Straight quantum waveguide with Robin boudary conditions

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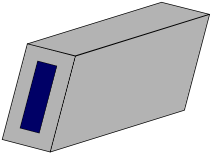
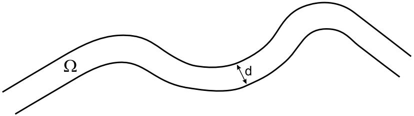
Physical motivation

- Fabrication of tiny semiconductor structures $\longrightarrow$ nanostructures



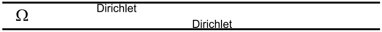
- Materials: pure, crystallic structure $\Rightarrow$ modelled by $H = -\frac{\hbar^2}{2m^*}\Delta \quad \text{in} \quad L^2(\Omega)$
- Important cathegory: **quantum waveguides**:



- Observation of vanishing of wavefunction near the interface $\Rightarrow$ imposing Dirichlet boundary conditions on $\partial\Omega$, *i.e.* $\psi = 0$ on $\partial\Omega$
- Spectral properties of H?

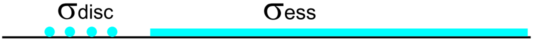
Known results - Dirichlet b.c.

- Simplest case:

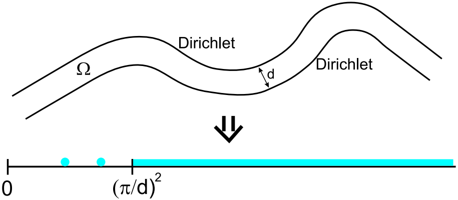


- Separation of variables:

- Interesting phenomenon: **bound states** , *i.e.* $\sigma_{disc}(H) \neq \emptyset$



- Exner, Šeba, Bound states in curved quantum waveguide, J. Math. Phys. (1989)
- Duclos, Exner, Curvature induced bound states in quantum waveguides in two and three dimensions, Rev. Math. Phys (1995)
- Krejčiřík, Kříž, On the spectrum of curved planar waveguides, Publ. RIMS Kyoto Univ. (2005)



Known results - Robin b.c.

- Dirichlet b.c. - special case. It is enough that the particle is confined to Ω, *i.e.*

$$n \cdot j = 0, \quad \text{where } j := \frac{i\hbar}{2m^*}\left[\psi \nabla \overline{\psi} - \overline{\psi} \nabla \psi\right]$$

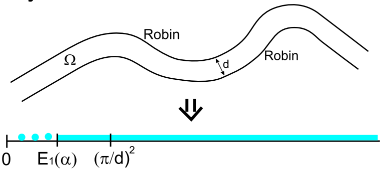
- Satisfied also by **Robin boundary conditions**, *i.e.*

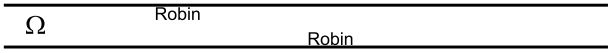
$$\frac{\partial \psi}{\partial n} + \alpha \psi = 0$$

- Simplest case: 

- Separation of variables: 

- My Bacherol thesis:

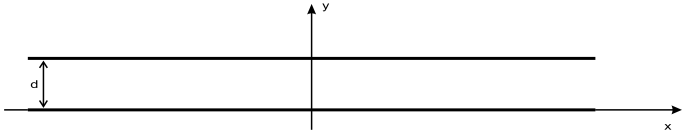


- Another possibility: 

, α varies along $\partial\Omega$

Definition of the Hamiltonian

- Let $\Omega := \mathbb{R} \times (0, d), \quad d > 0$



- It is natural to define

$$H_\alpha \psi := -\Delta \psi$$

$$D(H_\alpha) := \{\psi \in W^{2,2}(\Omega) \big| \forall x \in \mathbb{R}, \quad -\partial_y \psi(x,0) + \alpha(x)\psi(x,0) = 0, \quad \partial_y \psi(x,d) + \alpha(x)\psi(x,d) = 0\}$$

- $\alpha : \mathbb{R} \to [0, \infty)$
- H_α ... symmetric, non-negative
- Self-adjointness?

Self-adjointness of the Hamiltonian

- Let us define the quadratic form in $L^2(\Omega)$:

$$h_\alpha[\psi] := \int_\Omega |\nabla\psi(x,y)|^2 \mathrm{d}x\mathrm{d}y + \int_{\mathbb{R}} \alpha(x) \left(|\psi(x,0)|^2 + |\psi(x,d)|^2\right) \mathrm{d}x$$

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

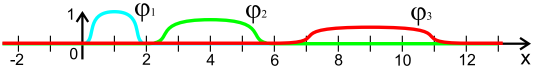
- h_α - densely defined, closed, symmetric, non-negative
- First representation theorem $\Rightarrow \exists$ unique self-adjoint $\tilde{H}_\alpha$ associated with h_α
- **Theorem**: If $\alpha \in W^{1,\infty}(\mathbb{R})$ then $H_\alpha = \tilde{H}_\alpha$.
- Proof. Based on *standard elliptic regularity theorems*

The stability of essential spectrum

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

a) $\inf \sigma_{ess}(H_\alpha) \geq E_1(\alpha_0)$ (Neumann bracketing)

b) $[E_1(\alpha_0), \infty) \subseteq \sigma_{ess}(H_\alpha)$
Weyl: $\lambda \in \sigma(H) \Leftrightarrow \exists \psi_n \in D(H), \|(H-\lambda)\psi_n\|_{L^2(\Omega)} \to 0$
Modified Weyl:
$\lambda \in \sigma_{ess}(H) \Leftrightarrow \exists \psi_n \in D(h), \|(H-\lambda)\psi_n\|_{D(h)^*} \to 0$
(Dermenjian,Durand,Iftimie, Commun. in Part. Diff. Eq. (1998))
$\psi_n(x,y) := \varphi_n(x)\chi_1(y;\alpha_0) \exp i\sqrt{\lambda - E_1(\alpha_0)}x$



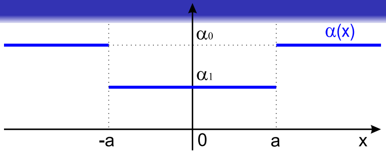
Existence of bound states

- **Theorem**: 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:
- find
  $\psi \in D(h_\alpha) = W^{1,2}(\Omega)$, $Q_\alpha[\psi] := h_\alpha[\psi] - E_1(\alpha_0)\|\psi\|^2_{L^2(\Omega)} < 0$
- $\psi_n(x,y) := \varphi_n(x)\chi_1(y;\alpha_0)$
- $\lim_{n\to\infty} Q_\alpha[\psi_n] =$
  $\left(|\chi_1(0;\alpha_0)|^2 + |\chi_1(d;\alpha_0)|^2\right) \int_{\mathbb{R}}(\alpha(x) - \alpha_0)\mathrm{d}x < 0$
- n - large enough

Mode-matching method



- A "rectangular well" example:

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

- Symmetry $\Rightarrow$ symmetric/antisymmetric solution:

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

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

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

- Continuity and normal derivative continuity at $x = a \Rightarrow a_n, b_m$

Numerical results - eigenvalues

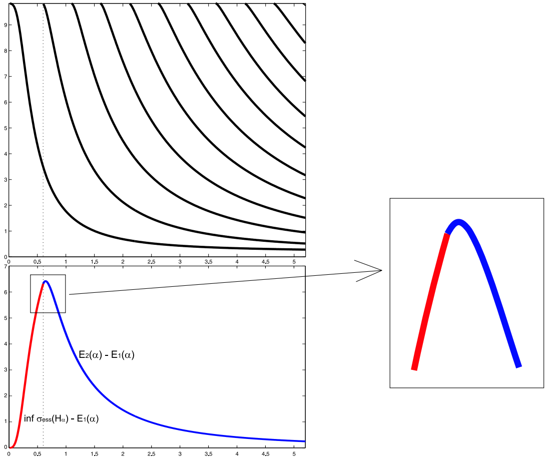


Figure: Bound states energies and first gap in dependence on a/d $(\alpha_1 = 0.1, \alpha_0 = 1000)$

Numerical results - eigenfunctions

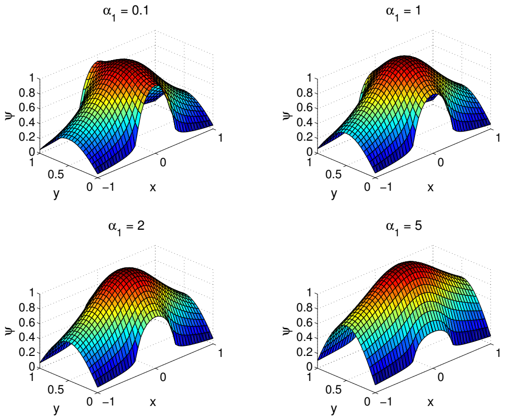


Figure: Ground state eigenfunctions ($a/d = 0.3, \alpha_0 = 20$)

Comparing with DN case

Dittrich, Kříž, Bound states in straight quantum waveguides with combined boundary condition, J. Math. Phys., (2002)

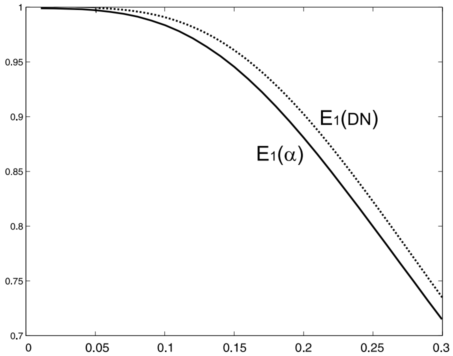


Figure: First eigenvalue in dependence on a/d $(\alpha_1 = 0.1, \alpha_0 = 1000)$ compared with DN-case