Mathematical Problems in Quantum Mechanics

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# CURVED QUANTUM WAVEGUIDES WITH COMBINED BOUNDARY CONDITIONS

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J. Dittrich, J K, J. Phys. A **35** (2002), L269–275.

D. Krejčiřík, J K, math-ph/0306008.

# Program

1. Introduction ( What are QW?; Various boundary conditions)

2. Preliminaries (Configuration space; Hamiltonian)

3. Energy spectrum (Essential spectrum; Existence (absence) of discrete spectrum)

4. Conclusions (Comparison with known results; Open problems)

# 1. Introduction

## What are quantum waveguides?

Semiconductor or metallic microstructures of the tube like shape.

(a) small size $10 - 100\ nm$;
(b) high purity ($e^-$ mean free path $\sim \mu m$);
(c) crystallic structure.

### Physical background:


1. J. T. Londergan, J. P. Carini, and D. P. Murdock, *Binding and scattering in 2-dimensional systems*, LNP, vol. m60, Springer, Berlin, 1999.

2. S. Datta, *Electronic transport in mesoscopic systems*, Camb.Univ.Press, Cambridge, 1995.

3. P. Duclos and P. Exner, *Curvature-induced bound states in quantum waveguides in 2 and 3 dimensions*, Rev.Math.Phys. **7** (1995), 73–102.

# Our model

free particle of an effective mass $m^*$ living in nontrivial spatial region $\Omega$
impenetrable walls: suitable b.c.

1. *Dirichlet b.c.* (semiconductor structures)

2. *Neumann b.c.* (metallic structures, acoustic or electromagnetic waveguides)

3. Waveguides with *combined* Dirichlet and Neumann b.c. on different parts of boundary

(more realistic models allow for quantum tunneling)

Mathematical point of view: spectrum of $-\triangle$ $(\hbar^2/(2m^*) = 1)$ acting in the Hilbert space $L^2(\Omega)$

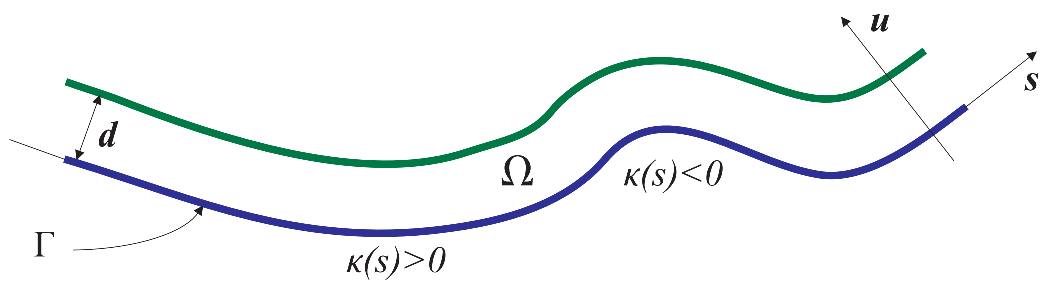
# 2. Preliminaries

## Configuration space

- $\Gamma : \mathbb{R} \to \mathbb{R}^2$ ... $C^2$ infinite plane curve
- $\nu := (-\dot{\Gamma}^2, \dot{\Gamma}^1)$ ... unit normal vector field
- $\kappa := \det(\dot{\Gamma}, \ddot{\Gamma})$ ... signed curvature
- $\Omega_0 := \mathbb{R} \times (0, d)$ ... straight strip of width $d$
- $\mathcal{L} : \mathbb{R}^2 \to \mathbb{R}^2 : \{(s, \; u) \mapsto \; \Gamma(s) + u\nu(s)\}$
- $\Omega := \mathcal{L}(\Omega_0)$ ... curved strip along $\Gamma$
- $\kappa_\pm := \max\{0, \pm\kappa\}$
- $\alpha := \int_{\mathbb{R}} \kappa(s) ds$ ...bending angle

Assumptions : ◇ $\Omega$ is not self − intersecting
◇ $\kappa \in L^\infty(\mathbb{R}),\ d\|\kappa_+\|_{L^\infty(\mathbb{R})} < 1$

$\mathcal{L} : \Omega_0 \to \Omega$ ... $C^1$-diffeomorphism;
$\mathcal{L}^{-1}$ defines natural coordinates $(s, u)$




— ... Dirichlet b.c. — ... Neumann b.c.

Hilbert space: $L^2(\Omega) \to L^2(\Omega_0, (1-u\kappa(s))du\,ds)$

<u>Hamiltonian</u>

unique s.-a. operator, whose quadratic form is

$$Q(\psi,\varphi) := \int_{\Omega_0} \left( \frac{\overline{\frac{\partial\psi}{\partial s}}\frac{\partial\varphi}{\partial s}}{(1-u\kappa)} + \overline{\frac{\partial\psi}{\partial u}}\frac{\partial\varphi}{\partial u}(1-u\kappa) \right) duds$$

$$\text{Dom}\, Q := \left\{ \psi \in W^{1,2}(\Omega_0) | \psi(s,0) = 0 \right\}$$

associated operator: $H$

$\Gamma \in C^3(\mathbb{R}) \implies$ Laplace–Beltrami operator

$$-\frac{1}{(1-u\kappa)^2}\partial_{ss}^2 - \frac{u\dot{\kappa}}{(1-u\kappa)^3}\partial_s - \partial_{uu}^2 + \frac{\kappa}{1-u\kappa)}\partial_u$$

operator domain Dom $H$

$$\left\{\psi \in W^{2,2}(\Omega_0) | \psi(s,0) = 0, \partial_u\psi(s,d) = 0\right\}$$

# 3. Energy spectrum

## Essential spectrum

**Theorem:**

$$\lim_{|s|\to\infty} \kappa(s) = 0 \implies \sigma_{\text{ess}}(H) = \left[\frac{\pi^2}{4d^2}, \infty\right)$$

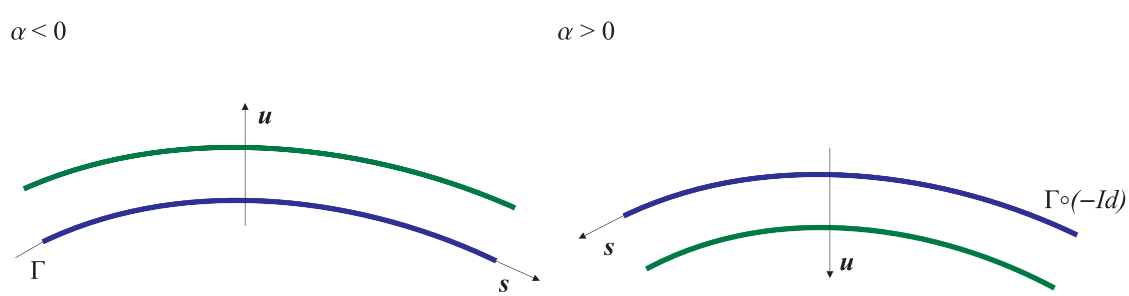
PROOF: 1. D-N Bracketing.
2. Generalized Weyl criterion. □

Y. Dermenjian, M. Durand, and V. Iftimie, Commun. in Partial Differential Equations **23** (1998), no. 1&2, 141–169.

# Discrete spectrum

**Theorem:**
(i) Assume $\kappa \not\equiv 0$. If one of
 (a) $\kappa \in L^1(\mathbb{R})$ and $\alpha \leq 0$
 (b) $\kappa_- \not\equiv 0$ and $d$ is small enough
is satisfied then $\inf \sigma(H) < \frac{\pi^2}{4d^2}$.

(ii) If $\kappa_- \equiv 0$ then $\inf \sigma(H) \geq \frac{\pi^2}{4d^2}$.




PROOF: Existence - variationally.
Absence - $\forall \psi \in \mathrm{Dom}\, Q^\kappa_{DN}$ :
$Q^\kappa_{DN}[\psi] - \frac{\pi^2}{4d^2}\|\psi\|_{L^2(\Omega_0, d\Omega)} \geq 0.$ $\square$

**Corollary:** Assume $\lim_{|s|\to\infty} \kappa(s) = 0$. Then
(i) $\Longrightarrow$ $H$ has an isolated eigenvalue;
(ii) $\Longrightarrow$ $\sigma_{\mathrm{disc}}(H) = \emptyset$.

## Some properties of discrete eigenvalues

**Proposition:** Assume $\kappa \not\equiv 0$, $\operatorname{supp}\kappa \subset [-s_0, s_0]$, $\alpha \leq 0$. Then $\inf \sigma(H) \leq \frac{\pi^2}{4d^2} - C\left(\frac{\alpha}{\pi}\right)^2$.

Remarks:

1. Dirichlet b.c. $\Longrightarrow$ $\inf \sigma(H) \leq \frac{\pi^2}{d^2} - \tilde{C}\left(\frac{\alpha}{\pi}\right)^4$

2. mildly curved strips Dirichlet strips: $\{\Gamma_\beta\}_{\beta>0}$
$\kappa_\beta := \beta\kappa \Longrightarrow \alpha_\beta = \beta\alpha$
$\inf \sigma(H) = \frac{\pi^2}{d^2} - \hat{C}\beta^4 + \mathcal{O}(\beta^5)$.

3. thin strips
Combined: $\frac{\pi^2}{4d^2} - \inf \sigma(H) \geq -\frac{\alpha}{2ds_0} + \mathcal{O}(d^{-1/2})$
Dirichlet: $\frac{\pi^2}{d^2} - \inf \sigma(H) \geq \tilde{C}_0\left(\frac{\alpha}{\pi}\right)^4 + \mathcal{O}(d)$
Exact asymptotic $\frac{\pi^2}{d^2} - \inf \sigma(H) = -\lambda + \mathcal{O}(d)$,
$\lambda$ ... 1.eigenvalue $-d^2/(ds^2) - \kappa^2/4$

P. Duclos and P. Exner, Rev. Math. Phys. **7** (1995), 73–102.

# 4. Conclusions

## Comparison with known results

Assume only asymptotically straight strips.

Dirichlet b.c.: $\kappa \not\equiv 0 \Longrightarrow \sigma_{\text{disc}}(H) \neq \emptyset$.

P. Exner and P. Šeba, J.Math.Phys.**30** (1989), 2574–2580.

J. Goldstone and R. L. Jaffe, Phys.Rev.B **45** (1992), 14100–14107.

Neumann b.c.: $\sigma_{\text{disc}}(H) = \emptyset$.

Combined b.c.: existence of $\sigma_{\text{disc}}$ depends on $\kappa$.

## Open problems

more complicated combination of b.c.

higher dimensions

b.c. $a\psi + b\partial_\nu\psi = 0$

nature of essential spectrum