Scattering through a quantum waveguide with combined boundary conditions

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1 Introduction

Quantum waveguides with combined boundary conditions

- possible new microelectronic elements (if boundary conditions realizable)
- mathematical challenge

Straight quantum waveguides with the combined Dirichlet and Neumann boundary conditions are studied for years:

Effectively for the wave functions of special symmetry

- D. V. Evans, M. Levitin, D. Vassiliev, J. Fluid Mech. **261** (1994), 21.
- P. Exner, P. Šeba, M. Tater, D. Vaněk, J. Math. Phys. **37** (1996), 4867.

Bound states

- J. Dittrich, J. Kříž, J. Math. Phys. **43** (2002), 3892.
- D. Borisov, G. Cardone, J. Math. Phys. **52** (2011), 123513.

3-D Dirichlet layer with Neumann windows

- H. Najar, O. Olendski, J. Phys **A44** (2011), 305304.

Heat equation time decay

- D. Krejčiřík, E. Zuazua, J. Diff. Eq. **250** (2011), 2334.

Infinitely many changes of boundary condition type

- D. Borisov, R. Bunoiu, G. Cardone, Ann. H. Poincaré **11** (2010), 1591; C. R. Acad. Sci. Paris, Ser. I **349** (2011), 53.

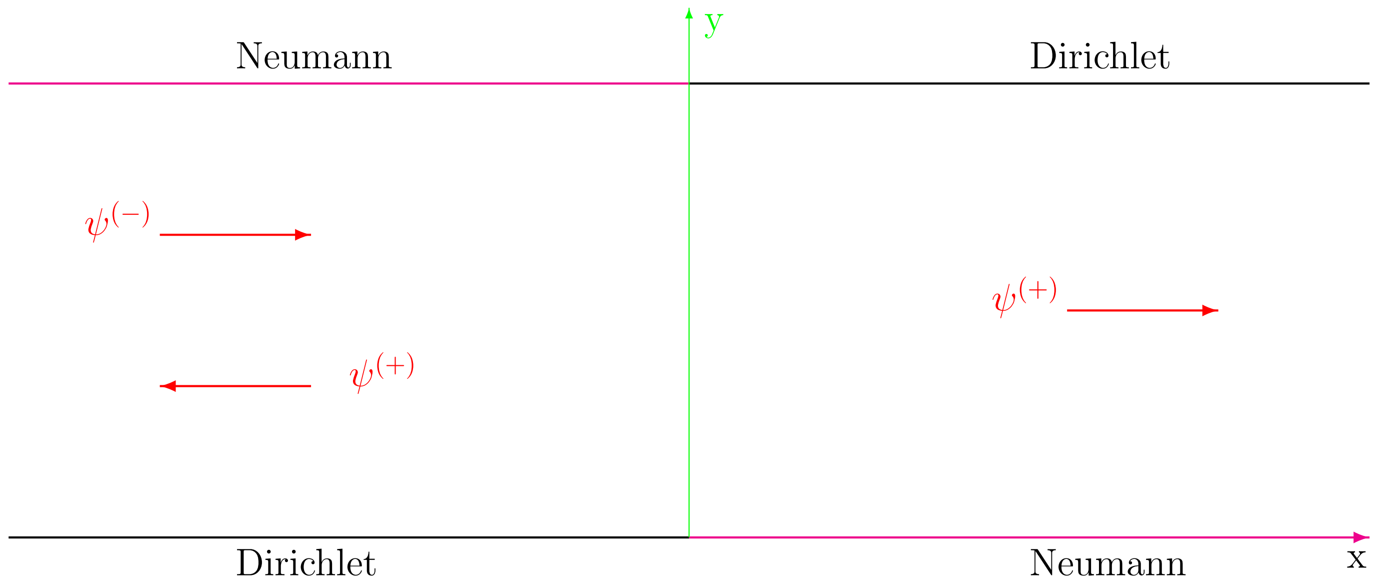
Limit of infinitely thin waveguide - Dirichlet-like decoupling

- D. Borisov, G. Cardone, J. Math. Phys. **53** (2012), 023503.

Review on many aspects of quantum waveguides in

- P. Ener, H. Kovařík: Quantum Waveguides, Springer, 2015
  Scattering: Chapter 2.

Our task:
Scattering in a planar straight waveguide
Ph. Briet, J. Dittrich, E. Soccorsi, J. Math. Phys. 55 (2014), 112104

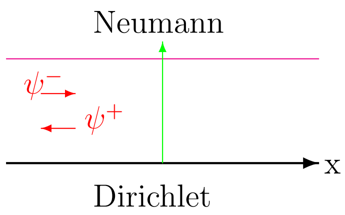

y
Neumann
Dirichlet
$\psi^{(-)}$
$\psi^{(+)}$
$\psi^{(+)}$
Dirichlet
Neumann
x

The Hamiltonian is the $H = -\Delta$, Laplace operator in the waveguide $\Omega = (-\infty, +\infty) \times (0, d)$ with the indicated combined boundary conditions.

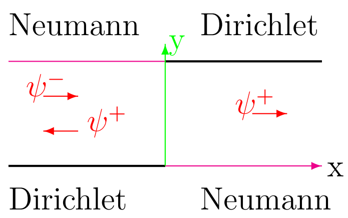
$$\mathcal{D}(H) = \Big\{ \psi \in W^{1,2}\Omega) \,|\, -\Delta\psi \in L^2(\Omega)\,,\; \psi(x,0) = 0\;,$$
$$\frac{\partial\psi(x,d)}{\partial y} = 0 \;\text{ for }\; x < 0\;,\; \psi(x,d) = 0\,,\; \frac{\partial\psi(x,0)}{\partial y} = 0 \;\text{ for }\; x > 0 \Big\}$$

Not $W^{2,2}(\Omega)$ but contained in $W^{2,2}_{loc}(\Omega)$
For any open $\Omega_1 \subset \Omega$,
$\overline{\Omega_1} \cap \{(0,0)\,,\; (0,d)\} = \emptyset \implies \mathcal{D}(H) \subset W^{2,2}(\Omega_1)$
- cf. M.S. Birman, G.E. Skvortsov, IVUZ, Mat. **30**(5) (1962), 12; J. Dittrich, J. Kříž, J. Math. Phys. **43** (2002), 3892.

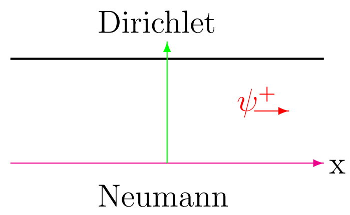
As reference (free motion) Hamiltonians for the scattering we use two – Laplace operators with Dirichlet boundary condition on the whole lower boundary $y = 0$ and Neumann boundary condition on the whole upper boundary $y = d$ or vice versa.



Hamiltonian H_1.



Hamiltonian H.



Hamiltonian H_2.

Transversal modes

$$\chi_n^{(-)}(y) = \sqrt{\frac{2}{d}} \sin\left((2n-1)\frac{\pi y}{2d}\right)$$
$$\chi_n^{(+)}(y) = \sqrt{\frac{2}{d}} \cos\left((2n-1)\frac{\pi y}{2d}\right) \quad , \quad n = 1, 2, \ldots$$

with eigenvalues $\mu_n = (2n-1)^2 \frac{\pi^2}{4d^2}$. We consider scattering from left ($x \to -\infty$) to right ($x \to +\infty$), formulas for energies between μ_1 and μ_2 shown here but similarly for any initial transversal mode.

2 Stationary scattering method

Let us look for the function f satisfying "stationary Schrödinger equation"

$$\left(-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2}\right) f(k,x,y) = (\mu_1 + k^2) f(k,x,y)$$

where

$$0 < k < \sqrt{\mu_2 - \mu_1} = \sqrt{2}\frac{\pi}{d}$$

$$
\begin{aligned}
f(k,x,y) &= e^{ikx}\chi_1^{(-)}(y) + r_1(k)e^{-ikx}\chi_1^{(-)}(y) + \sum_{n=2}^{\infty} r_n(k)e^{k_n x}\chi_n^{(-)}(y) \\
&\quad \text{for} \quad x < 0 \\
f(k,x,y) &= t_1(k)e^{ikx}\chi_1^{(+)}(y) + \sum_{n=2}^{\infty} t_n(k)e^{-k_n x}\chi_n^{(+)}(y) \\
&\quad \text{for} \quad x > 0 \\
k_n &= \sqrt{\mu_n - \mu_1 - k^2} \quad = \quad \sqrt{n(n-1)\frac{\pi^2}{d^2} - k^2}
\end{aligned}
$$

Expected matching conditions

$$
f(k,0^-,\cdot) = f(k,0^+,\cdot) \quad , \quad \frac{\partial}{\partial x}f(k,0^-,\cdot) = \frac{\partial}{\partial x}f(k,0^+,\cdot)
$$

in a sense to be precised.

The coefficients r_n and t_n should be derived from these conditions.

$$f \in W^{1,2}((-L,0)\times(0,d)) \implies$$
$$\sum_{n=1}^{\infty} n|r_n|^2 < \infty\ ,\ \sum_{n=1}^{\infty} n|t_n|^2 < \infty\ ,\ f(k,0^{\pm},\cdot) \in W_{\pm}^{\frac{1}{2},2}((0,d))$$

$$W_{\pm}^{\frac{1}{2},2}((0,d)) = \left\{ \sum_{n=1}^{\infty} a_n^{(\pm)} \chi^{(\pm)} \;\middle|\; \sum_{n=1}^{\infty} n|a_n^{(\pm)}|^2 < \infty \right\}$$

Hilbert spaces with scalar products

$$(f,g)_{\pm} = \sum_{n=1}^{\infty} n\, \overline{a_n^{(\pm)}}\, b_n^{(\pm)}$$

Common matching value

$$f(k,0,\cdot) \in W_0^{\frac{1}{2},2}((0,d)) := W_-^{\frac{1}{2},2}((0,d)) \cap W_+^{\frac{1}{2},2}((0,d))$$

Hilbert space if equipped with a scalar product and the corresponding norm

$$(f,g)_0 := (f,g)_- + (f,g)_+$$

$$\|f\|_0 = \sqrt{\|f\|_-^2 + \|f\|_+^2}$$

and therefore reflexive.

Might be our $W_0^{\frac{1}{2},2}$ smaller than "standard $W_0^{\frac{1}{2},2}$" which is the space of traces from $W_0^{1,2}$?

$$\frac{\partial}{\partial x} f(k,0^{\pm},\cdot) \in W_0^{-\frac{1}{2},2} = \left(W_0^{\frac{1}{2},2}\right)^*$$

Schrödinger equation in distributional sense $\Longrightarrow$

$$\langle \frac{\partial}{\partial x} f(k, 0^-, \cdot), \omega \rangle = \langle \frac{\partial}{\partial x} f(k, 0^+, \cdot), \omega \rangle$$

for $\omega \in C_0^\infty$.

Require equality in $W_0^{-\frac{1}{2},2}$

Let us define projectors

$$P_n = \chi_n^{(-)}(\chi_n^{(-)}, \cdot)\ ,\ Q_n = \chi_n^{(+)}(\chi_n^{(+)}, \cdot)\ ,\ n = 1, 2, \dots$$

and an operator

$$D = -ikP_1 + \sum_{n=2}^{\infty} k_n P_n - ikQ_1 + \sum_{n=2}^{\infty} k_n Q_n$$

$$D: \ W_0^{\frac{1}{2},2}((0,d)) \to W_0^{-\frac{1}{2},2}((0,d)) = W_0^{\frac{1}{2},2}((0,d))^*$$

Derivative matching condition reads

$$D\varphi = -2ik\chi_1^{(-)} \quad \text{for} \quad \varphi = \sum_{n=1}^{\infty} t_n \chi_n^{(+)} = \chi_1^{(-)} + \sum_{n=1}^{\infty} r_n \chi_n^{(+)}$$

Evidently at most one solution. To prove its existence consider first

$$D_2 = \sum_{n=2}^{\infty} k_n P_n + \sum_{n=2}^{\infty} k_n Q_n$$

D_2 is strictly positive as

$$\max(||(I-P_1)\varphi||, ||(I-Q_1)\varphi||) \geq \eta||\varphi|| \quad , \quad \eta = \sqrt{\frac{\pi^2 - 4\pi + 4}{2\pi^2 - 4\pi + 4}} > 0$$

for $\varphi \in L^2((0,d))$. Try to solve

$$D_2\varphi = \psi$$

where $\varphi \in W_0^{\frac{1}{2},2}((0,d))$ is unknown and $\psi \in W_0^{-\frac{1}{2},2}((0,d))$ is given. This is an equation for the extremals of the functional

$$F(\varphi) = \langle D_2\varphi, \varphi\rangle - \langle\psi, \varphi\rangle - \overline{\langle\psi, \varphi\rangle}$$

F is a real functional on a reflexive Banach space $W_0^{\frac{1}{2},2}((0,d))$, weakly lower semicontinuous, coercive, strictly convex. So unique minimum of F exists.

D_2^{-1} maps $W_0^{-\frac{1}{2},2}((0,d))$ onto $W_0^{\frac{1}{2},2}((0,d))$ and therefore is bounded.

The matching condition reads

$$\varphi - ikD_2^{-1}(P_1+Q_1)\varphi = -2ikD_2^{-1}\chi_1^{(-)}$$

Let us denote R the projector onto span$\{\chi_1^{(-)},\chi_1^{(+)}\}$ in $L^2((0,d))$,

$$\varphi_1 = \sqrt{P_1+Q_1}R\varphi \quad ,\varphi_2 = (I-R)\varphi$$

P_1+Q_1 invertible in $\mathcal{R}an(R)$

Projected matching condition

$$\begin{aligned}
\varphi_1 - ik\sqrt{P_1+Q_1}RD_2^{-1}R\sqrt{P_1+Q_1}\varphi_1 &= -2ik\sqrt{P_1+Q_1}RD_2^{-1}\chi_1^{(-)}\\
\varphi_2 - ik(I-R)D_2^{-1}R\sqrt{P_1+Q_1}\varphi_1 &= -2ik(I-R)D_2^{-1}\chi_1^{(-)}
\end{aligned}$$

φ_1 is solution of a linear equation in 2-dimensional space containing a Hermitian non-negative matrix

$$M = \sqrt{P_1 + Q_1} R D_2^{-1} R \sqrt{P_1 + Q_1}$$

φ_2 is expressed through φ_1. Sufficient to show that

$$\det(I_2 - ikM) = (1 - im_1)(1 - im_2) \neq 0$$

$m_1, m_2 \geq 0$ eigenvalues of M.
The determinant is non-zero in any case. Solutions φ and f exist.

An operator

$$A = \sum_{n=2}^{\infty} k_n P_n \quad , \quad k_n = \sqrt{n(n-1)\frac{\pi^2}{d^2} - k^2} \sim n$$

entered our equations

$$\frac{\partial A}{\partial k} = -\sum_{n=2}^{\infty} \frac{k}{k_n} P_n \quad , \quad \frac{k}{k_n} \sim \frac{1}{n}$$

Better convergency than in A.
Coefficients r_n, t_n are continuously differentiable functions of k (in our energy range at the least).
$||\varphi||$ is continuous in k.

3 Scattering states

Let $a \in C_0^\infty(\mathbb{R})$,

$\operatorname{supp} a \subset [A, B] \subset (0, \sqrt{\mu_2 - \mu_1}) \subset (0, +\infty) \backslash \{\sqrt{\mu_n - \mu_1}\}_{n=1}^{\infty}$.

Let us construct a state evolving according to our Hamiltonian

$$\psi(t, x, y) = \int_{\mathbb{R}} a(k) e^{-i(\mu_1 + k^2)t} f(k, x, y)\, dk$$

and asymptotic states which are superpositions of states evolving according to the reference Hamiltonians

$$\begin{aligned}
\psi^{(-)}(t, x, y) &= \int_{\mathbb{R}} a(k) e^{-i(\mu_1 + k^2)t} e^{ikx} \chi_1^{(-)}(y)\, dk \\
\psi^{(+)}(t, x, y) &= \int_{\mathbb{R}} a(k) e^{-i(\mu_1 + k^2)t} \left[r_1(k) e^{-ikx} \chi_1^{(-)}(y) + t_1(k) e^{ikx} \chi_1^{(+)}(y) \right] dk
\end{aligned}$$

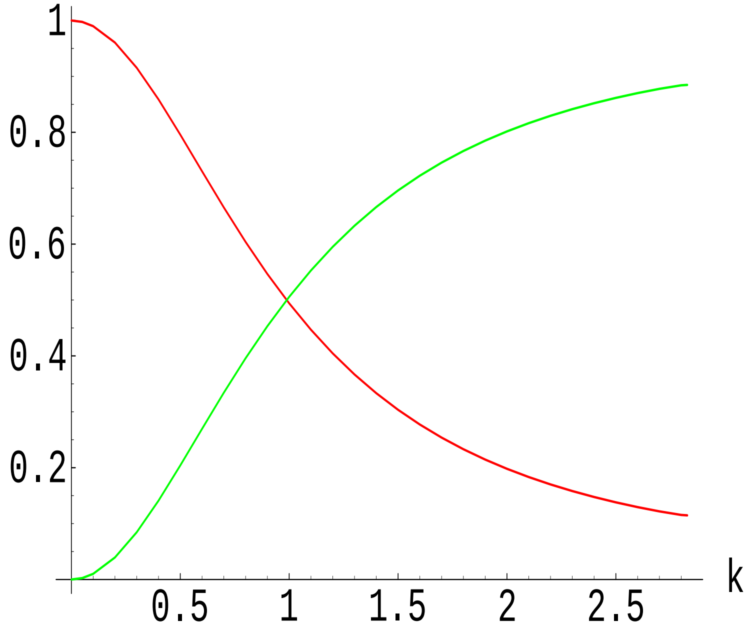
If r_n and t_n are continuously differentiable functions of k and $\sum_{n=1}^{\infty} |r_n(k)|^2$, $\sum_{n=1}^{\infty} |t_n(k)|^2$ locally bounded in k , then

$$\lim_{t \to -\infty} ||\psi(t, \cdot, \cdot) - \psi^{(-)}(t, \cdot, \cdot)||_{L^2(\Omega)} = 0$$

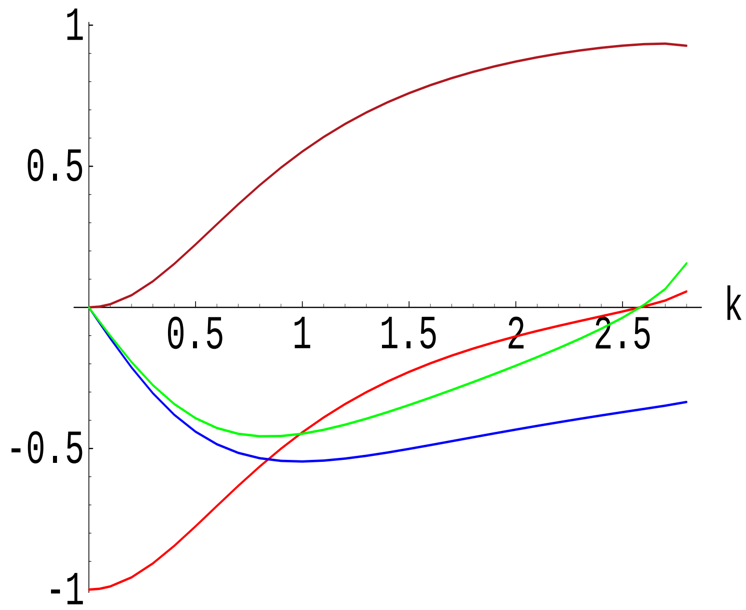
$$\lim_{t \to +\infty} ||\psi(t, \cdot, \cdot) - \psi^{(+)}(t, \cdot, \cdot)||_{L^2(\Omega)} = 0$$

This justifies the use of stationary scattering method for our system and shows that $r_1(k)$ and $t_1(k)$ are the reflection and transmission coefficients for the transversal modes $\chi_1^{(\pm)}$ and longitudinal momentum k.

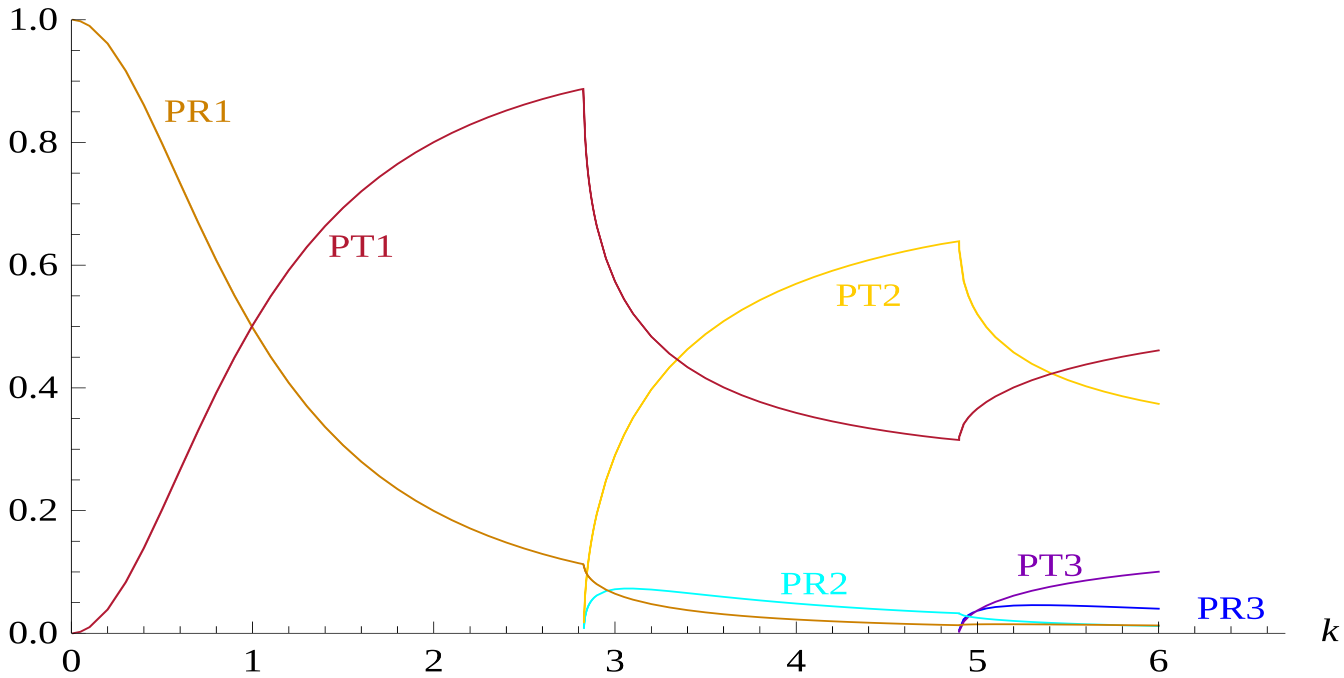
4 Numerical results



Reflection and transmission probabilities $|r_1(k)|^2$ and $|t_1(k)|^2$



Reflection and transmission coefficients $\Re\, r_1(k)$, $\Im\, r_1(k)$, $\Re\, t_1(k)$, $\Im\, t_1(k)$


1.0
0.8
0.6
0.4
0.2
0.0
0
1
2
3
4
5
6
k
PR1
PT1
PT2
PR2
PT3
PR3

5 Conclusions

- Scattering through a straight quantum waveguide with a simple combination of Dirichlet and Neumann boundary conditions is studied.
- Stationary scattering method is justified. The proof of the solution existence for the matching conditions is given.
- For the lowest energy ($k = 0$), the total reflection occurs in accordance with the Borisov and Cardone proof of the two halves of waveguide decoupling in the limit of zero width.

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