-1)^2-1-\lambda-c\right]\ \text{Clear}[f];$$
$$f[\lambda\text{\_}, \text{c\_}]{:=}\text{Det}[\text{Table}[\text{mmn}[m,n,\lambda,c],\{m,10\},\{n,10\}]]$$
$$\text{Clear}[c,\text{imax},\lambda 11,\lambda 0,\lambda 12,\lambda 02,\text{c2},\lambda 13,\lambda 03,\text{c3}];$$
$$\text{imax}=100;\lambda 0=-0.0001;$$
$$\text{Table}[\lambda 11[i],\{i,0,\text{imax}\}];\text{Table}[c[i],\{i,0,\text{imax}\}];$$
$$\text{For}[i=0,$$

$i < \text{imax} + 1,$
$i{+}{+},$
$c[i] = \frac{3.5}{99}(i - 1) + 0.5;$
$\lambda 0 = \lambda /.\text{FindRoot}[f[\lambda, c[i]] == 0, \{\lambda, \lambda 0\}];$
$\lambda 11[i] = \lambda 0];$
$\lambda 02 = -0.0001; \text{Table}[\lambda 12[i], \{i, 0, \text{imax}\}]; \text{Table}[\text{c2}[i], \{i, 0, \text{imax}\}];$
$\text{For}[i = 0,$
$i < \text{imax} + 1,$
$i{+}{+},$
$\text{c2}[i] = \frac{4}{99}(i - 1) + 3.5;$
$\lambda 02 = \lambda /.\text{FindRoot}[f[\lambda, \text{c2}[i]] == 0, \{\lambda, \lambda 02\}];$
$\lambda 12[i] = \lambda 02];$
$\text{p11} = \text{ListPlot}[\{\text{Table}[\{c[i], \lambda 11[i]\}, \{i, 0, \text{imax}\}],$
$\text{Table}[\{\text{c2}[i], \lambda 12[i]\}, \{i, 0, \text{imax}\}]\}, \text{AxesLabel} \to \{c, \lambda[c]\}]$

References

[1] R. A. Adams, *Sobolev spaces*, Academic Press, New York (1975).

[2] J. Blank, P. Exner, M. Havlíček, *Lineární operátory v kvantové fyzice*, Univerzita Karlova, vydavatelství Karolinum, Praha (1993).

[3] E. B. Davies, *Spectral theory and differential operators*, Camb. Univ. Press, Cambridge (1995).

[4] J. Dittrich and J. Kříž, *Bound states in straight quantum waveguides with combined boundary conditions*, J. Math. Phys. **43**, 3892-3915 (2002).

[5] J. Dittrich and J. Kříž, *Curved planar quantum wires with Dirichlet and Neumann boundary conditions*, J. Phys. A: Math. Gen. **35**, 269-275, (2002).

[6] P. Duclos and P. Exner, *Curvature-induced bound states in quantum waveguides in two and three dimensions*, Rev. Math. Phys. **7**, 73-102 (1995).

[7] T. Ekholm and H. Kovařík, *Stability of the magnetic Schrödinger operator in a waveguide*, Commun. in Partial Differential Equations **30** (2005).

[8] T. Ekholm, H. Kovařík and D. Krejčiřík, *A Hardy inequality in twisted waveguides*, Arch. Ration. Mech. Anal. **188**, No. 2, 245-264 (2008).

[9] P. Exner and P. Šeba, *Bound states in curved quantum waveguides*, J. Math. Phys. **30**, 2574-2580 (1989).

[10] P. Freitas and D. Krejčiřík, *Waveguides with combined Dirichlet and Robin boundary conditions*, Math. Phys. Anal. Geom. **9** (2006), no. 4, 335-352.

[11] D. Gilbarg, N. S. Trudinger, *Elliptic partial differential equations of second order*, Springer-Verlag, Berlin (1983).

[12] G. H. Hardy, *Note on a theorem of Hilbert*, Math. Zeit. **6** (1920), 314-317.

[13] V. Jarník, *Integrální počet II.*, Nakladatelství Československé Akademie věd, Praha (1955).

[14] H. Kovařík and D. Krejčiřík, *A Hardy inequality in a twisted Dirichlet-Neumann waveguide*, Math. Nachr. **281** (2008), 1159-1168.

[15] D. Krejčiřík, *Quantum strips on surfaces*, J. Geom. Phys. **45** (2003), no. 1-2, 203-217.

[16] D. Krejčiřík, *Twisting versus bending in quantum waveguides*, Proc. of Symp. in Pure Math. **44** (2008), 617-636.

[17] D. Krejčiřík and J. Kříž *On the spectrum of curved quantum waveguides*, Publ. RIMS, Kyoto University, **41** (2005), no. 3.

[18] D. Krejčiřík, E. Zuazua, *The Hardy inequality and the heat equation in twisted tubes*, J. de Math. Pures et Appl. 0906.3359 , to appear.

[19] A. Laptev, T. Weidl, *Hardy inequalities for magnetic Dirichlet forms*, Operator Theory: Advances Applications **108**, 299-305 (1999).

[20] B. Opic, A. Kufner, *Hardy-type inequalities*, Longman Scientific & Technical; Harlow (1990).

[21] T. Pfrommer, *Analytische und numerische Untersuchungen von Hardyungleichungen auf gedrehten Wellenleitern*, Diploma thesis, supervisor: Prof. TeknD. Timo Weidl; Universität Stuttgart (2008).

[22] M. Reed, B. Simon, *Methods of modern mathematical physics, IV. Analysis of operators*, Academic Press, New York (1978).