Charles University in Prague
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BACHELOR'S THESIS

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Perturbations of bound states in broken waveguides

Institute of Theoretical Physics

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Prohlašuji, že jsem svou bakalářskou práci napsal samostatně a výhradně s použitím citovaných pramenů. Souhlasím se zapůjčováním práce a jejím zveřejňováním.

V Praze dne 26.5.2009 Martin Váňa

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Abstrakt: V předložené práci studujeme existenci vázaného stavu ve vlnovodu s tvrdými stěnami tvaru L a hraniční podmínky této existence při umístění lokálního konstantího potenciálu nebo lokálního magnetického pole v ohybu vlnovodu. Vlastní výpočet pak vede na řešení parciální diferenciální rovnice druhého řádu s dirichletovskou okrajovou podmínkou. Podmínky pro existenci získáváme metodou sešívání vlnových funkcí na hranicích oblastí umístěných potenciálů. Výsledkem jsou pak numerické modely vlnových funkcí a garfy energetických hladin těchto stavů.

Klíčová slova: Vlnovod, vázaný stav, Laplaceův operátor, Dirichletovy okrajové podmínky.

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Abstract: In present thesis we study existence of bound state in L-shaped waveguide with hard walls and its stability to simple perturbations i.e. to a local constant potential and to a local magnetic potential, placed in the corner of the waveguide. Mathematically we solve partial differential equations of second order with Dirichlet boundary condition. The conditions for existence of the bound state we receive by mode matching of the wavefunctions on borders of placed potentials. The results are numerical models of wavefunctions and graphs of energy values with respect to field strength.

Keywords: Waveguide, bound state, Laplace operator, Dirichlet boundary conditions.

Chapter 1

Introduction

In recent decades the technical development of microelectronics allowed us to create tiny microscopic devices with highly pure materials. These nanostructures revealed that even geometric configuration of the structure may exhibit quantum effects. Studies of these structures may be found under term *mesoscopic physics*. Existence of bound state is one of quantum effects, which might be exhibited in such structures. Studying behaviour of a particle in these structures would lead to many-body Schrödinger equation, which would be very complicated to solve, unless we could make a sufficient approximation. If we consider very small devices with highly pure materials, crystallic structure and with smooth walls, we may approximate the device as a region with zero or constant potential with infinite potential outside the region. Without loss of generality we may consider the inner potential to be equal to zero, hence the Schrödinger operator is given by:

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

where Δ denotes Laplace operator and m^* denotes effective mass, which depends also on conductor material. In present thesis we use standard units, i.e. we put $\frac{\hbar^2}{2m^*} = 1$. We focus on "opened" shapes with asymptotically straight branches with perfect hard walls. Such structures are often called *quantum waveguides*. Studying bound states in this approximation leads to stationary Schrödinger equation of a free particle with Dirichlet boundary conditions. From mathematical point of view we study the spectrum of linear self-adjoint operator on a Hilbert space.

In presented thesis we study two dimensional case of a waveguide with one break and two straight external leads. It has been known for a long time that bending or breaking of two dimensional waveguide induces the existence of bound state with energy below the threshold of continuous spectrum [2],[1]. From mathematical point of view, an eigenvalue of finite multiplicity appears in the discrete part of the spectrum below the threshold.

In past two decades a relation between bound states and electromagnetic confined modes has been proved [3]. Some results of quantum studies were proven in experiments with microwave resonance in waveguides [3]. In this thesis we study the stability of break-induced bound state to perturbations, e.g., constant and magnetic potential in the corner of an L-shaped waveguide. Many of two dimensional problems can be straightforwardly extended to three-dimension systems [3], but it is not discussed in present thesis.

Chapter 2

Definition of operators

In presented thesis we study discrete part of spectrum of energy operator corresponding to open subset $\Omega \subset \mathbb{R}^2$ with Dirichlet boundary conditions. We define a *linear operator* $\hat{H}$ on Hilbert space $\mathscr{H}$ with *scalar product* $(\cdot,\cdot)$ and *norm* $||\cdot|| = \sqrt{(\cdot,\cdot)}$ as a linear mapping from $D(\hat{H}) \subseteq \mathscr{H}$ into $\mathscr{H}$, where $D(\hat{H})$ is called the *domain* of the operator $\hat{H}$. Operator is *densely defined* if $D(\hat{H})$ is dense in $\mathscr{H}$. An operator is said to be *symmetric* if it is densely defined and:

$$(\hat{H}\psi,\phi) = (\psi,\hat{H}\phi),\ \forall\phi,\psi \in D(\hat{H}) \tag{2.1}$$

For densely defined operator we define an *adjoint* operator $\hat{H}^*$ with domain $D(\hat{H}^*)$ by condition:

$$(\hat{H}\psi,\phi) = (\psi,\hat{H}^*\phi),\ \forall\psi \in D(\hat{H}) \text{ and } \forall\phi \in D(\hat{H}^*) \tag{2.2}$$

Where the domain $D(\hat{H}^*)$ is defined to be a set of all $\phi \in \mathscr{H}$ for which there exists $\eta \in \mathscr{H}$ such that:

$$(\hat{H}\psi,\phi) = (\psi,\eta)\ \forall\psi \in D(\hat{H}) \tag{2.3}$$

We define the *self-adjoint* operator to be symmetric and

$$D(\hat{H}^*) = D(\hat{H}) \tag{2.4}$$

We define the *spectrum* $\sigma(\hat{H})$ of self-adjoint operator to be a set of points $\lambda \in \mathbb{C}$ for which the operator $(\hat{H}-\lambda)^{-1}$ either does not exists or if it exists it is not bounded on $D(\hat{H})$. It is easy to prove that for self-adjoint operator $\sigma(\hat{H}) \subseteq \mathbb{R}$.

We define a *point spectrum* $\sigma_p(\hat{H})$ to be a set of all eigenvalues of $\hat{H}$, i.e. of all $\lambda \in \mathbb{R}$, for which there exists $\psi \in D(\hat{H})$ with $||\psi|| = 1$ such that $\hat{H}\psi = \lambda\psi$. It is obvious that $\sigma_p(\hat{H}) \subseteq \sigma(\hat{H})$.

We define the *geometric multiplicity* of $\lambda \in \sigma_p(\hat{H})$ to be the dimension of kernel of operator $(\hat{H} - \lambda)$.

We define the *discrete spectrum* σ_d to be a set of all isolated eigenvalues with finite multiplicity and the essential spectrum to be $\sigma_e(\hat{H}) = \sigma(\hat{H}) \setminus \sigma_d(\hat{H})$.

We define a *closed* operator to be an operator $\hat{H}$ defined on domain $D(\hat{H}) \subseteq \mathscr{H}$ if whenever ψ_n is a sequence in $D(\hat{H})$ with limit ψ in $\mathscr{H}$ and there exist $\phi \in \mathscr{H}$ such that $\lim_{n\to\infty} \hat{H}\psi_n = \phi$, it follows that $\psi \in D(\hat{H})$ and $\hat{H}\psi = \phi$.

We define an *extension* $\tilde{H}$ of an operator $\hat{H}$ if $D(\tilde{H}) \supseteq D(\hat{H})$ and $\tilde{H}\psi = \hat{H}\psi$, $\forall\psi \in D(\hat{H})$. (For such $\tilde{H}$ we say $\hat{H}$ is a restriction.)

We define a *closure* $\overline{H}$ of an operator $\hat{H}$ to be the smallest closed extension of $\hat{H}$.

We say the operator $\hat{H}$ is *positive* if $(\psi, \hat{H}\psi) \geq 0$, $\forall\psi \in D(\hat{H})$. (It is often written simply $\hat{H} \geq 0$)

We say the operator is *lower semi-bounded* if there is $c \in \mathbb{R}$ such that $(\psi, \hat{H}\psi) \geq c$. ($\hat{H} \geq c$) We may point out that the lower semi-bounded operator can be turned into a positive operator by translation.

We define a core $\mathscr{D}$ of a closed linear operator $\hat{H}$ to be a subset of $D(\hat{H})$ if $\hat{H}$ is the closure of its restriction on $\mathscr{D}$.

Studying the behavior of a linear self-adjoint operator, its domains and their cores may be in many cases very difficult. To avoid these difficulties we will use the quadratic form approach. Before defining quadratic forms we give a condition of segment property:

Let Ω be a bounded open set in $\mathbb{R}^m$ and let $\partial\Omega = \overline{\Omega}\backslash\Omega$ be its topological boundary. Ω is said to have a *segment property* if $\partial\Omega$ has a finite open covering $\{O_i\}$ and corresponding nonzero vectors $\{y_i\}$ so that for $0 < t < 1$, $x + ty_i$ is in Ω if $x \in \overline{\Omega} \cap O_i$.

2.1 Self-adjoint Operator as a quadratic form

In this part of the thesis we define associated quadratic forms, which are powerful tools for studying self-adjoint operators, yet their rigorous definitions and detail study is out of scope of present thesis. We give only basic results, for more information we refer to [5]. We define a *non-negative sesquilinear* form Q' on dense domain $\mathscr{D}$ in Hilbert space $\mathscr{H}$ is a map $Q' : \mathscr{D} \times \mathscr{D} \to \mathbb{C}$ such that:

$$Q'(\psi, \phi) \text{ is linear in } \psi \tag{2.5}$$

$$Q'(\psi, \phi) \text{ is conjugate linear in } \phi \tag{2.6}$$

$$Q'(\psi, \phi) = \overline{Q'(\phi, \psi)} \ \forall \psi, \phi \in \mathscr{D} \tag{2.7}$$

$$Q'(\psi, \psi) \geq 0 \ \forall \psi \in \mathscr{D} \tag{2.8}$$

We define *quadratic form* to be:

$$Q(\psi) = \begin{cases} Q'(\psi, \psi) & \text{if } \psi \in \mathscr{D} \\ +\infty & \text{otherwise} \end{cases} \tag{2.9}$$

Theorem 2.1.1 *(The Friedrichs Extension) Let $\hat{H}$ be a positive symmetric operator and let $Q(\phi, \psi) = (\phi, \hat{H}\psi)$ for $\phi, \psi \in D(\hat{H})$. Then Q is a closable quadratic form and its closure $\tilde{Q}$ is the quadratic form of a unique self-adjoint operator $\tilde{H}$. $\tilde{H}$ is a positive extension of $\hat{H}$, and the lower bound of its spectrum is the lower bound of Q. Further, $\tilde{H}$ is the only self-adjoint extension of $\hat{H}$ whose domain is contained in the form domain of $\tilde{Q}$.*

This theorem with proof might be found as Theorem X.23 in [6]. Since we are concerned of open subsets $\Omega \subset \mathbb{R}$ we have therefore Hilbert space $\mathscr{H} = L^2(\Omega)$. The considered Hamiltonian is $\hat{H}^D_\Omega = -\Delta^D_\Omega$ with domain $D(\Delta^D_\Omega) = C^\infty_0(\Omega)$ and we identify the associated quadratic form with:

$$Q_\Omega(\psi) = \int_\Omega |\nabla \psi|^2 \, \mathrm{d}x \tag{2.10}$$

If Ω has segment property the set of all ψ that are infinitely smooth in the interior of Ω and vanish on its boundary forms a core of $-\Delta^D_\Omega$ [1]. We may point out that if we add a constant potential in subset $\Sigma \subset \Omega$ the Hamiltonian on Σ is connected with above defined one by translation. For vector potential we consider Hamiltonian $\hat{H}^D_{\Sigma,\vec{A}} = (-i\nabla+\vec{A})^2$ with associated quadratic form:

$$Q^{\vec{A}}_{\Sigma}(\psi) = \int_{\Sigma} |(-i\nabla + \vec{A})\psi|^2 \, \mathrm{d}^2 x \tag{2.11}$$

defined on magnetic Sobolev space $H^1_{0,\vec{A}}(\Sigma)$. We may point out that gradient in above definitions is defined in distributional sense, i.e. in $\mathbb{R}^n$:

$$\int (\nabla\phi)\psi \, \mathrm{d}^n x = (-1)^n \int \phi\nabla\psi \, \mathrm{d}^n x \tag{2.12}$$

Chapter 3

Domain Decomposition

In this part of thesis we define a two dimensional waveguide as an open subset $\Omega \subseteq \mathbb{R}^2$. We consider an L-shaped waveguide to be a planar strip of constant width d with one right-angled break. It is useful to decompose the region in three new subregions: $\Omega = \Omega_I \cup \Omega_{II} \cup \Omega_{III}$, where $\Omega_I = (0, d) \times (d, \infty)$, $\Omega_{II} = (d, \infty) \times (0, d)$ and $\Omega_{III} = (0, d) \times (0, d)$. It is clear that this domain has segment property. See figure 3.1.

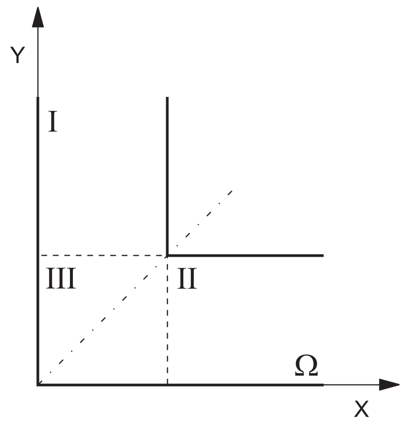

Figure 3.1: Domain decomposition

As a point in $\mathbb{R}^2$ we denote (x, y). In further text we give the solutions of Schrödinger equation for each region separately, then we connect them by *mode matching* method, i.e. through equality of wavefunctions and its first derivate on borders of subregions (see Chapter 4). We consider the wavefunction $\Psi(x, y)$ to be:

$$\Psi(x,y) = \begin{cases} \Psi_I(x,y) \text{ if } (x,y) \in \Omega_I \\ \Psi_{II}(x,y) \text{ if } (x,y) \in \Omega_{II} \\ \Psi_{III}(x,y) \text{ if } (x,y) \in \Omega_{III} \end{cases} \tag{3.1}$$

The symmetry of the given shape (with respect to axis $x = y$) gives us great simplification: The wavefunction is either symmetric or antisymmetric with respect to above defined axis.

3.1 External leads

With respect to above defined symmetry it is sufficient to study the wavefunction only on half of Ω (divided by the symmetry axis). The wavefunction can be then straightforwardly extended to the second half. Therefore we will study the solution in one external lead. In our case we consider the potential in external lead to be equal to zero, hence the Schrödinger operator can be identified with Hamiltonian of a free particle and Schrödinger equation can be written as:

$$\hat{H}\psi = -\Delta\psi = \lambda\psi \tag{3.2}$$

The infiniteness of potential outside considered region provides vanishing of wavefunction outside Ω, hence we consider Dirichlet boundary conditions, i.e. for external lead Ω_{II}: $\psi(x, 0) = 0,\ \psi(x, d) = 0,\ \forall x \in (d, \infty)$. Considering the zero potential we can separate variables and divide the problem into two independent problems.

$$\psi(x,y) = \eta(x)\phi(y) \tag{3.3}$$

$$\Rightarrow \quad \frac{\eta''(x)}{\eta(x)} + \lambda = c \tag{3.4}$$

$$\Rightarrow \quad -\frac{\phi''(y)}{\phi(y)} = c \tag{3.5}$$

First we will solve the *transversal* case (3.5).

3.1.1 Transversal solution

As a transversal Hamiltonian we consider operator defined as $\hat{H}\phi = -\phi''$, defined on $L^2(0,d)$. The solution of Schrödinger equation with zero boundary condition is:

$$\phi(y) = \sqrt{\frac{2}{d}} \sin\left(\frac{j\pi y}{d}\right),\ j \in \mathbb{N} \tag{3.6}$$

At this point we may point out that we have complete orthogonal set of eigenfunctions, hence the energy operator $\hat{H}$ is essentially self-adjoint. The solution gives the value of a constant c in (3.5), (3.4), $c = \frac{j^2\pi^2}{d^2}$ where $j = 1, 2..., \infty$.

3.1.2 Longitudinal solution

Now we can give a solution to longitudinal part of the problem. The solution to (3.4) is bounded with zero condition in infinity, and therefore is:

$$\psi = \exp^{\pi\sqrt{j^2-\kappa}(1-\frac{x}{d})}, \tag{3.7}$$

where $\kappa = \frac{d^2}{\pi^2}\lambda_0$ and the threshold of continuous spectrum is given by the first transversal mode: $\lambda_0 = \frac{\pi^2}{d^2}$.

3.1.3 Wavefunction

The wavefunction on Ω_{II} is therefore:

$$\Psi_{II}(x,y) = \sum_{j=1}^{\infty} (-1)^{j+1} r_j\ e^{q_j(1-x/d)} \sqrt{\frac{2}{d}} \sin\left(\frac{j\pi y}{d}\right), \tag{3.8}$$

where r_j are coefficients. As it was mentioned above, the wavefunction on Ω_I is given by the same expression with swapped variables and coefficients t_j. Due to the symmetry of the problem we consider the wavefunctions to be symmetric resp. antisymmetric to the axis $x = y$. The symmetry resp. antisymmetry can be expressed with relation of the coefficients: $r_j = t_j$ resp. $r_j = -t_j$.

Chapter 4

Mode matching

Let $\Psi(x, y)$ is the wavefunction on Ω defined in (3.1). Since the Schrödinger equation is a second order partial differential equation with piecewise continuous potential, its solution have to be continuous and continuous in its prime derivates for all $(x, y) \in \Omega$. Above defined separated solutions satisfy these conditions on their domains. The mode matching method gives us necessary conditions for wavefunctions on borders of their domains. Since we know the relation between wavefunctions Ψ_I and Ψ_{II}, we focus on relation between Ψ_{III} and Ψ_{II}.

$$\Psi_{III}(d, y) = \Psi_{II}(d, y) \ , \ \frac{\partial \Psi_{III}}{\partial x}(d, y) = \frac{\partial \Psi_{II}}{\partial x}(d, y) \tag{4.1}$$

If the conditions given by these relations and condition between Ψ_I and Ψ_{II} are satisfied, than the conditions given by relations between Ψ_{III} and Ψ_I are satisfied automatically. (In further work, we add a potential in region Ω_{III}, thus we may point out that this relation is true only if the inner potential in Ω_{III} is also symmetric to the axis $x = y$.)

4.1 Constant potential

First perturbation studied in presented thesis is constant potential of given strength V_0 placed in region Ω_{III}. Hence the Schrödinger operator is:

$$\hat{H}_{\Omega_{III}} = -\Delta_D^{\Omega_{III}} + V_0 \tag{4.2}$$

with zero conditions on borders $x = 0$ and $y = 0$. We can also see that the solution respects the symmetry to the axis $x = y$. Using the same method as in external leads case can express the solution as:

$$\Psi_{III}(x,y) = \sum_{j=1}^{\infty}(-1)^{j+1}\left[r_j\frac{\sinh(p_j\frac{y}{d})}{\sinh(p_j)}\phi_j(x) + t_j\frac{\sinh(p_j\frac{x}{d})}{\sinh(p_j)}\phi_j(y)\right], \quad (4.3)$$

where $p_j = \pi\sqrt{j^2 - \kappa + V_0}$ and functions $\phi_j(\cdot)$ are defined as in (3.6). In next section we will show, that for sufficiently strong negative potential antisymmetric bound states appears. Coefficients t_j can therefore be equal to either to r_j or $-r_j$, dependant on to which state they belong. Using conditions (4.1) with relation of orthogonality of functions ϕ_j leads us to equation:

$$Cr = r, \quad (4.4)$$

where r is an infinite vector of coefficients r_j and C denotes a matrix operator C_{jk} defined as:

$$C_{jk} = \pm\frac{jk}{(k^2 + \frac{p_j}{\pi^2})}\frac{1}{(q_k + p_k\coth(p_k))} \quad (4.5)$$

The sign of the operator depends on the symmetry resp. antisymmetry of the state.

4.2 Numerical solutions

In this part (of present thesis) we give numerical solution to equation (4.4). From mathematical point of view we will study a matrix operator $(C_{jk} - 1)$, which depends on V_0 and κ. For each value of the potential we will use the parameter κ as independent variable. If the solution fulfils all conditions the matrix operator $(C_{jk} - 1)$ is singular, hence:

$$\det(C_{jk} - 1) = 0 \quad (4.6)$$

For further computing we used computer program MATLAB 6.5. For finding zero point we used built-in function "fzero", which is using standard bisection method. For computing energy values we have to confine ourselves to a finite row of coefficients. This restriction leads to condition of rapid convergence of coefficients, which is satisfied automatically if the resulting

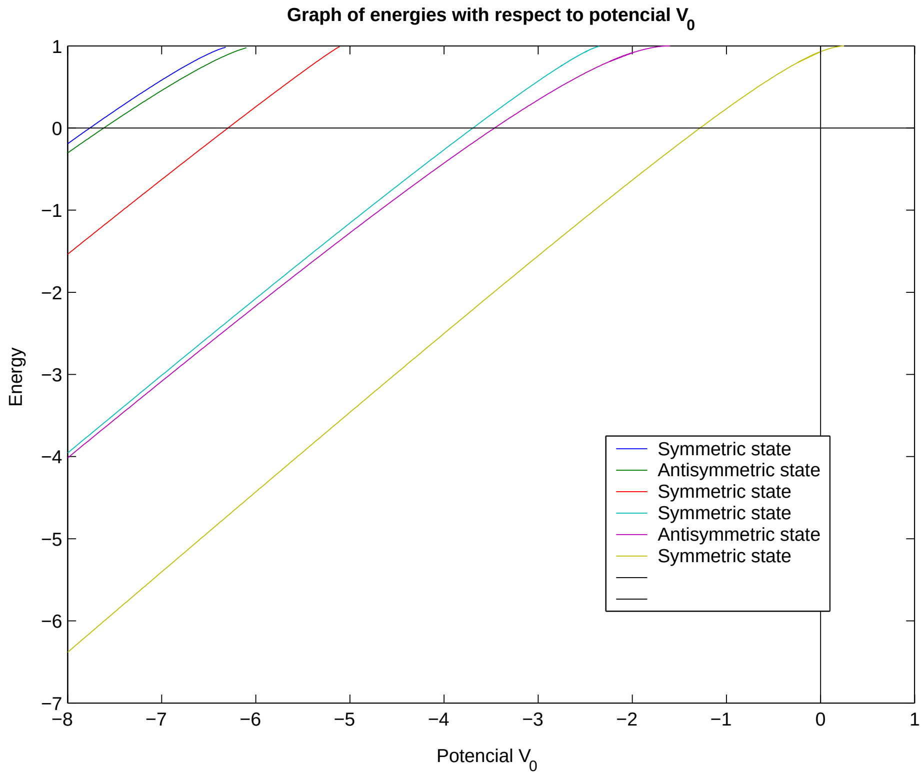

Figure 4.1: Energy levels with respect to constant potential strength V_0, with width of the strip $d = \pi$.

wavefunction is in $L^2(\Omega)$, and which was formerly discussed by prof. Exner et al. in [1]. Computed values we arranged in following graph:

The graph shows the first symmetric state crossing zero potential line in point $E \doteq 0.93\lambda_0$ which corresponds to former computation performed by prof. P. Exner et al. [1]. One may find interesting that the positive potential must be surprisingly strong to make the state vanish. The graph also shows that new states appear for sufficiently strong negative potential. Some examples of wavefunctions follows in figure 4.2

Studying the first symmetric state shows that the potential pushes the wavefunction inside external leads. When the repulsive potential is strong enough the wavefunction cannot be normalised, i.e. cannot be in $L^2(\Omega)$. The highest value of potential strength for which we were able to find bound state was $V_0^{max} \doteq 0,266$.

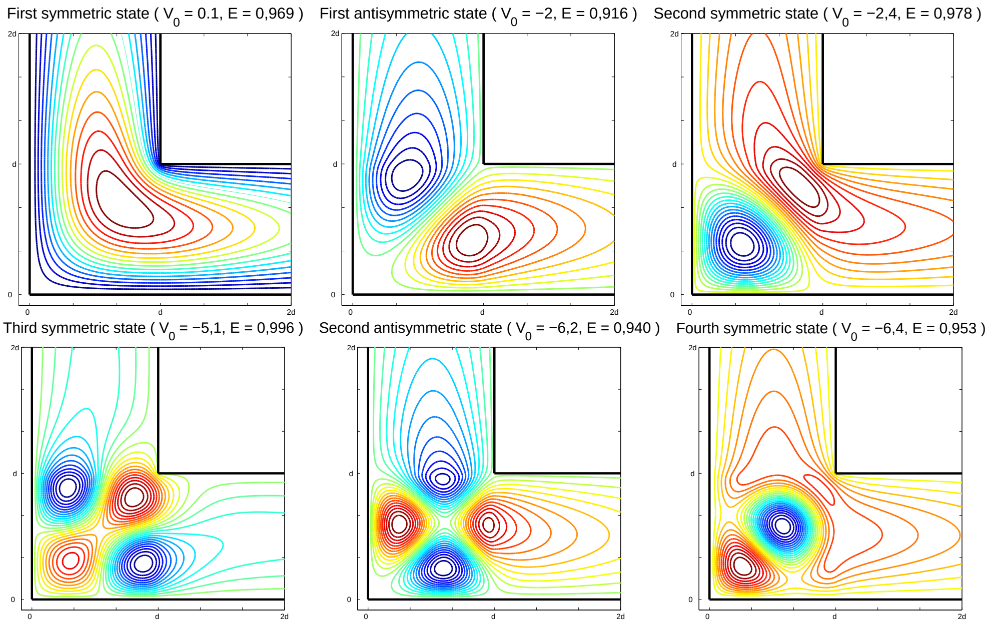

Figure 4.2: Examples of wavefunctions of bound states for different potential strength V_0 and with width of the strip $d = \pi$.

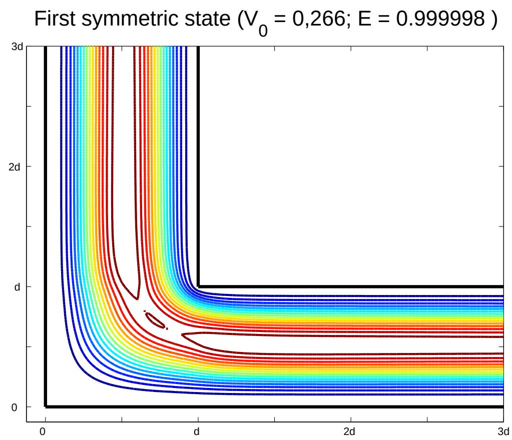

Figure 4.3: Model of a wavefunction of a ground state with repulsive constant potential in the corner near the threshold of continuous energy spectrum and with width of the strip $d = \pi$.

4.3 Magnetic field

Next perturbation studied in present thesis is magnetic field. It's potential given by formula:

$$\vec{A} = -\frac{1}{2}By\vec{e}_x + \frac{1}{2}Bx\vec{e}_y, \tag{4.7}$$

where B denotes a parameter of field strength. One would expect that the solution would be easily found by mode-matching method. It is easy to find solution on region Ω_{III} and to formulate necessary conditions as integral equations. Unfortunately it is not that easy to find numerical solutions.

Chapter 5

Finite element method

Due to numerical complications we decided to use easier approach. In the text below we give a brief overview of the *Finite Element Method* (*FEM*), used for solving the magnetic field case. We do not describe the method exactly. Proper description including used formulas might be found in [7].

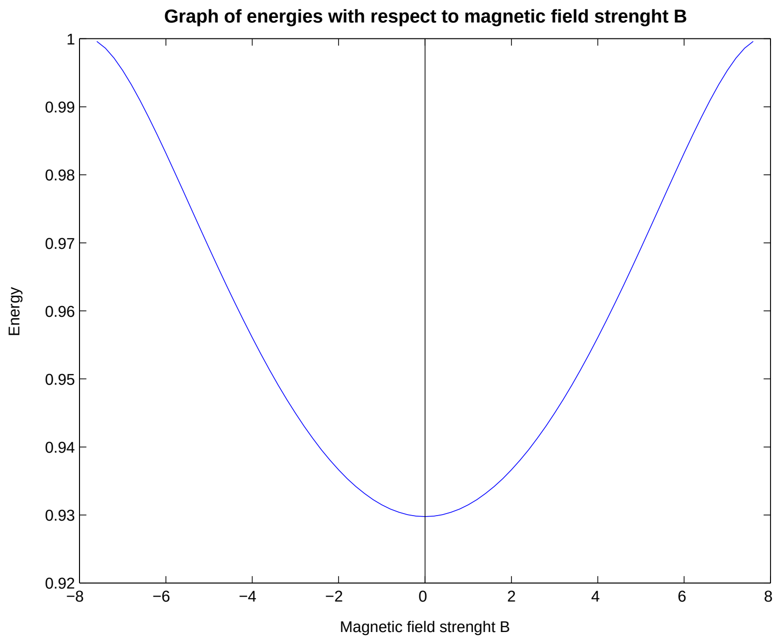

Figure 5.1: Energy level of ground state with respect to magnetic field strength B in L-shaped waveguide with width $d = \pi$.

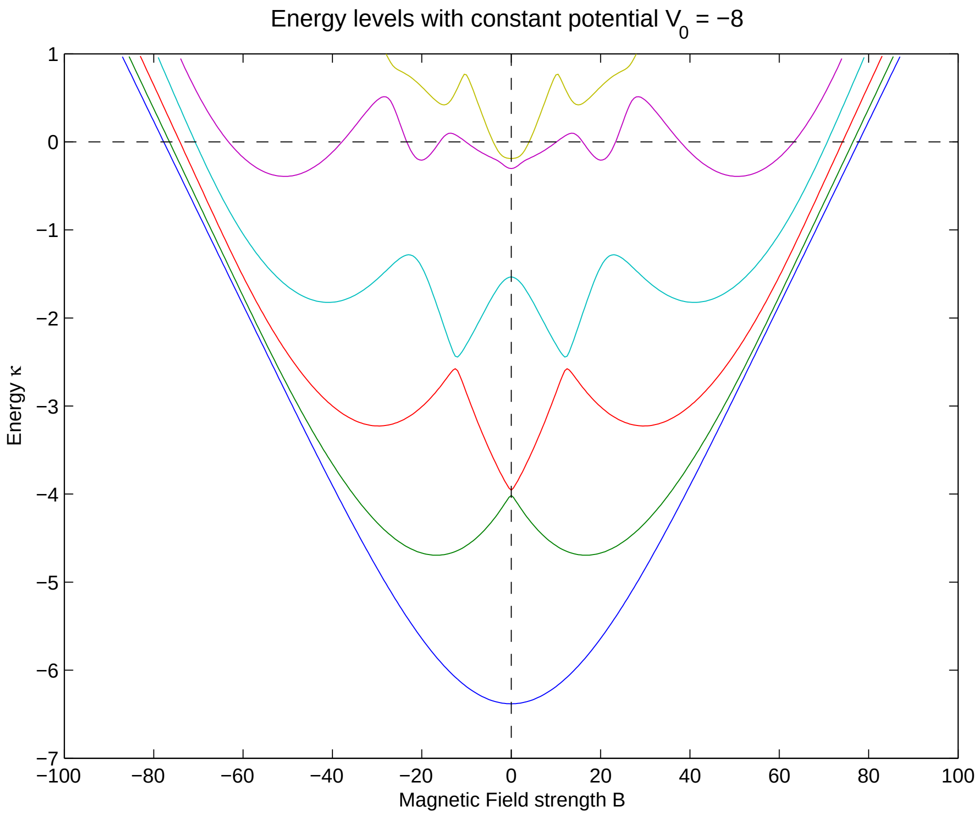

Figure 5.2: Graph of energy levels with respect to magnetic field strength B in L-shaped waveguide with attractive constant potential $V_0 = -8$ in the corner and with width $d = \pi$.

The finite element method is based on approximation computational domain Ω with a union of simple geometric object, in this case triangles. The main proposition is that the solution is simple on each triangle and that solutions are continuously connected to each other across the edges. The simplest function which can be connected are linear. The resolving function is than approximated by piecewise linear function. The Dirichlet boundary conditions are simply added as zero value of the function on triangle edges which lie on borders of defined region. The partial differential equation is than reformulated in a finite set of linear equations. The approximate solution is hence given by algebraic computation, which is much easier to solve.

For computing numerical solution we used specialised COMSOL Multi-Physics 3.4 software. The software does not allow us to compute equations on infinite objects, hence we have to approximate infinite external leads with sufficiently long but finite. After defining the problem we received solutions, which we arranged in a graph (see Fig. 5.1). Graph shows us how the energy depends on magnetic field's strength. As control point we can use the situation when magnetic field vanishes, as we did before for constant potential. We were also interested in combining both perturbations. The following graph shows us energy behavior for one value of constant potential.

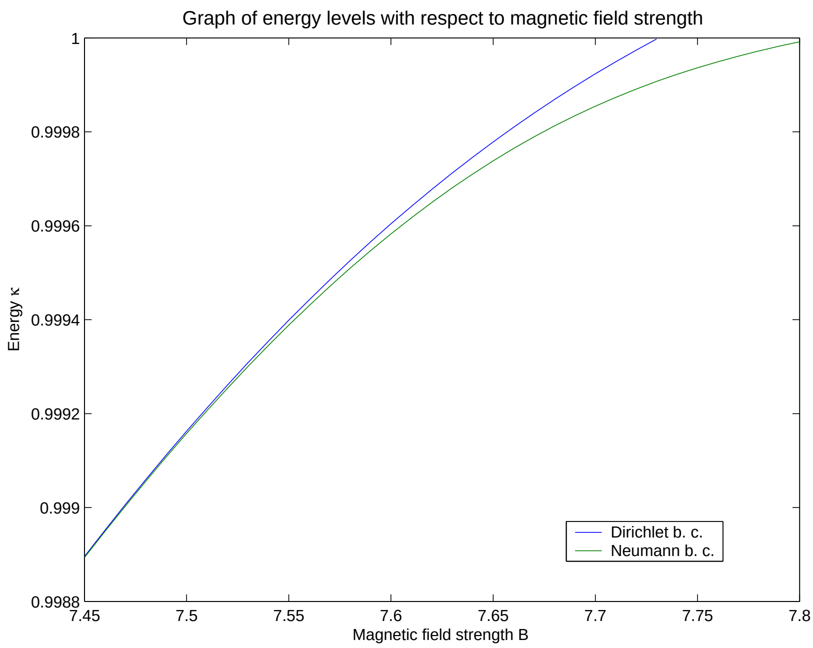

Figure 5.3: Graph of energy levels near continuous spectrum with respect to Magnetic field strength in L-shaped waveguide with width $d = \pi$ and zero constant potential.

We may point out that values in Fig. 5.1 and Fig. 5.2 are approximative only, particularly values close to threshold of essential spectrum. It is easy to identify the sources of these inaccuracies. One source is given by the method itself, with its approximation of the considered region by a mesh. This inaccuracy can be suppressed by refining the mesh. Unfortunately this refinement significantly increases the computation time. Second inaccuracy is given by the restriction to finite shape with Dirichlet condition at the ends of the leads. When the probability density is pushed inside external leads and the wavefunction is slowly decaying, the finite external lead is no longer sufficient approximation. This inaccuracy cannot be suppressed, but we can replace the Dirichlet boundary condition with Neumann boundary condition, i.e. $\nabla\Psi = 0$, $\forall(x, y) \in \partial\Omega$. Using Proposition 4 in chapter 13 in [6]:

$$0 \leq -\Delta_N^{\Omega} \leq -\Delta_D^{\Omega}, \tag{5.1}$$

for all $\Omega \subseteq \mathbb{R}^n$ and considering the wavefunction to be decaying in external leads, we may suggest the energy level lies between Dirichlet and Neumann boundary condition levels. We performed detail computation for values close to continuous spectrum with zero constant potential (see Fig 5.3)

Chapter 6

Conclusions

In present thesis we have studied the stability of geometrically induced bound state in L-shaped waveguide with respect to perturbations. For constant potential we have performed computation of values for energy of the state with respect to potential strength (Fig. 4.1). We have showed that with increasing strength of attractive constant potential the number of bound states increases and the symmetry resp. antisymmetry is manifested in wavefunctions (Fig. 4.2). We have also showed that the repulsive potential have to be surprisingly strong to destroy the bound state and that the state is very weakly coupled for strong repulsive potential (Fig. 4.3). These computations were performed on MATLAB 6.5 software. We have also studied the magnetic field perturbation. We have showed that for sufficiently strong field the bound state vanishes (Fig. 5.1) and the symmetry of the graph shows that energy values are not dependant on orientation of the magnetic field. We have also studied the combination of negative constant potential and magnetic field (Fig. 5.2). The energy values manifests avoided crossing in several points. The independence to orientation of magnetic field is kept. These computations were performed on COMSOL MultiPhysics 3.4 software.

Bibliography

[1] P. Exner, P. Šeba, P. Šťovíček: *On existence of a bound state in an L-shaped waveguide*, Czech. J. Phys. B39 (1989), 1181-1191

[2] P. Duclos, P. Exner: *Curvature-Induced Bound States in Quantum waveguides in Two and Three Dimensions*, Rev. Math. Phys. 7, 73-102 (1995)

[3] J.T. Londergan, J.P. Carini, D.P. Murdoc:*Binding and Scattering in Two-Dimensional Systems*, Springer (1999)

[4] Kvasnica J.: *Teorie elektromagnetického pole*, Academia, Praha, 1985.

[5] E. B. Davies: *Spectral Theory and Differential Operators*, Cambridge University Press (1995)

[6] M. Reed, B. Simon: *Methods of Modern Mathematical Physics II: Fourier Analysis, Self-Adjointness*, Academic press, New York, San Francisco, London, (1975)

[7] J. M. Cooper: *Introduction to Partial Differential Equations with MATLAB*, Birkhauser, Boston, Basel, Berlin (1997)