Straight quantum waveguide with Robin boundary conditions

by

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Abstract

We investigate spectral properties of a quantum particle confined to an infinite straight planar strip by imposing Robin boundary conditions with variable coupling. Assuming that the coupling function tends to a constant at infinity, we localise the essential spectrum and derive a sufficient condition which guarantees the existence of bound states. Further properties of the associated eigenvalues and eigenfunctions are studied numerically by the mode-matching technique.

1 Introduction

Modern experimental techniques make it possible to fabricate tiny semiconductor structures which are small enough to exhibit quantum effects. These systems are sometimes called *nanostructures* because of their typical size in a direction and they are expected to become the building elements of the next-generation electronics. Since the used materials are very pure and of crystallic structure, the particle motion inside a nanostructure can be modeled by a free particle with an effective mass m^* living in a spatial region Ω. That is, the quantum Hamiltonian can be identified with the operator

$$H = -\frac{\hbar^2}{2m^*}\Delta \tag{1.1}$$

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in the Hilbert space $L^2(\Omega)$, where $\hbar$ denotes the Planck constant. We refer to [20, 10] for more information on the physical background.

An important category of nanostructures is represented by *quantum waveguides*, which are modeled by Ω being an infinitely stretched tubular region in $\mathbb{R}^2$ or $\mathbb{R}^3$. In principle, one can consider various conditions on the boundary of Ω in order to model the fact that the particle is confined to Ω. However, since the particle wavefunctions ψ are observed to be suppressed near the interface between two different semiconductor materials, one usually imposes Dirichlet boundary conditions, *i.e.* $\psi = 0$ on $\partial\Omega$. Such models were extensively studied. The simplest possible system is a straight tube. The spectral properties of corresponding Hamiltonian in this case are trivial in the sense that the discrete spectrum is empty.

It is known, that a deviation from the straight tube can give rise to non-trivial spectral properties like existence of bound states, by bending it [5, 10, 13, 16, 19], introducing an arbitrarily small 'bump' [2, 4] or impurities modeled by Dirac interaction [12], coupling several waveguides by a window [14], *etc.*

Another possibility of generating bound states is the changing of boundary conditions. It can be done by imposing a combination of Dirichlet and Neumann boundary conditions on different parts of the boundary. Such models were studied in [9, 8, 15, 18].

In this paper, we introduce and study the model of straight planar quantum waveguide with Robin conditions on the boundary. While to impose the Dirichlet boundary conditions means to require the vanishing of wavefunction on the boundary of Ω, the Robin conditions correspond to the weaker requirement of vanishing of the probability current, in the sense that its normal component vanishes on the boundary, *i.e.*

$$j \cdot n = 0 \quad \text{on} \quad \partial\Omega,$$

where the probability current j is defined by

$$j := \frac{i\hbar}{2m^*}\left[\psi\nabla\overline{\psi} - \overline{\psi}\nabla\psi\right].$$

This less restrictive requirement may in principle model different types of interface in materials.

The system we are going to study is sketched on Figure 1. We consider the quantum particle whose motion is confined to a straight planar strip of width d. For definiteness we assume that it is placed to the upper side of the x-axis. On the boundary the Robin conditions are imposed. More precisely, we suppose that every wave-function ψ satisfies

$$
\begin{aligned}
-\psi_{,y}(x,0) + \alpha(x)\psi(x,0) &= 0, \\
\psi_{,y}(x,d) + \alpha(x)\psi(x,d) &= 0,
\end{aligned} \tag{1.2}
$$

for all $x \in \mathbb{R}$. The coma with the index marks the partial derivative. Notice that the parameter α depends on the x-coordinate and this dependence is the same on both "sides" of the strip. We require that $\alpha(x)$ is non-negative for all $x \in \mathbb{R}$. Moreover, in Theorem 2.2 we will show that a sufficient condition for the self-adjointness of the Hamiltonian is the requirement that $\alpha \in W^{1,\infty}(\mathbb{R})$. We shall denote this configuration space by $\Omega := \mathbb{R} \times (0,d)$.

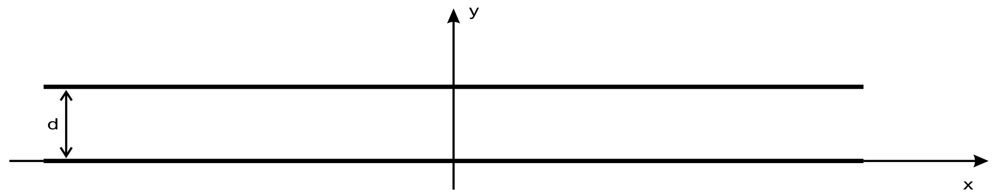

Figure 1: Straight waveguide with Robin boundary conditions

Putting $\hbar^2/2m^* = 1$ in (1.1), we may identify the particle Hamiltonian with the self-adjoint operator on the Hilbert space $L^2(\Omega)$, defined in the following way

$$
H_\alpha\psi := -\Delta\psi, \quad \forall \psi \in D(H_\alpha) := \left\{ \psi \in W^{2,2}(\Omega) \middle| \psi \text{ satisfies (1.2)} \right\}, \tag{1.3}
$$

where $D(H_\alpha)$ denotes the domain of the Hamiltonian.

While it is easy to see that H_α is symmetric, it is quite difficult to prove that it is self-adjoint. This will be done in the next section. Section 3 is devoted to localisation of the essential spectrum and proving the existence of discrete spectrum. In the final section we study an example numerically to illustrate the spectral properties.

2 The self-adjointness of the Robin Laplacian

For showing the self-adjointness of the Hamiltonian, we were inspired by [3, Sec. 3]. Our strategy is to show that H_α is, in fact, equal to another operator $\tilde{H}_\alpha$, which is self-adjoint and defined in following way.

Let us introduce a sesquilinear form

$$h_\alpha(\phi,\psi) := \int_\Omega \overline{\nabla\phi(x,y)}\cdot\nabla\psi(x,y)\,\mathrm{d}x\,\mathrm{d}y + \int_{\mathbb{R}} \alpha(x)\big(\overline{\phi(x,0)}\psi(x,0) + \overline{\phi(x,d)}\psi(x,d)\big)\,\mathrm{d}x$$

with the domain

$$D(h_\alpha) := W^{1,2}(\Omega).$$

Here the dot denotes the scalar product in $\mathbb{R}^2$ and the boundary terms should be understood in the sense of traces [1, Sec. 4]. We shall denote the corresponding quadratic form by $h_\alpha[\psi] := h_\alpha(\psi,\psi)$. In view of the first representation theorem [17, Thm. VI.2.1], there exists the unique self-adjoint operator $\tilde{H}_\alpha$ in $L^2(\Omega)$ such that $h_\alpha(\phi,\psi) = (\phi, \tilde{H}_\alpha\psi)$ for all $\psi \in D(\tilde{H}_\alpha) \subset D(h_\alpha)$ and $\phi \in D(h_\alpha)$, where

$$D(\tilde{H}_\alpha) = \left\{\psi \in D(h_\alpha) \middle| \exists F \in L^2(\Omega), \forall\phi \in D(h_\alpha), h_\alpha(\phi,\psi) = (\phi, F)\right\}.$$

For showing the equality between H_α and $\tilde{H}_\alpha$ we will need following result.

Lemma 2.1. *Let $\alpha \in W^{1,\infty}(\mathbb{R})$ and $\forall x \in \mathbb{R},\ \alpha(x) \geq 0$. For each $F \in L^2(\Omega)$, a solution ψ to the problem*

$$\forall\phi \in W^{1,2}(\Omega),\ h_\alpha(\phi,\psi) = (\phi, F) \tag{2.1}$$

belongs to $D(H_\alpha)$.

Proof. For any function $\psi \in W^{1,2}(\Omega)$, we introduce the difference quotient

$$\psi_\delta(x,y) := \frac{\psi(x+\delta,y) - \psi(x,y)}{\delta},$$

where δ is a small real number [11, Chap. 5.8.2]. Since

$$|\psi(x+\delta,y) - \psi(x,y)| = \left|\delta \int_0^1 \psi_{,x}(x+\delta t,y)\,\mathrm{d}t\right| \leq |\delta| \int_0^1 |\psi_{,x}(x+\delta t,y)|\ \mathrm{d}t,$$

we get the estimate

$$\begin{aligned}\int_\Omega |\psi_\delta|^2 \leq \int_\Omega \left(\int_0^1 |\psi_{,x}(x+\delta t,y)|\ \mathrm{d}t\right)^2 \mathrm{d}x\,\mathrm{d}y \leq \int_\Omega \left(\int_0^1 |\psi_{,x}(x+\delta t,y)|^2\ \mathrm{d}t\right) \mathrm{d}x\,\mathrm{d}y \\ = \int_0^1 \left(\int_\Omega |\psi_{,x}(x+\delta t,y)|^2\ \mathrm{d}x\,\mathrm{d}y\right) \mathrm{d}t = \int_\Omega |\psi_{,x}(x,y)|^2\ \mathrm{d}x\,\mathrm{d}y.\end{aligned}$$

Therefore the inequality

$$\|\psi_\delta\|_{L^2(\Omega)} \leq \|\psi\|_{W^{1,2}(\Omega)} \tag{2.2}$$

holds true.

If ψ satisfies (2.1), then ψ_δ is a solution to the problem

$$h_\alpha(\phi, \psi_\delta) = (\phi, F_\delta) - \int_{\mathbb{R}} \alpha_\delta(x) \left(\overline{\phi(x,0)}\psi(x+\delta,0) + \overline{\phi(x,d)}\psi(x+\delta,d) \right) \mathrm{d}x,$$

where $\phi \in W^{1,2}(\Omega)$ is arbitrary. Letting $\phi = \psi_\delta$ and using the "integration-by-parts" formula for the difference quotients, $(\phi, F_\delta) = -(\phi_{-\delta}, F)$, we get

$$h_\alpha[\psi_\delta] = -((\psi_\delta)_{-\delta}, F) - \int_{\mathbb{R}} \alpha_\delta(x) \left(\overline{\psi_\delta(x,0)}\psi(x+\delta,0) + \overline{\psi_\delta(x,d)}\psi(x+\delta,d) \right) \mathrm{d}x. \tag{2.3}$$

Using Schwarz inequality, Cauchy inequality, estimate (2.2), boundedness of α and α_δ, and embedding of $W^{1,2}(\Omega)$ in $L^2(\partial\Omega)$ [1, Sec 4], we can make following estimates

$$|((\psi_\delta)_{-\delta}, F)| \le \|F\| \|(\psi_\delta)_{-\delta}\| \le \frac{1}{2}\|F\|^2 + \frac{1}{2}\|\psi_\delta\|^2_{W^{1,2}(\Omega)},$$

$$\left| \int_{\mathbb{R}} \alpha_\delta(x) \left(\overline{\psi_\delta(x,0)}\psi(x+\delta,0) + \overline{\psi_\delta(x,d)}\psi(x+\delta,d) \right) \mathrm{d}x \right| \le C_1 \|\psi_\delta\|_{L^2(\partial\Omega)} \|\psi\|_{L^2(\partial\Omega)}$$

$$\le C_2 \|\psi_\delta\|_{W^{1,2}(\Omega)} \|\psi\|_{W^{1,2}(\Omega)},$$

$$\left| \int_{\mathbb{R}} \alpha(x) \left(|\psi_\delta(x,0)|^2 + |\psi_\delta(x,d)|^2 \right) \mathrm{d}x \right| \le C_3 \|\psi_\delta\|^2_{L^2(\partial\Omega)} \le C_4 \|\psi_\delta\|^2_{W^{1,2}(\Omega)}$$

with constants C_1–C_4 independent of δ. Giving these estimates together, the identity (2.3) yields

$$-\|\psi_\delta\|^2_{W^{1,2}(\Omega)} \le C_4 \|\psi_\delta\|^2_{W^{1,2}(\Omega)} + C_2 \|\psi_\delta\|_{W^{1,2}(\Omega)} \|\psi\|_{W^{1,2}(\Omega)} + \frac{1}{2}\|F\|^2 + \frac{1}{2}\|\psi_\delta\|^2_{W^{1,2}(\Omega)}.$$

We get the inequality

$$\|\psi_\delta\|_{W^{1,2}(\Omega)} \le C,$$

where the constant C is independent of δ. This estimate implies

$$\sup_\delta \|\psi_{-\delta}\|_{W^{1,2}(\Omega)} < \infty;$$

and, therefore, by [11, § D.4] there exists a function $v \in W^{1,2}(\Omega)$ and a subsequence $\delta_k \to 0$ such that $\psi_{-\delta_k} \xrightarrow{w} v$ in $W^{1,2}(\Omega)$. But then

$$-\int_\Omega \psi_{,x}\phi = \int_\Omega \psi\phi_{,x} = \int_\Omega \psi \lim_{\delta_k \to 0} \phi_{\delta_k} = \lim_{\delta_k \to 0} \int_\Omega \psi\phi_{\delta_k} = -\lim_{\delta_k \to 0} \int_\Omega \psi_{-\delta}\phi = -\int_\Omega v\phi.$$

Thus, $\psi_{,x} = v$ in the weak sense, and so $\psi_{,x} \in W^{1,2}(\Omega)$. Hence, $\psi_{,xx} \in L^2(\Omega)$ and $\psi_{,xy} \in L^2(\Omega)$.

It follows from the standard elliptic regularity theorems (see [11, § 6.3]) that $\psi \in W^{2,2}_{loc}(\Omega)$. Hence, the equation $-\Delta\psi = F$ holds true a.e. in Ω. Thus, $\psi_{,yy} = -F - \psi_{,xx} \in L^2(\Omega)$, and therefore $\psi \in W^{2,2}(\Omega)$.

It remains to check boundary conditions for ψ. Using integration by parts, one has

$$\begin{aligned}(\phi, F) = h_\alpha(\psi, \phi) = (\phi, -\Delta\psi)\\ + \int_{\mathbb{R}} \overline{\phi(x,0)}\,[-\psi_{,y}(x,0) + \alpha(x)\psi(x,0)]\ \mathrm{d}x\\ + \int_{\mathbb{R}} \overline{\phi(x,d)}\,[\psi_{,y}(x,d) + \alpha(x)\psi(x,d)]\ \mathrm{d}x\end{aligned}$$

for any $\phi \in W^{1,2}(\Omega)$. This implies the boundary conditions because $-\Delta\psi = F$ a.e. in Ω and ϕ is arbitrary. □

Theorem 2.2. *Let $\alpha \in W^{1,\infty}(\mathbb{R})$ and $\forall x \in \mathbb{R},\ \alpha(x) \geq 0$. Then $\tilde{H}_\alpha = H_\alpha$.*

Proof. Let $\psi \in D(H_\alpha)$, *i.e.*, $\psi \in W^{2,2}(\Omega)$ and ψ satisfies the boundary conditions (1.2). Then $\psi \in D(h_\alpha) = W^{1,2}(\Omega)$ and by integration by parts and (1.2) we get for all $\phi \in D(h_\alpha)$ the relation

$$\begin{aligned}h_\alpha(\phi,\psi) = \int_{\mathbb{R}} \overline{\phi(x,d)}\psi_{,y}(x,d)\,\mathrm{d}x - \int_{\mathbb{R}} \overline{\phi(x,0)}\psi_{,y}(x,0)\,\mathrm{d}x -\\ - \int_{\Omega} \overline{\phi(x,y)}\Delta\psi(x,y)\,\mathrm{d}x\,\mathrm{d}y + \int_{\mathbb{R}} \alpha(x)\overline{\phi(x,d)}\psi(x,d)\,\mathrm{d}x +\\ + \int_{\mathbb{R}} \alpha(x)\overline{\phi(x,0)}\psi(x,0)\,\mathrm{d}x = -\int_{\Omega} \overline{\phi(x,y)}\Delta\psi(x,y)\,\mathrm{d}x\,\mathrm{d}y.\end{aligned}$$

It means that there exists $\eta := -\Delta\psi \in L^2(\Omega)$ such that $\forall \phi \in D(h_\alpha),\ h_\alpha(\phi,\psi) = (\phi,\eta)$. That is, $\tilde{H}_\alpha$ is an extension of H_α.

The other inclusion holds as a direct consequence of Lemma 2.1 and the first representation theorem. □

3 The spectrum of Hamiltonian

In this section we will investigate the spectrum of the Hamiltonian with respect to the behavior of the function α. In whole section we suppose that $\alpha \in W^{1,\infty}(\mathbb{R})$ and $\forall x \in \mathbb{R},\ \alpha(x) \geq 0$. We start with the simplest case.

3.1 Unperturbed system

If $\alpha(x) = \alpha_0 \geq 0$ is a constant function, the Schrödinger equation can be easily solved by separation of variables. The spectrum of hamiltonian is then $\sigma(H_{\alpha_0}) = [E_1(\alpha_0), \infty)$, where $E_1(\alpha_0)$ is the first transversal eigenvalue. The transversal eigenfunctions have the form

$$\chi_n(y;\alpha) = N_\alpha \left(\frac{\alpha}{\sqrt{E_n(\alpha)}} \sin\left(\sqrt{E_n(\alpha)}y\right) + \cos\left(\sqrt{E_n(\alpha)}y\right)\right), \tag{3.1}$$

where N_α is a normalisation constant and the eigenvalues $E_n(\alpha)$ are determined by the implicit equation

$$f(E_n;\alpha) = 2\alpha\sqrt{E_n(\alpha)}\cos(\sqrt{E_n(\alpha)}d) + (\alpha^2 - E_n(\alpha))\sin(\sqrt{E_n(\alpha)}d) = 0.$$

Note that there are no eigenvalues below the bottom of the essential spectrum, *i.e.*, $\sigma_{disc}(H_{\alpha_0}) = \emptyset$.

3.2 The stability of essential spectrum

As we have seen, if α is a constant function, the essential spectrum of the Hamiltonian is the interval $[E_1(\alpha_0), \infty)$. Now we prove that the same spectral result holds if α tends to α_0 at infinity.

Theorem 3.1. *If* $\lim_{|x|\to\infty} \alpha(x) - \alpha_0 = 0$ *then* $\sigma_{ess}(H_\alpha) = [E_1(\alpha_0), \infty)$.

The proof of this theorem is achieved in two steps. Firstly, in Lemma 3.3, we employ a Neumann bracketing argument to show that the threshold of essential spectrum does not descent below the energy $E_1(\alpha_0)$. Secondly, in Lemma 3.4, we prove that all values above $E_1(\alpha_0)$ belongs to the essential spectrum by means of the following characterisation of essential spectrum which we have adopted from [7].

Lemma 3.2. *Let H be a non-negative self-adjoint operator in a complex Hilbert space $\mathcal{H}$ and h be the associated quadratic form. Then $\lambda \in \sigma_{ess}(H)$ if and only if there exists a sequence $\{\psi_n\}_{n=1}^\infty \subset D(h)$ such that*

(i) $\forall n \in \mathbb{N} \setminus \{0\},\ \|\psi_n\| = 1,$

(ii) $\psi_n \xrightarrow[n\to\infty]{w} 0$ in $\mathcal{H}$,

(iii) $(H - \lambda)\psi_n \xrightarrow[n\to\infty]{} 0$ in $D(h)^*$.

Here $D(h)^*$ denotes the dual of the space $D(h)$. We note that

$$\|\psi\|_{D(h)^*} = \sup_{\phi \in D(h) \setminus \{0\}} \frac{|(\phi, \psi)|}{\|\phi\|_1}$$

with

$$\|\phi\|_1 := \sqrt{h[\phi] + \|\phi\|^2_{L^2(\Omega)}}.$$

The main advantage of Lemma 3.2 is that it requires to find a sequence from the form domain of H only, and not from $D(H)$ as it is required by the Weyl criterion [6, Lem. 4.1.2]. Moreover, in order to check the limit from (iii), it is still sufficient to consider the operator H in the form sense, *i.e.* we will not need to assume that α is differentiable in our case.

Lemma 3.3. *If* $\lim_{|x|\to\infty} \alpha(x) - \alpha_0 = 0$ *then* $\inf \sigma_{ess}(H_\alpha) \geq E_1(\alpha_0)$.

Proof. Since $\alpha(x) - \alpha_0$ vanishes at infinity, for any fixed $\varepsilon > 0$ there exists $a > 0$ such that

$$|x| > a \;\Rightarrow\; |\alpha(x) - \alpha_0| < \varepsilon. \tag{3.2}$$

Cutting Ω by additional Neumann boundary parallel to the y-axis at $x = \pm a$, we get new operator $H_\alpha^{(N)}$ defined using quadratic form. We can decompose this operator

$$H_\alpha^{(N)} = H_{\alpha,t}^{(N)} \oplus H_{\alpha,c}^{(N)},$$

where the "tail" part $H_{\alpha,t}^{(N)}$ corresponds to the two halfstrips ($|x| > a$) and the rest, $H_{\alpha,c}^{(N)}$, to the central part with the Neumann condition on the vertical boundary. Using Neumann bracketing, *cf* [21, Sec. XIII.15], we get

$$H_\alpha^{(N)} \leq H_\alpha$$

in the sense of quadratic forms.

We denote

$$\alpha_{min}(a) := \inf_{|x|>a} \alpha(x).$$

Since $\sigma_{ess}(H^{(N)}_{\alpha_{min},t}) = [E_1(\alpha_{min}), \infty)$ and

$$H^{(N)}_{\alpha_{min},t} \leq H^{(N)}_{\alpha,t}$$

in the sense of quadratic forms, we get the following estimate of the bottom of the essential spectrum of the "tail" part

$$E_1(\alpha_{min}) \leq \inf \sigma_{ess}(H^{(N)}_{\alpha,t}). \tag{3.3}$$

Since the spectrum of $H^{(N)}_{\alpha,c}$ is purely discrete, *cf* [6, Chap. 7], the minimax principle gives the inequality

$$\inf \sigma_{ess}(H^{(N)}_{\alpha,t}) \leq \inf \sigma_{ess}(H_\alpha). \tag{3.4}$$

Since the assertion (3.2) yields

$$\alpha_0 - \varepsilon < \alpha_{min}$$

and E_1 is an increasing function of α, we have

$$E_1(\alpha_0 - \varepsilon) < E_1(\alpha_{min}). \tag{3.5}$$

Giving together (3.3), (3.4), and (3.5) we get the relation

$$E_1(\alpha_0 - \varepsilon) < \inf \sigma_{ess}(H_\alpha).$$

The claim then follows from the fact that $E_1 = E_1(\alpha)$ is a continuous function and ε can be made arbitrarily small. □

Lemma 3.4. *If* $\lim_{|x|\to\infty} \alpha(x) - \alpha_0 = 0$ *then* $[E_1(\alpha_0), \infty) \subseteq \sigma_{ess}(H_\alpha)$.

Proof. Let $\lambda \in [E_1(\alpha_0), \infty)$. We shall construct a sequence $\{\psi_n\}_{n=1}^{\infty}$ satisfying the assumptions (i)–(iii) of Lemma 3.2. We define the following family of functions

$$\psi_n(x, y) := \varphi_n(x)\chi_1(y; \alpha_0) \exp\left(i\sqrt{\lambda - E_1(\alpha_0)}x\right),$$

where χ_1 is the lowest transversal function (3.1) and $\varphi_n(x) := n^{-1/2}\varphi(x/n - n)$ with φ satisfying

1. $\varphi \in C_0^\infty(\mathbb{R})$,
2. $\forall x \in \mathbb{R},\ 0 \leq \varphi(x) \leq 1$,
3. $\forall x \in (-1/4, 1/4)\,,\ \varphi = 1$,
4. $\forall x \in \mathbb{R} \setminus [-1/4, 1/4]\,,\ \varphi = 0$,
5. $\|\varphi\|_{L^2(\mathbb{R})} = 1$.

Note that supp $\varphi_n \subset (n^2 - n, n^2 + n)$. It is clear that ψ_n belongs to the form domain of H_α. The assumption (i) of Lemma 3.2 is satisfied due to the normalisation of χ_1 and φ.

The point (ii) of Lemma 3.2 requires that $(\phi, \psi_n) \to 0$ as $n \to \infty$ for all $\phi \in C_0^\infty(\Omega)$, a dense subset of $L^2(\Omega)$. However, it follows at once because ϕ and ψ_n have disjoint supports for n large enough.

Hence, it remains to check that $\|(H_\alpha - \lambda)\psi_n\|_{D(h)^*} \to 0$ as $n \to \infty$. An explicit calculation using integration by parts, boundary conditions (1.2) and the relations

$$\|\dot\varphi_n\|_{L^2(\mathbb{R})} = n^{-1}\|\dot\varphi\|_{L^2(\mathbb{R})}, \qquad \|\ddot\varphi_n\|_{L^2(\mathbb{R})} = n^{-2}\|\ddot\varphi\|_{L^2(\mathbb{R})} \tag{3.6}$$

yields

$$\begin{aligned} \left|\Big(\phi, (H_\alpha - \lambda)\psi_n\Big)\right| = \Bigg| \int_\Omega \overline{\phi(x,y)}\chi_1(y;\alpha_0)\ddot\varphi_n(x) \exp\left(i\sqrt{\lambda - E_1(\alpha_0)}x\right) \mathrm{d}x\, \mathrm{d}y \\ + 2i \int_\Omega \overline{\phi(x,y)}\chi_1(y;\alpha_0)\dot\varphi_n(x)\sqrt{\lambda - E_1(\alpha_0)} \exp\left(i\sqrt{\lambda - E_1(\alpha_0)}x\right) \mathrm{d}x\, \mathrm{d}y\Bigg| \\ \leq n^{-2}\|\phi\|_{L^2(\Omega)}\|\chi_1\|_{L^2((0,d))}\|\ddot\varphi\|_{L^2(\mathbb{R})} \\ +2n^{-1}\|\phi\sqrt{\lambda - E_1(\alpha_0)}\|_{L^2(\Omega)}\|\chi_1\|_{L^2((0,d))}\|\dot\varphi\|_{L^2(\mathbb{R})} \end{aligned}$$

for all $\phi \in D(h_\alpha)$. The claim then follows from the fact that both terms at the r.h.s. go to zero as $n \to \infty$. ☐

3.3 The existence of bound states

Now we show that if $\alpha - \alpha_0$ vanishes at infinity, some behavior of the function α may produce a non-trivial spectrum below the energy $E_1(\alpha_0)$. Note that this together with the assumption of Theorem 3.1 implies that the spectrum below $E_1(\alpha_0)$ consists of isolated eigenvalues of finite multiplicity, *i.e.* $\sigma_{disc}(H_\alpha) \neq \emptyset$. Sufficient condition that pushes the spectrum of the Hamiltonian below $E_1(\alpha_0)$ is introduced in following theorem.

Theorem 3.5. *Suppose*

1. $\alpha(x) - \alpha_0 \in L^1(\mathbb{R})$,
2. $\int_{\mathbb{R}} (\alpha(x) - \alpha_0)\, \mathrm{d}x < 0$.

Then $\inf \sigma(H_\alpha) < E_1(\alpha_0)$.

Proof. The proof is based on the variational strategy of finding a trial function ψ from the form domain of H_α such that

$$Q_\alpha[\psi] := h_\alpha[\psi] - E_1(\alpha_0)\|\psi\|^2_{L^2(\Omega)} < 0. \tag{3.7}$$

We define a sequence

$$\psi_n(x,y) := \varphi_n(x)\chi_1(y;\alpha_0), \quad \varphi_n(x) := n^{-1/2}\varphi(x/n),$$

where the function φ was defined in the proof of Lemma 3.4. Using the relations (3.6) and the integration by parts we get

$$Q_\alpha[\psi_n] = n^{-2}\|\dot{\varphi}\|^2_{L^2(\mathbb{R})} + \left(|\chi_1(0;\alpha_0)|^2 + |\chi_1(d;\alpha_0)|^2\right)\int_{\mathbb{R}}(\alpha(x)-\alpha_0)\varphi_n(x)\,\mathrm{d}x.$$

Since the integrand is dominated by the L^1-norm of $\alpha-\alpha_0$ we have the limit

$$\lim_{n\to\infty} Q_\alpha[\psi_n] = \left(|\chi_1(0;\alpha_0)|^2 + |\chi_1(d;\alpha_0)|^2\right)\int_{\mathbb{R}}(\alpha(x)-\alpha_0)\,\mathrm{d}x$$

by dominated convergence theorem. This expression is negative according to the assumptions. Now, it is enough to take n sufficiently large to satisfy inequality (3.7). □

4 A 'rectangular well' example

To illustrate the above results and to understand the behavior of the spectrum of the Hamiltonian in more detail, we shall now numerically investigate an example. Inspired by [12] we choose the function α to be a steplike function which make it possible to solve the corresponding Schrödinger equation numerically by employing the mode-matching method. The simplest non-trivial case concerns a 'rectangular well' of a width $2a$,

$$\alpha(x) = \begin{cases} \alpha_1 & \text{if } |x| < a \\ \\ \alpha_0 & \text{if } |x| \geq a \end{cases}$$

with $a > 0$ and $0 \leq \alpha_1 < \alpha_0$. In view of Theorem 3.5 this waveguide system has bound states. In particular, one expects that in the case when α_1 is close to zero and α_0 is large the spectral properties will be similar to those of the situation studied in [8].

Since the system is symmetric with respect to the y-axis, we can restrict ourselves to the part of Ω in the first quadrant and we may consider separately the symmetric and antisymmetric solutions, *i.e.* to analyse the halfstrip with the Neumann or Dirichlet boundary condition at the segment $(0,d)$ on y-axis, respectively.

4.1 Preliminaries

Theorem 3.1 enable us to localise the essential spectrum in the present situation, *i.e.*, $\sigma_{ess}(H_\alpha) = [E_1(\alpha_0), \infty)$. Moreover, according to the minimax principle we know that isolated eigenvalues of H_α are squeezed between those of $H_{a,c}^{(N)}$ and $H_{a,c}^{(D)}$, the Hamiltonians in the central part with Neumann or Dirichlet condition on the vertical boundary, respectively. The Neumann estimate tells us that $\inf \sigma(H_\alpha) \geq E_1(\alpha_1)$. One finds that the n-th eigenvalue E_n of H_α is estimated by

$$E_1(\alpha_1) + \left(\frac{(n-1)\pi}{2a}\right)^2 \leq E_n \leq E_1(\alpha_1) + \left(\frac{n\pi}{2a}\right)^2.$$

4.2 Mode-matching method

Let us pass to the mode-matching method. A natural Ansatz for the solution of an energy $\lambda \in [E_1(\alpha_1), E_1(\alpha_0))$ is

$$\psi_{s/a}(x,y) = \sum_{n=1}^{\infty} a_n^{s/a} \left\{ \begin{array}{c} \frac{\cosh(l_n x)}{\cosh(l_n a)} \\ \\ \frac{\sinh(l_n x)}{\sinh(l_n a)} \end{array} \right\} \chi_n(y;\alpha_1) \qquad \text{for } 0 \leq x < a$$

$$\psi_{s/a}(x,y) = \sum_{n=1}^{\infty} b_n^{s/a} \exp(-k_n(x-a))\chi_n(y;\alpha_0) \qquad \text{for } x \geq a$$

where the subscripts and superscripts s, a distinguish the symmetric and antisymmetric case, respectively. The longitudinal momenta are defined by

$$l_n := \sqrt{E_n(\alpha_1) - \lambda}, \qquad k_n := \sqrt{E_n(\alpha_0) - \lambda}.$$

As an element of the domain (1.3), the function ψ should be continuous together with its normal derivative at the segment dividing the two regions, $x = a$. Using the orthonormality of $\{\chi_n\}$ we get from the requirement of continuity

$$\sum_{n=1}^{\infty} a_n \int_0^d \chi_n(y,\alpha_1)\chi_m(y;\alpha_0)\,\mathrm{d}y = b_m. \tag{4.1}$$

In the same way, the normal-derivative continuity at $x = a$ yields

$$\sum_{n=1}^{\infty} a_n l_n \left\{ \begin{array}{c} \tanh \\ \coth \end{array} \right\} (l_n a) \int_0^d \chi_n(y;\alpha_1)\chi_m(y;\alpha_0)\,\mathrm{d}y + b_m k_m = 0. \tag{4.2}$$

Substituting (4.1) to (4.2) we can write the equation as

$$\mathbf{Ca} = \mathbf{0}, \tag{4.3}$$

where

$$C_{mn} = \left(l_n \left\{ \begin{array}{c} \tanh \\ \coth \end{array} \right\} (l_n a) + k_m \right) \int_0^d \chi_n(y;\alpha_1)\chi_m(y;\alpha_0)\,\mathrm{d}y.$$

In this way we have transformed a partial-differential-equation problem to a solution of an infinite system of linear equations. The latter will be solved numerically by using in (4.3) an N by N subblock of $\mathbf{C}$ with large N (in our computations, typically $N = 10$).

4.3 Numerical results

The dependence of the ground state wavefunction with respect to α_1 for the central part of the halfwidth $a/d = 0.3$ is illustrated in Figure 2.

Figure 3 shows the bound-state energies as functions of the 'window' halfwidth a/d for $\alpha_0 = 1000$ and $\alpha_1 = 0.1$. We see that the energies decrease monotonously with the increasing 'window' width. Their number increases as a function of a/d. For illustration, the first gap, *i.e.* the difference between first and second eigenvalue (or between first eigenvalue and the bottom of the essential spectrum if there is only one eigenvalue), is plotted in the bottom part of the figure.

We can compare the dependence of the first eigenvalue on the 'window' halfwidth with the model studied in [8]. The authors there studied the model of straight quantum waveguide with combined Dirichlet and Neumann boundary conditions. Figure 4 shows that if we take α_0 sufficiently large and α_1 sufficiently small (in our case $\alpha_0 = 1000, \alpha_1 = 0.1$), the first eigenvalue is closed to the Dirichlet-Neumann case.

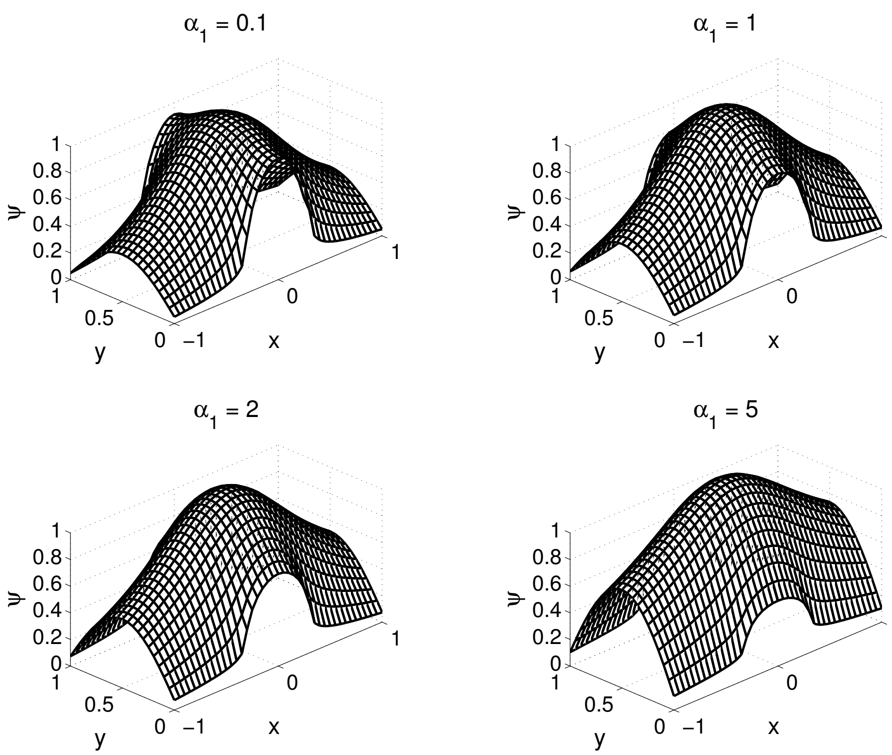

Figure 2: Ground state eigenfunctions for $a/d = 0.3$, $\alpha_0 = 20$.

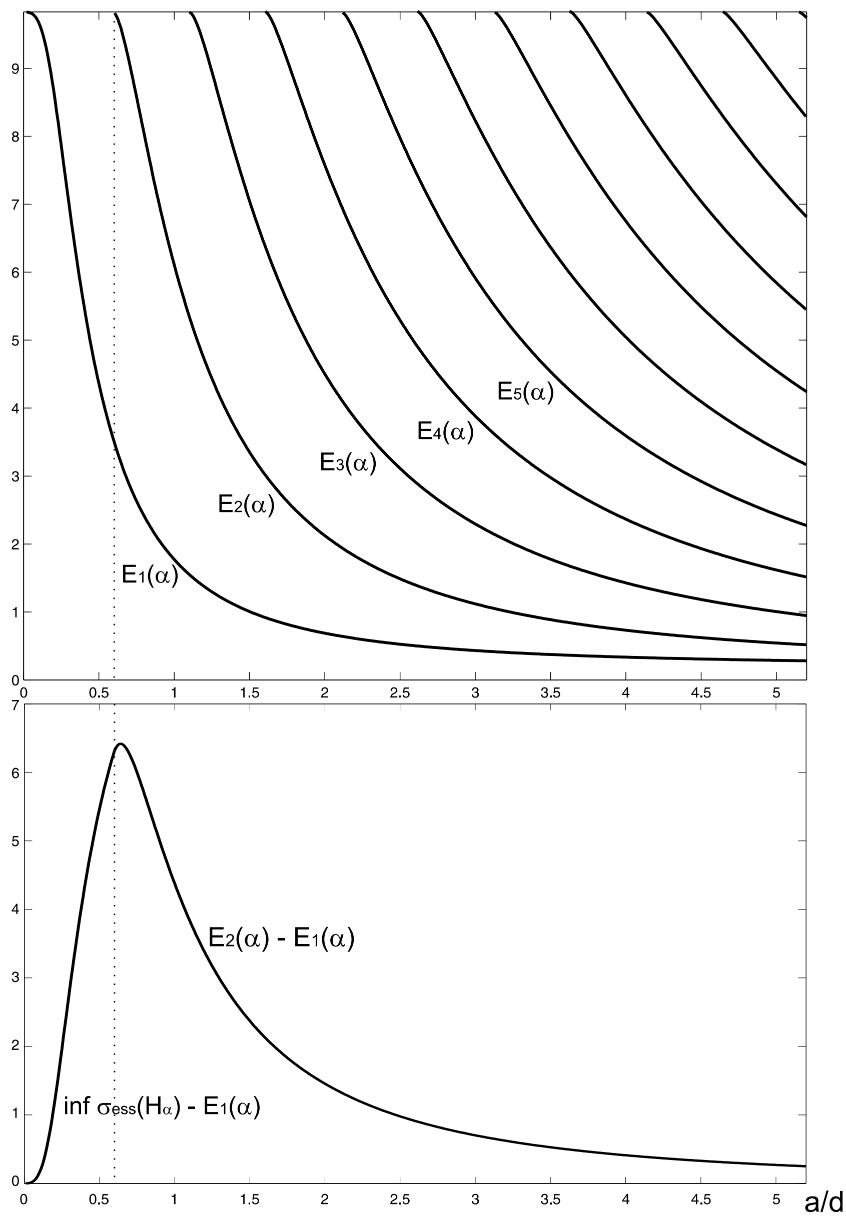

Figure 3: Bound states energies and the first gap (in the units of $1/d^2$) in dependence on a/d for $\alpha_1 = 0.1$ and $\alpha_0 = 1000$.

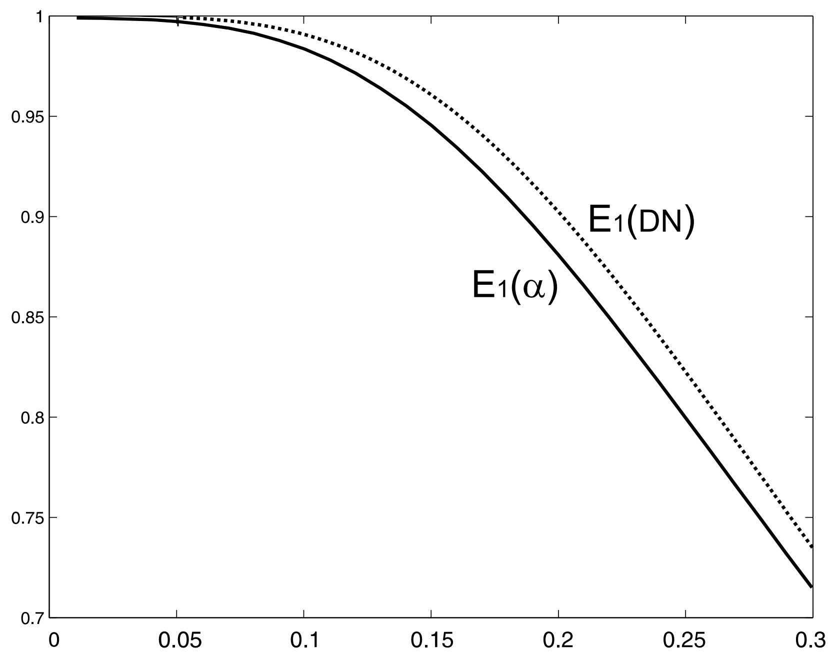

Figure 4: First eigenvalue (in the units of π^2/d^2) in dependence on a/d for $\alpha_1 = 0.1$ and $\alpha_0 = 1000$ compared with the Dirichlet-Neumann case (dotted curve) adopted from [8].

Appendix A: The source code of the Matlab program

We have solved the equation (4.3) numerically using Matlab. The main m-function called eigenvalues has 4 parameters. n is the size of the matrix $\mathbf{C}$. As an output we get the list of eigenvalues.

```
function y=eigenvalues(n,alpha0,alpha1,a)
Ealpha0=chieigenvalues(n,alpha0);
Ealpha1=chieigenvalues(n,alpha1);
for k=1:n
    normalpha0(k)=sqrt(quad(@(x)(chi(alpha0,Ealpha0(k),x)
    .*chi(alpha0,Ealpha0(k),x)),0,1));
    normalpha1(k)=sqrt(quad(@(x)(chi(alpha1,Ealpha1(k),x)
    .*chi(alpha1,Ealpha1(k),x)),0,1));
end
%
for f=1:n
    for g=1:n
        X(f,g)=quad(@(x)(chi(alpha0,Ealpha0(f),x)./normalpha0(f)
        .*chi(alpha1,Ealpha1(g),x)./normalpha1(g)),0,1);
    end
end
%
rootsmin=0; rootsmax=0; rootamin=0; rootamax=0;
%
aa=[Ealpha1(1)+0.001:0.001:Ealpha0(1)-0.001,Ealpha0(1)
    -0.0009:0.0001:Ealpha0(1)-0.0001,Ealpha0(1)
    -0.00009:0.00001:Ealpha0(1)-0.00001,Ealpha0(1)
    -0.000009:0.000001:Ealpha0(1)-0.000001];
%
for f=1:length(aa)
    bs(f)=det(matrixs(aa(f),n,Ealpha0,Ealpha1,a,X));
    ba(f)=det(matrixa(aa(f),n,Ealpha0,Ealpha1,a,X));
end
%
signbs=sign(bs); signba=sign(ba); for f=2:length(signbs)
```

```
    if signbs(f-1)>signbs(f)
        rootsmax=[rootsmax,aa(f)];
        rootsmin=[rootsmin,aa(f-1)];
    end
end for f=2:length(signba)
    if signba(f-1)>signba(f)
        rootamax=[rootamax,aa(f)];
        rootamin=[rootamin,aa(f-1)];
    end
end
%
rootsmin=rootsmin(2:end); rootsmax=rootsmax(2:end); for
f=1:length(rootsmax)
    rootsym(f)=fzero(@(lambda)real(det
    (matrixs(lambda,n,Ealpha0,Ealpha1,a,X))),
    [rootsmin(f),rootsmax(f)],optimset('TolX',0.00000000001));
end
%
if rootamax==0
  y=rootsym(1);
  return;
end
%
rootamin=rootamin(2:end); rootamax=rootamax(2:end); for
f=1:length(rootamax)
    roota(f)=fzero(@(lambda)real(det(
    matrixa(lambda,n,Ealpha0,Ealpha1,a,X))),
    [rootamin(f),rootamax(f)],optimset('TolX',0.00000000001));
end
%
for f=1:length(roota)
    root(f*2-1)=rootsym(f);
    root(f*2)=roota(f);
end if length(rootsym)>length(roota)
    root=[root,rootsym(end)];
end y=root;
```

```
function y=implchi(lambda,alpha0)
y=(lambda-alpha0.^2).*sin(sqrt(lambda))
 -2.*alpha0.*sqrt(lambda).*cos(sqrt(lambda));

function l=chieigenvalues(n,alpha) k=0; for f=1:n
  k=[k,fzero(@(x)implchi(x,alpha),[(f-1)^2.*pi^2+0.001,f^2.*pi^2])];
end l=k(2:end);

function M=matrixs(lambda,n,Ealpha0,Ealpha1,a,X)
M=(ones(n,1)*(sqrt(Ealpha1-lambda).*tanh(sqrt(Ealpha1-lambda).*a))
 +(sqrt(Ealpha0-lambda))'*ones(1,n)).*X;

function M=matrixa(lambda,n,Ealpha0,Ealpha1,a,X)
M=(ones(n,1)*(sqrt(Ealpha1-lambda).*coth(sqrt(Ealpha1-lambda).*a))
 +(sqrt(Ealpha0-lambda))'*ones(1,n)).*X;

function y=chi(A,L,X) a=A; l=L; x=X;
y=a./sqrt(l).*sin(sqrt(l).*x)+cos(sqrt(l).*x);
```

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