Abstract:

Spectral properties of a quantum particle in a straight planar waveguide are studied. Dirichlet and Neumann boundary conditions are imposed on different parts of the waveguide's boundary. The particle Hamiltonian is identified with the Laplace operator with corresponding boundary conditions. Its domain is shown to contain also some functions which do not belong to the Sobolev space $W^{2,2}$*. The existence of discrete bound states depends on the specific geometrical configuration of the waveguide. For some simple configurations, the conditions for the existence of discrete bound states below the essential spectrum threshold are found.*

What are quantum waveguides?

Semiconductor or metallic microstructures of the tube like shape. Their characteristic properties are:

(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.

The model

We study a free particle of an effective mass m^* living in nontrivial spatial region. The impenetrable walls are modelled by suitable boundary condition:

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

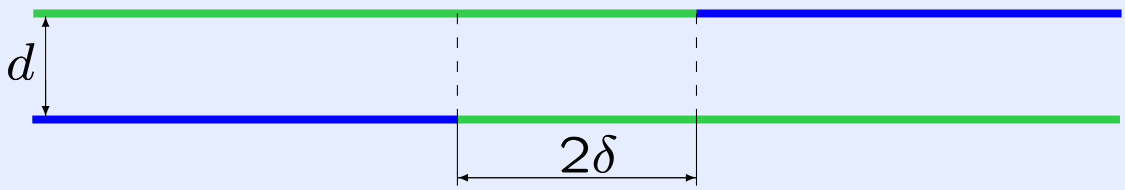
More realistic models allow for quantum tunneling.

From the mathematical point of view, we are interested in the spectral properties of the operator $-\Delta$ (putting $\hbar^2/(2m^*) = 1$) acting in the Hilbert space $L^2(\Omega)$.

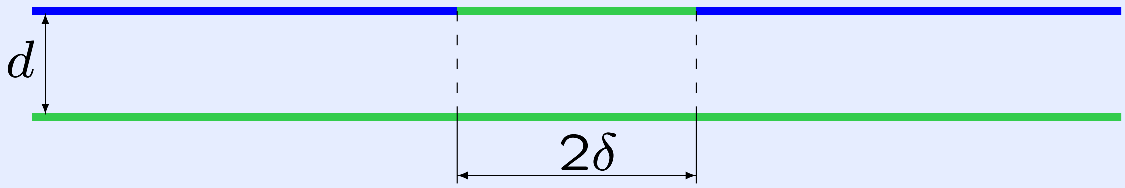
Our examples

Studied spatial regions are straight planar strips of a constant width d.

A)



B)



Green color denotes the Neumann b.c., blue one denotes the Dirichlet b.c..

Natural parameter of the problems is $\Lambda := \delta/d$. Both strips differ only in symmetry, however their spectral properties differ essentially at least for small values of Λ.

The Hamiltonian

Let us denote the planar strip by Ω, i.e. $\Omega := \mathbb{R} \times d$. Our Hilbert space is $L^2(\Omega)$. We denote the Dirichlet part of the boundary $\partial\Omega$ by $\mathcal{D}_\iota$ and the Neumann one by $\mathcal{N}_\iota$ for $\iota \in \{A, B\}$. Thus,

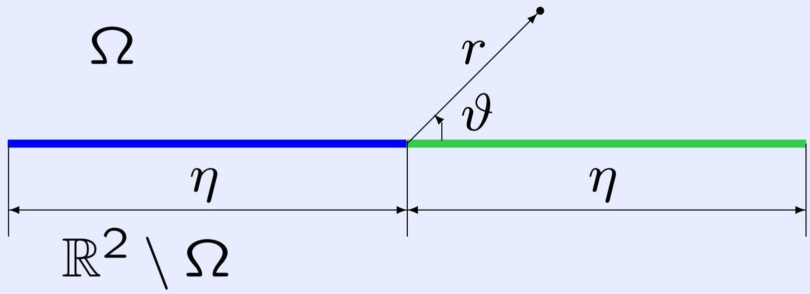
$$\begin{aligned} \mathcal{D}_A &= ((-\infty, -\delta] \times \{0\}) \cup ([\delta, \infty) \times \{d\})\,, \\ \mathcal{D}_B &= ((-\infty, -\delta] \times \{d\}) \cup ([\delta, \infty) \times \{d\})\,, \\ \mathcal{N}_A &= \partial\Omega \setminus \mathcal{D}_A, \qquad \mathcal{N}_B = \partial\Omega \setminus \mathcal{D}_B. \end{aligned}$$

We define Hamiltonians of our systems using the one-to-one correspondence between the closed, symmetric, semibounded quadratic forms and semibounded self-adjoint operators.

Definition: For $\iota \in \{A, B\}$, H_ι is the unique self-adjoint operator whose quadratic form is $Q_\iota(\psi, \varphi) := (\nabla\psi, \nabla\varphi)_{L^2(\Omega)}$ on the domain $\operatorname{Dom} Q_\iota = \{\psi \in W^{1,2}(\Omega) | \psi \restriction \mathcal{D}_\iota = 0\}$.

Theorem: For $\iota \in \{A, B\}$, H_ι acts as negative Laplacian on the domain $\operatorname{Dom} H_\iota = \{\psi \in W^{1,2}(\Omega) | \Delta\psi \in L^2(\Omega), \psi\restriction \mathcal{D}_\iota = 0, \partial_\nu\psi\restriction \mathcal{N}_\iota = 0\}$.

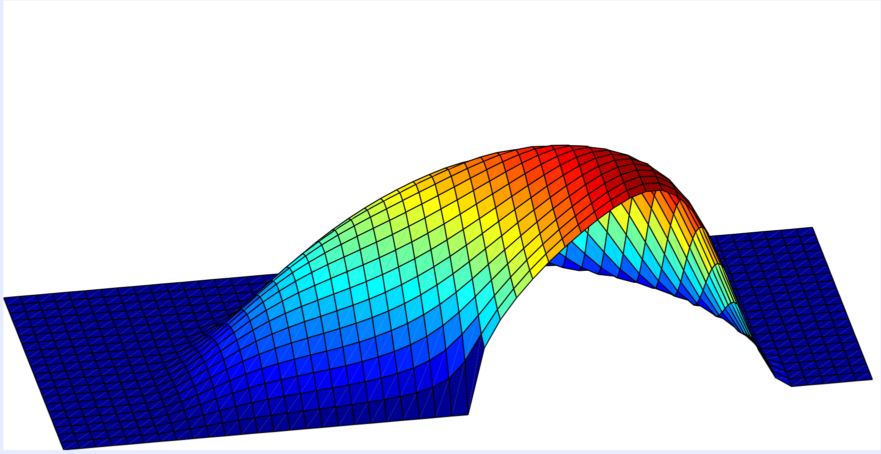
The inclusion Dom $H_\iota \subset W^{2,2}(\Omega)$ is not obeyed for our operators. Let us consider the following part of the region's boundary together with the polar coordinates (r,ϑ), $\eta < \min\{2\delta, d\}$.



Let ξ be such $C^\infty(0,\infty)$ function that $\xi(r) = 1$ for $r \in (0, \eta/2)$ and $\xi(r) = 0$ for $r > \eta$. Then

$$f(r,\vartheta) := \xi(r)\, r^{1/2} \cos(\vartheta/2)$$

belongs to the operator domain, $f \notin W^{2,2}(\Omega)$.



The energy spectrum

Essential spectrum

The essential spectrum of both our models coincides with the one of the straight strip with the Dirichlet b.c. on one boundary line and the Neumann b.c. on the other one.

Theorem: For $\iota \in \{A, B\}$, $\sigma_{\mathrm{ess}}(H_\iota) = \left[\frac{\pi^2}{4d^2}, \infty\right)$.

Number of discrete bound states

Dirichlet-Neumann bracketing gives us the estimate

$$-[-\Lambda] - 1 \leq N_\iota \leq -[-\Lambda],$$

where N_ι denotes the number of discrete eigenvalues of H_ι, $\iota \in \{A, B\}$.

The existence of bound states below σ_{ess}

The following statement was for the first time proved in [D. V. Evans, M. Levitin, D. Vassiliev, *Existence theorems for trapped modes*, J. Fluid Mech. **261** (1994), 21–31] .

Theorem: For any $\Lambda > 0$, $\inf \sigma(H_B) < \frac{\pi^2}{4d^2}$. Consequently, H_B has an isolated eigenvalue.

The situation in our model **A)** is more complicated.

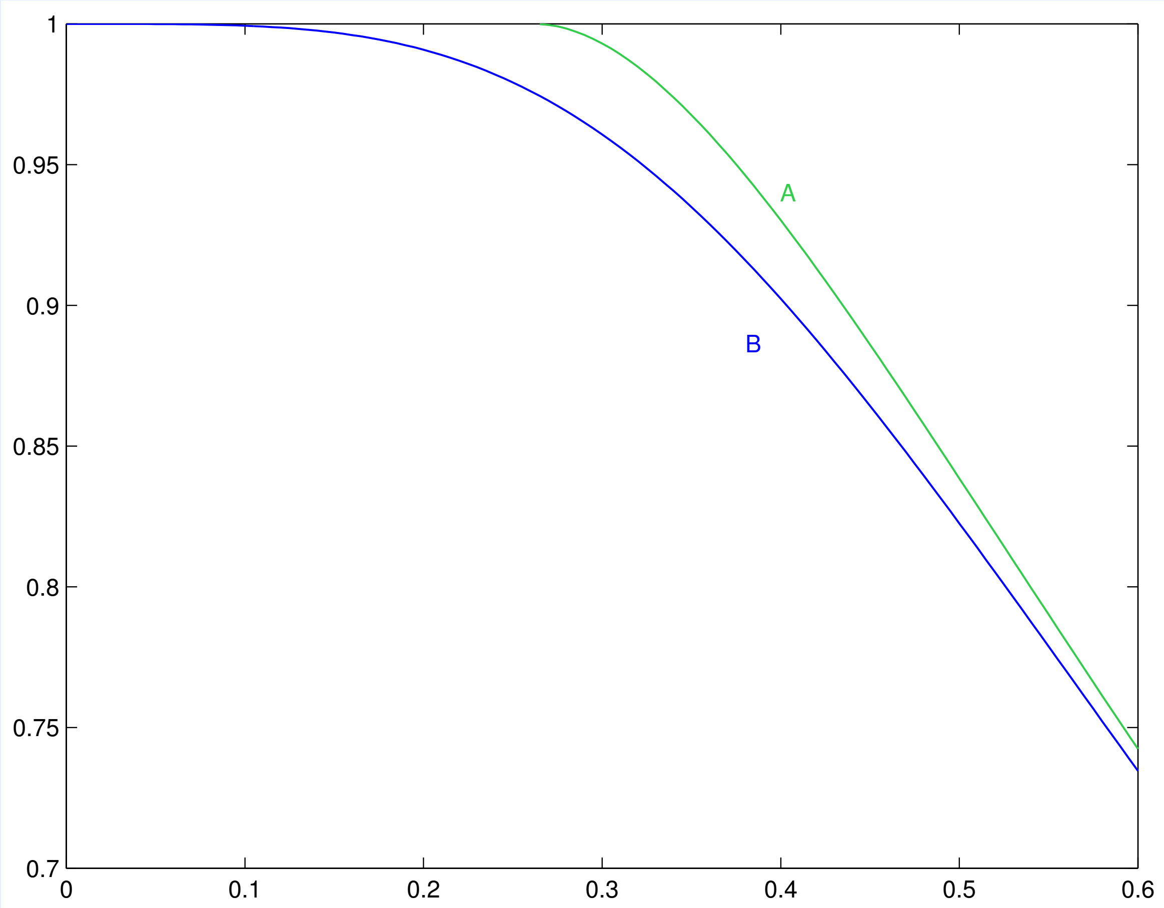
Theorem: There exists $\Lambda_0 \in (0, 1)$, such that for every $\Lambda \in (0, \Lambda_0]$, $\sigma_{\mathrm{disc}}(H_A) = \emptyset$ and for every $\Lambda > \Lambda_0$, $\sigma_{\mathrm{disc}}(H_A) \neq \emptyset$.

The continuity of discrete eigenvalues

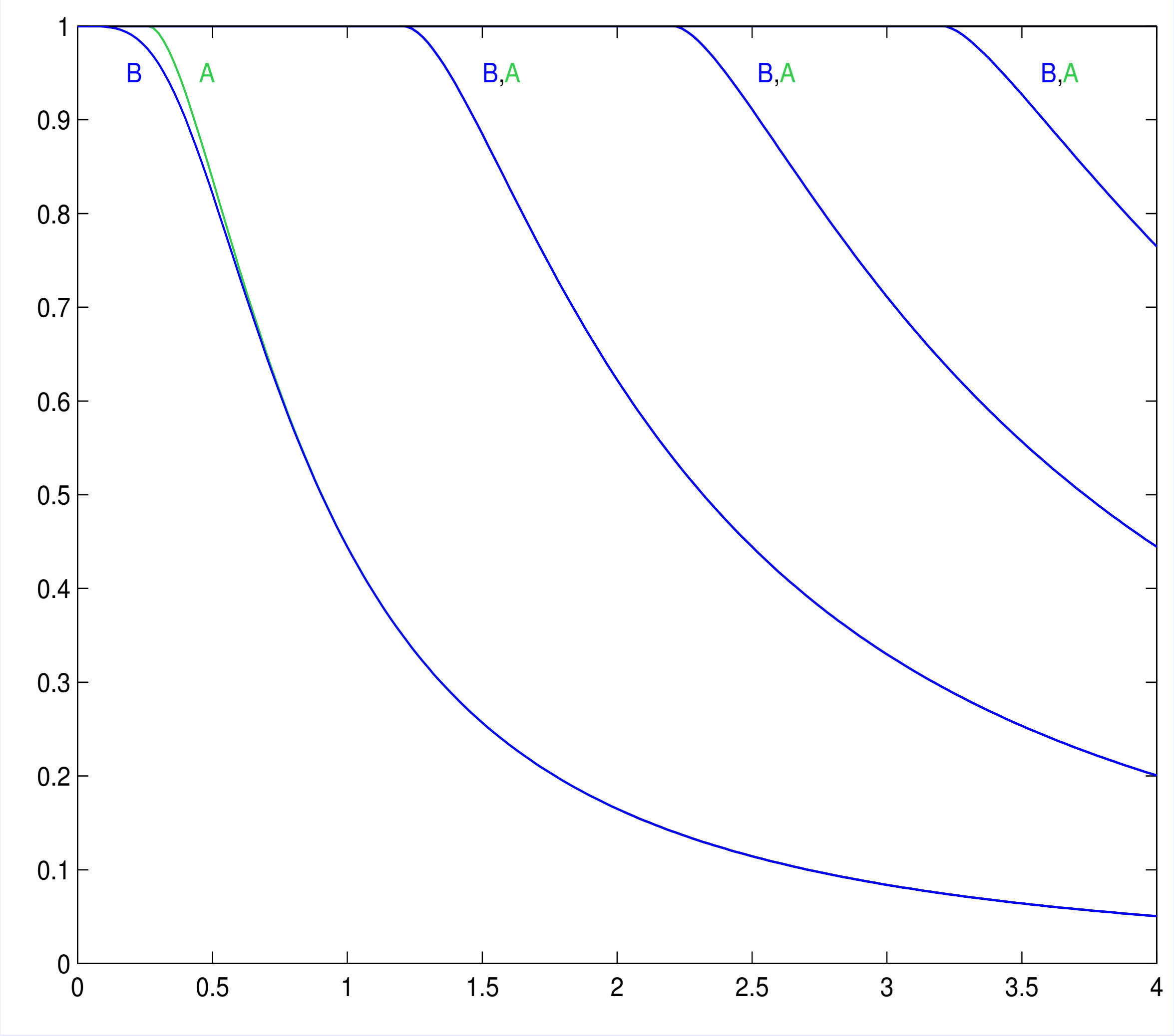
Theorem: All discrete eigenvalues of H_ι, $\iota \in \{A, B\}$, emerge at the essential spectrum threshold and they are nonincreasing, finite and continuous functions of Λ.

Numerical illustration

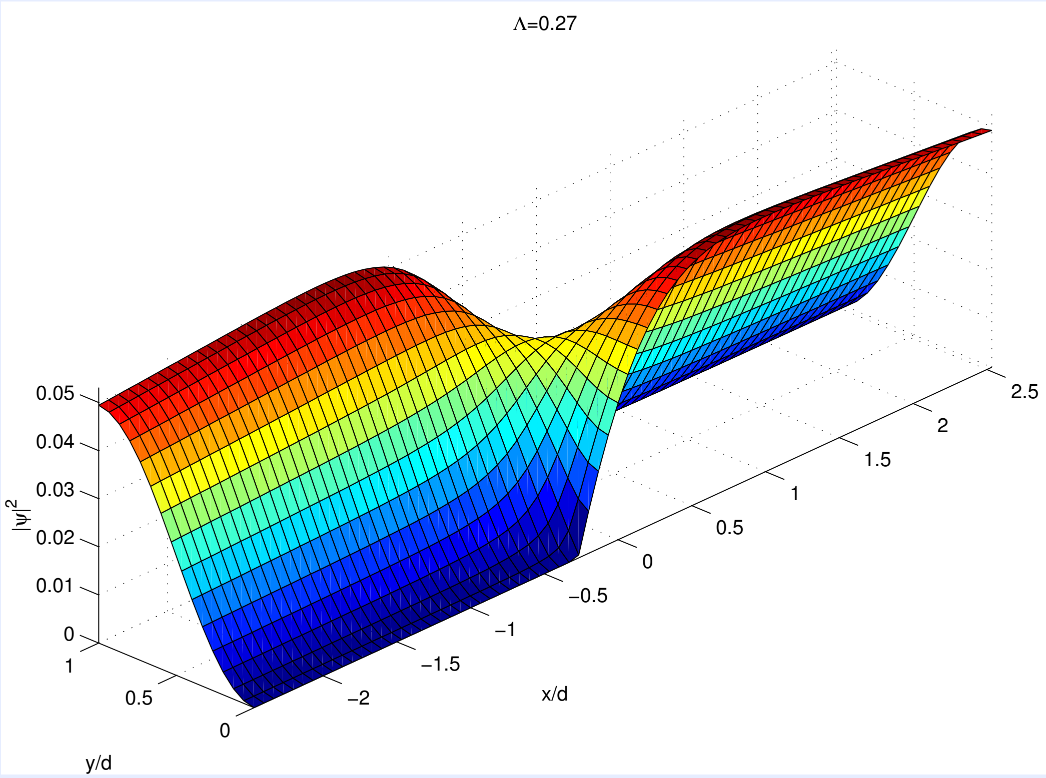
The first figure shows the first eigenvalues (in the units of $\frac{\pi^2}{4d^2}$) for both models in dependence on Λ. While in the model **B)** the eigenvalue exists for any $\Lambda > 0$, in the model **A)** appears at $\Lambda_0 \doteq 0.26$.

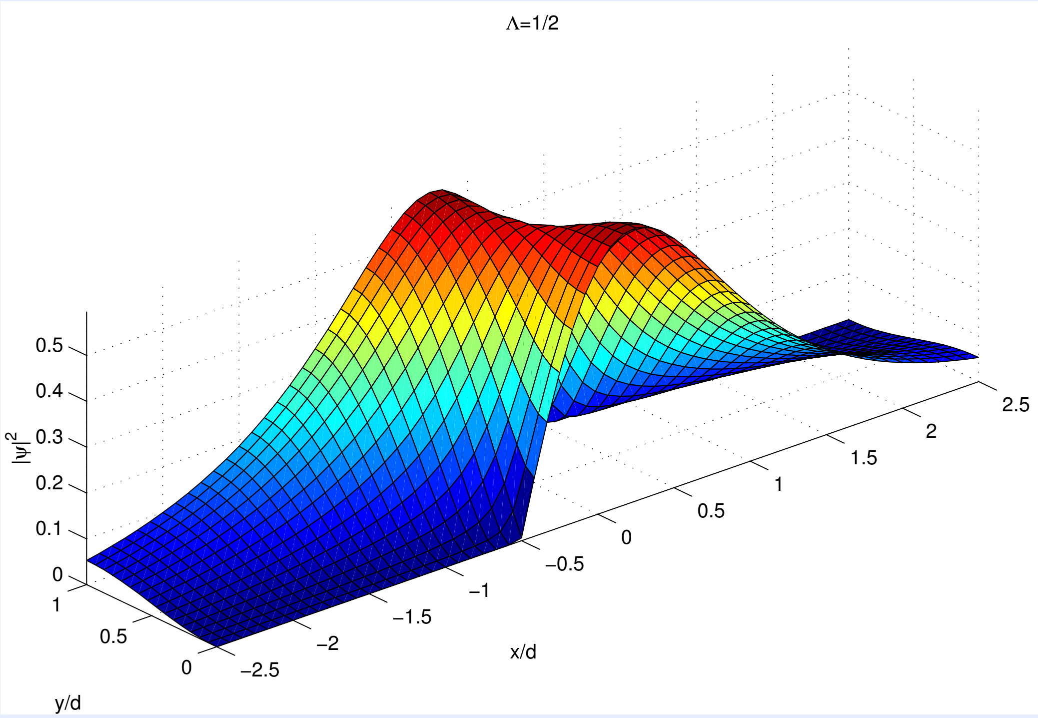


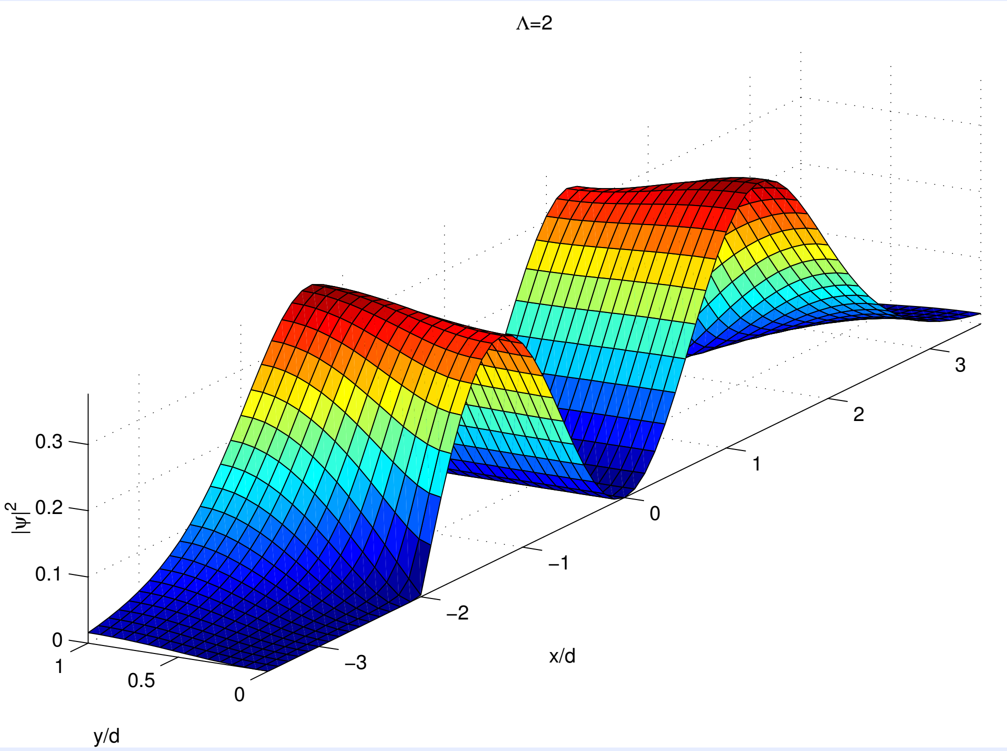
A few lowest eigenvalues (in the units of $\frac{\pi^2}{4d^2}$) for models **A)** and **B)** in dependence on Λ are drawn in the second figure. Higher eigenvalues in both models are very close to each other and cannot be distinguish within the scale of the graph.



The following three pictures show the examples of the probability density $|\psi|^2$ in the units of d^{-2} for the bound states in the model A) with three different values of the parameter Λ. The first example shows the probability density of the only one bound state for $\Lambda = 0.27$, which is close to the threshold for bound states appearance. The second example is computed for $\Lambda = \frac{1}{2}$ and the third one for $\Lambda = 2$, where we have already two bound states.




Λ=1/2
|ψ|^2
0
0.1
0.2
0.3
0.4
0.5
y/d
1
0.5
0
x/d
−2.5
−2
−1.5
−1
−0.5
0
0.5
1
1.5
2
2.5


Λ=2
|ψ|^2
0
0.1
0.2
0.3
y/d
1
0.5
0
x/d
−3
−2
−1
0
1
2
3