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BAKALÁŘSKÁ PRÁCE

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Vázané stavy v kuželovité vrstvě

Ústav teoretické fyziky

Vedoucí bakalářské práce: Prof. RNDr. Pavel Exner, DrSc.,
Ústav jaderné fyziky AV ČR

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Zde bych rád poděkoval svému vedoucímu práce Prof. RNDr. Pavelu Exnerovi, DrSc. za jeho neocenitelnou pomoc při tvorbě tohoto textu a trpělivost, s jakou zodpovídal mé často neodborné a triviální otázky. Neméně díků patří také RNDr. Miloši Taterovi, CSc., bez jehož pomoci bych si numerické řešení tohoto problému nedokázal představit.

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

V Praze dne 24.5.2007 Jan Švarcbach

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Abstrakt: V této práci studujeme existenci vázaných stavů kvantové částice uvězněné v trojdimenzionální kuželovité vrstvě s Dirichletovskými hraničními podmínkami. Podáváme referenci o dřívějších výsledcích v literatuře, které ukazují, že diskrétní spektrum je neprázdné pro jakýkoliv netriviální kužel, a přidáváme nová pozorování. Současně prezentujeme numerickou metodu, která by měla poskytnout hodnoty energií vázaných stavů.

Klíčová slova: vázané stavy, kužel, esenciální spektrum

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Abstract: We study the existence of bound states of a quantum particle confined within the 3-dimensional conical layer with Dirichlet boundary. We review earlier results in the literature showing that the discrete spectrum of such systems is nonempty whenever the cone is nontrivial and add new observations. We also present a numerical method which yields values of bound-state energy.

Keywords: bound states, cone, essential spectrum

1 Introduction

If we wanted to study energies of a quantum particle trapped in a bounded region Γ in $\mathbb{R}^n$, we would have to ask about the eigenvalues of the operator minus the Dirichlet Laplacian acting on $L^2(\Gamma)$. According to Theorem 6.2.3 in [1] the essential spectrum is empty and thus the particle possesses only discrete energy spectrum. If we "open" this domain in such a way that the particle can escape, one would naturally expect that the spectrum would be continuous because the particle has now space enough to escape and far from Γ there is no external effective potential induced by the geometry. In fact the question of the character of energy spectrum is much more complicated and leads to nontrivial mathematical constructions and assumptions.

The problem is more mathematically accessible in two dimensions where the Laplace operator as well as the geometries have a simpler shape and therefore these cases were studied at first. In [2] it was proved the existence of one bound state with energy $\lambda_0 = 0.93\lambda_1$ under the threshold λ_1 of continuous spectrum in an L-shaped strip. More general case of an broken strip (two half-wires joined together) was discussed in [3] with result that for any angle there is at least one bound state (of course except the case when the broken strip becomes just a strip). In addition it is proved that the number of energy eigenvalues under the threshold of the essential spectrum can be made arbitrarily large for very sharp angles.

The articles [4] and [5] deal with 3-dimensional problems. The authors were interested in curved layers with constant width built over the surface with certain properties. In the article [4] it is studied thin layers, whose half-width is less then the minimum normal curvature radius, built over a C^2-smooth complete simply connected non-compact surface with a pole. If the surface Ω is in addition nontrivially asymptotically planar and one of the following conditions holds

- integrability of the Gauss curvature, the integral is non-positive

- surface is C^3-smooth and the layer is sufficiently thin
- surface is C^3-smooth, the total Gauss curvature and the square of the gradient of the mean curvature are integrable, the total mean curvature is infinite
- integrability of the total Gauss curvature, surface is cylindrically symmetric,

then the existence of at least one isolated eigenvalue below $\inf \sigma_{ess}(-\triangle_D^\Omega)$ is ensured.

Unfortunately, the authors make an assumption in that paper on the surface which should be parameterizable by geodesic polar coordinates, i.e. the existence of at least one pole is needed. The later article [5] generalizes the spectral results to the situation when the surface needn't have a pole. In this work we were particularly concerned with Theorem 2 of that paper which states that if Ω' is obtained by any compact deformation of Ω, where Ω is a layer satisfying

- integrability of the Gauss curvature
- half width a is less than $(\max\{\| k_1 \|_\infty, \| k_2 \|_\infty\})^{-1}$; k_1, k_2 are the main curvatures
- the Gauss and mean curvatures vanish at infinity
- the reference surface Ω contains $N \geq 1$ cylindrically symmetric ends, each of them having total Gauss curvature,

then the infimum of the essential spectrum equals $\pi^2/4a^2$ and there will be at least N eigenvalues in the interval $(0, \pi^2/4a^2)$. This interesting property is established by means of special trial functions and the Rayleigh-Ritz variational principle, which limits the energies from above. In Chapter 6 of [4] cylindrically symmetric layers were studied and the assertion that the infimum of the spectrum is less than $\pi^2/4a^2$ was proven with help of special trial functions which were localized at infinity, that is for any compact there was a function from the sequence supported out of the compact. The scheme was employed in more complicated layers where the trial functions can be localized only at the ends which satisfy conditions of the theorem. Once the trial functions are at infinity, they don't interfere into the compact part of the layer and this compact can be changed without loss of spectral results, even into an object without smooth boundary.

In our paper we don't make any general conclusions but we use the results of previous papers to investigate a special object in $\mathbb{R}^3$, *viz.* a conical layer. As the other authors we are especially interested in bound states and properties of the layer that are sufficient for their existence. The conical layer arises by rotations of the two-dimensional object investigated already in [3]. In the next text we use the bracketing argument almost in the same way as in this article to investigate the cone layers with small angles, the only difference is the dimension of a decomposition object.

The mentioned Theorem 2 appears to be a more general tool for the determination of spectrum behavior because it doesn't limit us on some interval of small angles and permits us to make conclusions for any nontrivial cone layer. We will check the assumptions and the very content of the theorem is the result we wanted to achieve.

2 Survey of the layer

Let's have a conical layer with vertex angle φ and with the width $d = \pi$. The border of this object is assumed to be an infinitely high potential wall to which the Dirichlet boundary conditions correspond. The set of coordinates will be the axis of symmetry z and r, θ which are the polar coordinates of an annulus (or a circle) arisen as an intersection of the conical layer and a plane orthogonal to the axis. Parameter z lays in $(0,\infty)$, $\theta \in (0, 2\pi)$ and $r \in (r_0, r_1)$. Radii r_0, r_1 are determined by the geometry of our problem, in the concrete $r_0(z) = \max(0, z\tan\varphi - \frac{\pi}{\cos\varphi})$, $r_1(z) = z\tan\varphi$.

2.1 Bracketing method

We conjecture that the essential spectrum σ_{ess} begins from the value of the first transverse mode, which is equal to, providing $\frac{\hbar^2}{2m} = 1$, one thanks to the proper choice of the width. Our first goal is to figure out whether there is at least one discrete energy under the threshold of σ_{ess} for some angle φ. The easiest way is to use Proposition 4 in chapter 13 of [6], the bracketing argument. In short, this proposition states that if we divide some domain Ω into two disjoint subsets Ω_1, Ω_2 that $\overline{(\Omega_1 \cup \Omega_2)}^{int} = \Omega$ and $\Omega \setminus (\Omega_1 \cup \Omega_2)$ has measure 0, then

$$0 \leq -\triangle_D^{\Omega} \leq -\triangle_D^{\Omega_1 \cup \Omega_2}. \tag{2.1}$$

In other words, by adding an extra Dirichlet surface $\Omega \setminus (\Omega_1 \cup \Omega_2)$ (its dimension is dim(Ω)-1), we add an extra condition on the wave function which gives rise to the operator inequality because we limit ourselves to the subset of $C_0^\infty(\Omega)$. By the minimax principle the analogous inequality is valid between the respective eigenvalues of the two operators; for this inequality was the definition $A < B$, A and B self-adjoint operators, actually motivated. The spectrum of $-\triangle_D^{\Omega_1 \cup \Omega_2}$ is the union of $\sigma(-\triangle_D^{\Omega_1})$ and $\sigma(-\triangle_D^{\Omega_2})$, so it

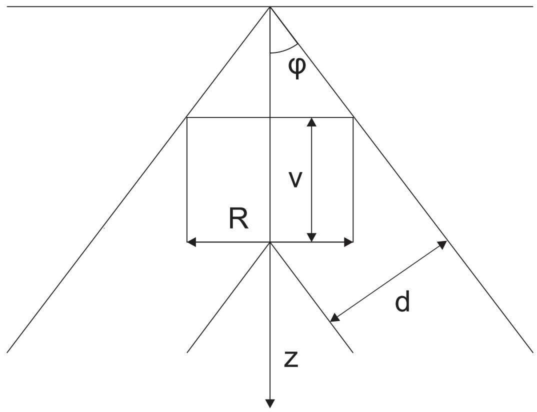

Figure 2.1: Bound states in a sharply tipped cone: a bracketing argument

suffices to bring the spectrum of some bounded object Ω_1 under the threshold σ_{ess}.

In our case Ω is the cone layer and Ω_1 will be some object which spectrum can be easily enumerated. Since we are interested in small values of energy, the inserted object should be big enough to satisfy our request for bringing $\inf\sigma$ under one. We will thus try to insert a cylinder Σ into this layer and according to its spectrum we hope we will be able to find the interval of angles (φ_1, φ_2) sufficient for the existence of at least one bound state. The inserted cylinder is localized near the vertex in the position shown in Fig. (2.1) and can be described by radius R and height v. From the geometry of our problem it is clear that the height is the function of the radius

$$v = \frac{\pi}{\sin\varphi} - \frac{R}{\tan\varphi}, \quad R \in (0, \frac{\pi}{\cos\varphi}). \tag{2.2}$$

We now ask about the spectrum of the cylinder with Dirichlet boundary conditions, i.e. setting $\frac{\hbar^2}{2m} = 1$ we seek a solution to

$$-\triangle_D^\Sigma \psi = E\psi. \tag{2.3}$$

The Laplace operator $\triangle$ in polar coordinates (r, θ, z) has the form $\triangle = \frac{\partial^2}{\partial z^2} + \triangle_{r,\theta}$. If we separate variables, we get $E = E_z + E_{r,\theta}$ and the equation transforms into the set of equations

$$-\frac{\partial^2}{\partial z^2}\psi_z(z) = E_z\psi_z(z) \tag{2.4}$$

$$-\triangle_{r,\theta}\psi_{r,\theta}(r,\theta) = E_{r,\theta}\psi_{r,\theta}(r,\theta) \tag{2.5}$$

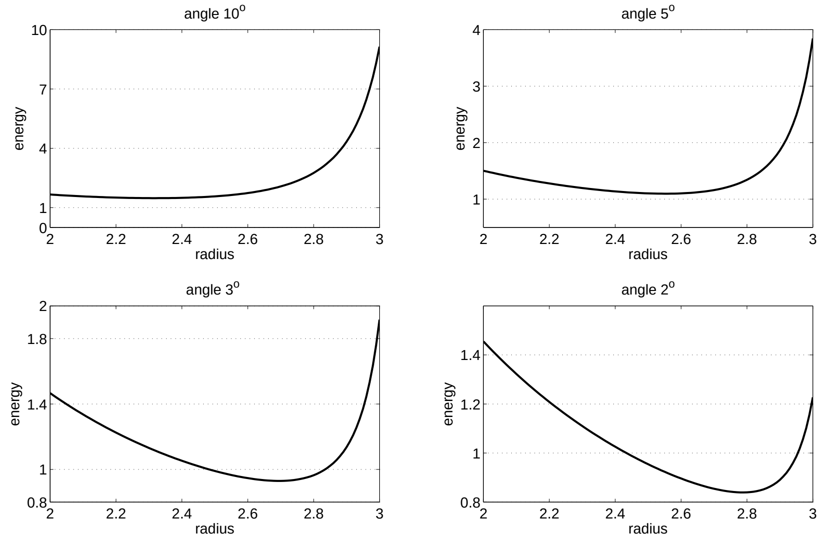

Figure 2.2: Ground state energy dependence on radius for inserted column

with boundaries taken from the geometry of the cylinder. Therefore our sought energy E is the sum of energies of a one-dimensional well and a two-dimensional round well with an infinite potential boundary. These two typical quantum cases can be found for example in [7] or [8], so

$$E = \left(\frac{\pi}{v}\right)^2 + \left(\frac{j_{m,n}}{R}\right)^2, \tag{2.6}$$

where $j_{m,n}$ denotes the n-th root of the first Bessel function of m-th order. If we look at the graphs of the Bessel functions, we see that the smallest possible energy will be that with the first root of J_0, Figure (2.2) shows dependence of the smallest possible energy E on R for angles 10^o, 5^o, 3^o and 2^o, respectively.

In this figures we can notice that for certain small angles there exist radii R allowing the energy to be smaller than one. It is also obvious that there is some angle between 3 and 5 degrees, for which our method with a decomposition column near the vertex stops to work. To be sure about the interval, let's fix the radius, for example R=2.8, and see how the lowest energy depends on angle φ. As we can see in Figure (2.3), if the angle is small enough, the energy in the cylinder can be smaller than one and from what was said before for these angles there is at least one bound state in the

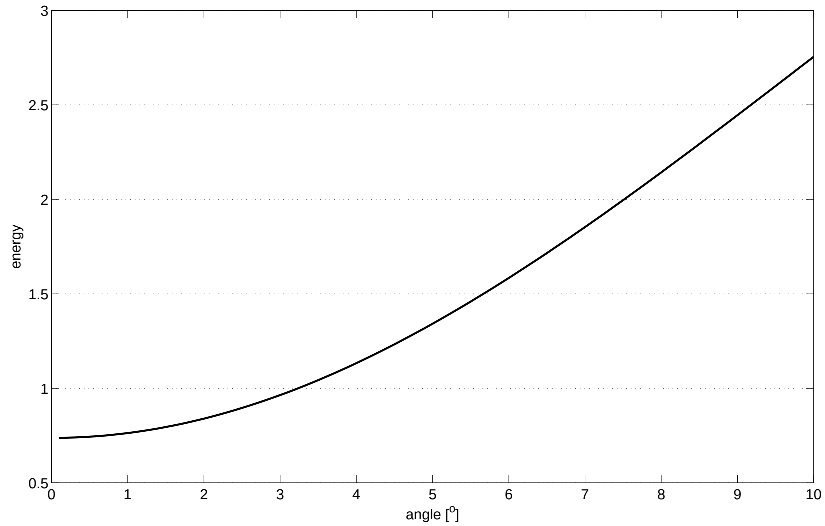

Figure 2.3: Energy dependence on angle for fixed radius

conical layer.

If the angle is small enough, we can estimate the spectrum by more than only a single lowest energy of the column. The energies of a higher level can be characterized by quantum numbers m, n, o

$$E_{m,n,o} = m^2 \left(\frac{\pi}{v}\right)^2 + \left(\frac{j_{o,n}}{R}\right)^2. \tag{2.7}$$

The geometry of our problem doesn't permit us to increase much the quantum numbers of the circle because the radii cannot exceed the width of the layer, which equals π. In fact, the total energy is already greater than one for all possible m and R whenever $n \geq 2$ and $o \geq 1$. Quantum number m is on the contrary very flexible and for small angles can be very big which is the matter of the geometry too. Given m, n and o, energy E is the function of height v and radius R which have a unique correspondence between themselves. It is hence possible to investigate function $E(R)$ and find the lowest energy estimate for a given angle φ. When we set the derivative of $E(R)$ equal to zero

$$0 = \frac{\pi^2 \sin^2\varphi \cos\varphi}{(\pi - R\cos\varphi)^3} - \frac{j_{o,n}^2}{R^3}, \tag{2.8}$$

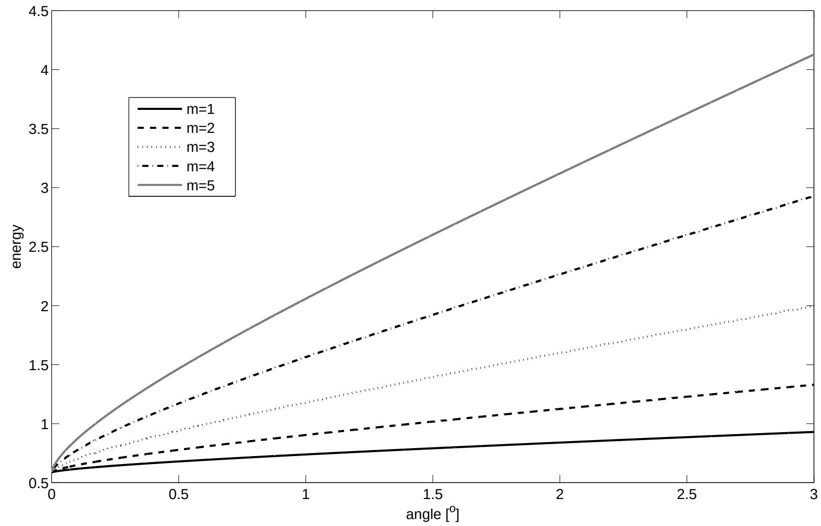

Figure 2.4: Dependence of the lowest energy estimate on the angle for different quantum number m

we solve a polynomial equation of the third order with only one real solution

$$R = \frac{j_{o,n}^{2/3}\pi}{\left(\pi^2 \sin^2\varphi\cos\varphi\right)^{1/3} + j_{o,n}^{2/3}\cos\varphi}. \tag{2.9}$$

Dependence of the lowest energy estimate on the angle (o=0, n=1) is shown in Figure (2.4), it is very interesting that all the functions converge to the number 0.586 when φ approaches zero. With this knowledge we can evidently claim that we have proved the existence of arbitrary number of bound states for small angles. The lowest energy estimate also shows that the method of the decomposition column begins to fail for angles above 3.8^o where we aren't able to ensure the bound state even for the system in the ground state, as was already predicted from Fig. (2.2).

2.2 General cone layer

Because the previous method limit us on small angles, we would like to use some different approach to our problem which would be independent of the angle. We will see that Theorem 2 in [5] is the right tool for investigation of the cone layer. Denote Ω' our conical layer and Ω an object which arises from the conical layer by transformation of the compact part around the vertex into a cap layer. This new object can be described as a set of points in R^3 whose distance from Σ is smaller than $\pi/2$, Σ is the surface made of the cap and a part of the cone surface. Σ is not C^2 smooth surface because of the shifting between its two parts but this shift can be smoothed and this change is so small that we can handle Σ as an object before smoothing. Another approach to this problem could be that we could construct a sequence of smooth layers which converge to Σ and require that other assumptions needed for the theorem can be fulfilled for some another layer from this sequence very close to Σ.

At the beginning we should find out how the main curvatures k_1, k_2 look because this characteristic of the surface Σ seems crucial in the above mentioned theorem. It is obvious that the cap described with radius r has both main curvatures equal $1/r$, which follows immediately from the definition. The latter part of Σ can be parameterized by projection γ

$$\gamma : (z, \theta) \to (z \tan\varphi \cos\theta, z \tan\varphi \sin\theta, z), \tag{2.10}$$

$z \in (a, \infty)$, $\theta \in (0, 2\pi)$, $a > 0$. The main curvatures can be enumerated as roots of the equation[9]

$$\det (F_{II} - \lambda F_I) = 0, \tag{2.11}$$

where F_I, F_{II} are the matrices of the first and second fundamental forms of the surface. F_I is a symmetric matrix

$$\mathbf{F_I} = \begin{pmatrix} E & F \\ F & G \end{pmatrix},$$

with elements $E = \vec{\gamma_z}.\vec{\gamma_z}$, $F = \vec{\gamma_z}.\vec{\gamma_\theta}$, $G = \vec{\gamma_\theta}.\vec{\gamma_\theta}$. After performing corresponding partial derivatives and the scalar product we get

$$\mathbf{F_I} = \begin{pmatrix} \tan^2\varphi + 1 & 0 \\ 0 & z^2 \tan^2\varphi \end{pmatrix}.$$

Matrix F_{II} can be described similarly

$$\mathbf{F_{II}} = \begin{pmatrix} L & M \\ M & N \end{pmatrix},$$

where the elements are $L = \vec{\gamma_{zz}}.\vec{n}$, $M = \vec{\gamma_{z\theta}}.\vec{n}$, $N = \vec{\gamma_{\theta\theta}}.\vec{n}$, $\vec{n}$ is the unit normal vector to the surface

$$\vec{n} = \frac{\vec{\gamma_z} \times \vec{\gamma_\theta}}{|\vec{\gamma_z} \times \vec{\gamma_\theta}|}. \tag{2.12}$$

After some calculation we obtain

$$\vec{n} = (-z\tan\varphi\cos\theta, -z\tan\varphi\sin\theta, z\tan^2\varphi)\frac{\cos\varphi}{z\tan\varphi} \tag{2.13}$$

and matrix F_{II} looks

$$\mathbf{F_{II}} = \begin{pmatrix} 0 & 0 \\ 0 & z\sin\varphi \end{pmatrix}.$$

Substituting F_I and F_{II} into (2.11) we solve the quadratic equation in λ

$$-\lambda(1+\tan^2\varphi)(z\sin\varphi - \lambda z^2\tan^2\varphi) = 0 \tag{2.14}$$

with result $\lambda_1 = 0 = k_1$, $\lambda_2 = \cos^2\varphi/(z\sin\varphi) = k_2$. These two values of the main curvatures could have been found more elementary if we had recalled that the curvature is the reciprocal of the radius of the osculation circle. It is evident from the geometry of our problem that the main curves, to which the main curvatures correspond, will be the intersections of the cone surface with normal planes, from which the first is passing through the vertex and the second is perpendicular to the first one. The first main curve is a line and therefore its osculating radius is infinity and the curvature zero. The second curve is an ellipse.

The integral of the Gauss curvature $G := k_1k_2$ on the whole Σ, the total Gauss curvature $\mathcal{G}$

$$\mathcal{G} := \int_\Sigma G d\Sigma, \tag{2.15}$$

doesn't depend on the radius r and because the cap is determined only with this one variable, we can choose arbitrary cap and be always sure about the total Gauss curvature. This result we simply get from definition (2.15). G outside the cap is zero everywhere thanks to k_1 and on the cap with surface $2\pi r^2(1-\sin\varphi)$ we integrate constant $1/r^2$. Let's discuss this proposition a little. G is surely constant $1/r^2$ because we have already agreed that both k_1, k_2 equal $1/r$ on the cap. In order to enumerate the surface we have parameterized the cap by the polar coordinates

$$\begin{aligned} x &= r\sin\theta\cos\phi \\ y &= r\sin\theta\sin\phi \\ z &= r\cos\theta \end{aligned}$$

$\theta \in (0, \pi/2 - \varphi)$, $\phi \in (0, 2\pi)$. Surface element dS in the new coordinates equals $r^2 \sin\theta$ and consequently

$$S_{cap} = \int_0^{2\pi} \int_0^{(\pi/2-\varphi)} r^2 \sin\theta d\theta d\phi = 2\pi r^2 [-\cos\theta]_0^{\pi/2-\varphi} = 2\pi r^2 (1 - \sin\varphi). \quad (2.16)$$

From (2.16) follows that $\mathcal{G}$ is really radius-independent and equals $2\pi(1 - \sin\varphi)$.

Since the main curvatures vanish at infinity, K and $M := (k_1 + k_2)/2$ vanish too and sure there exists radius $r > 2/\pi$ that

$$\pi/2 < (\max\{\| k_1 \|_\infty, \| k_2 \|_\infty\})^{-1}. \quad (2.17)$$

Condition $r > 2/\pi$ guarantees (2.17) on the cap and $k_1, k_2 \to 0$ when $r \to \infty$ says that $\| k_{1,2} \|_\infty$ can be made arbitrarily small by choosing some right r, therefore the term on the right side of (2.17) can be arbitrarily big, hence bigger than half-width $\pi/2$ of the layer.

We can also notice that Ω is cylindrically symmetric and the total Gauss curvature is positive (we have already enumerated it).

By this we have fulfilled the premises of the cited theorem and thereby we can claim that $\inf \sigma_{ess}(-\triangle_D^{\Omega'}) = 1$ and there is at least one eigenvalue in $(0, 1)$ for our cone layer.

3 Wave function

Since we do not consider any external field but infinite high walls, the hamiltonian of the system consists only of the kinetic energy of the particle and is time-independent. Hence we can pass from the time-dependent Schrödinger equation to the stationary Schrödinger equation

$$H\psi(z,r,\varphi) = -\frac{\hbar^2}{2m}\triangle\psi(z,r,\varphi) = E\psi(z,r,\varphi). \tag{3.1}$$

Setting $\frac{\hbar^2}{2m} = 1$ the equation reduces to

$$-\triangle\psi(z,r,\varphi) = E\psi(z,r,\varphi). \tag{3.2}$$

Laplacian in the cylindrical coordinates consists of the sum of $\frac{\partial^2}{\partial z^2}$ and derivatives with respect to φ and r. We shall use the method when we study the Laplacian on the transversal sections and then the wave function decompose into the basis of transversal modes. So now we will investigate Dirichlet Laplacian on the circle and the annulus.

3.1 Annulus

Consider an annulus with Dirichlet boundary conditions. We put the center of this annulus on the origin of coordinates and designate the radii of the border as r_0 and r_1, $r_0 < r_1$. When we set $\frac{\hbar^2}{2m} = 1$, the stationary Schrödinger equation looks

$$-\triangle_D\psi = \nu\psi. \tag{3.3}$$

Let us use the form of the Laplacian in polar coordinates and assume that the wave function has the form $\psi(r,\varphi) = \chi(r)\omega(\varphi)$. In the new equation

$$\frac{1}{r}\frac{\partial}{\partial r}\left[r\frac{\partial}{\partial r}\chi(r)\omega(\varphi)\right] + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\chi(r)\omega(\varphi) = -\nu\chi(r)\omega(\varphi) \tag{3.4}$$

we separate variables with the result

$$\frac{r\left(\chi_r + r\chi_{rr}\right)}{\chi} + r^2\nu = -\frac{\omega_{\varphi\varphi}}{\omega}, \tag{3.5}$$

where subscripts mean partial derivatives. Equation (3.5) holds for every r and φ, so the terms on both sides equal constant K and we get two ordinary differential equations

$$\begin{aligned} \omega_{\varphi\varphi} + K\omega &= 0 && (3.6) \\ r^2\chi_{rr} + r\chi_r + (r^2\nu - K)\chi &= 0 && (3.7) \end{aligned}$$

On function $\omega(\varphi)$ we impose periodic boundary condition $\omega(\varphi) = \omega(\varphi+2\pi)$, because if we go around the origin and stop at the same point, we should get the same value of $\omega(\varphi)$. It is very helpful to divide the cases when (let $j > 0$) $K = -j^2$, $K = j^2$ or $K = 0$. If K were positive, the solution to (3.6)

$$\omega(\varphi) = Ae^{j\varphi} + Be^{-j\varphi} \tag{3.8}$$

couldn't be periodic for any A, B because $|\omega(\varphi)| \to \infty$ when $\varphi \to \pm\infty$, therefor this solution is forbidden. From the same reason the solution to $K = 0$ with a nontrivial linear function is also invalid (but $K = 0$, $\omega(\varphi) = \mathit{const}$ reads). For K positive we get

$$\omega(\varphi) = Ae^{ij\varphi} + Be^{-ij\varphi}. \tag{3.9}$$

After resolving the complex exponential into the sum of trigonometrical functions and applying the same condition $\omega(\varphi) = \omega(\varphi + 2\pi)$ once more we can compare the real and complex terms

$$\begin{aligned} (A - B)\sin j\varphi &= (A - B)\sin j(\varphi + 2\pi) && (3.10) \\ (A + B)\cos j\varphi &= (A + B)\cos j(\varphi + 2\pi). && (3.11) \end{aligned}$$

It is easy to see that either $(A - B)$ or $(A + B)$ is nonzero because at least one of A, B must be nonzero. Salvo commonness let $(A + B) \neq 0$, then

$$\cos j\varphi = \cos j(\varphi + 2\pi) \quad \forall\varphi. \tag{3.12}$$

Condition (3.12) holds for all φ, when we choose $\varphi = 0$, then the equation requires $j(2\pi)$ be the integer multiple of 2π, i.e. j must be an integer. This condition is sufficient for all other angles too. We will write $\omega(\varphi)$ as $Ce^{\pm ij\varphi}$ where C is a normalization constant $\frac{1}{\sqrt{2\pi}}$.

After the substitution $r \to r/\sqrt{\nu} =: x$, $\psi(r) \to y(x)$ equation (3.7) transforms into Bessel equation

$$x^2\frac{d^2y}{dx^2} + x\frac{dy}{dx} + (x^2 - j^2)y = 0. \tag{3.13}$$

As was said before, j is an integer 0,1,2, ... and thus there are two linear independent solutions J_j and Y_j, which are Bessel functions of the first and second order, respectively. Let $\chi_j(r)$ be a solution to (3.13) with some chosen j, this solution will look as

$$\chi_j(r) = A_jJ_j(\sqrt{\nu_j}r) + B_jY_j(\sqrt{\nu_j}r). \tag{3.14}$$

Boundary conditions for $\chi_j(r)$ are $\chi_j(r_0) = 0$, $\chi_j(r_1) = 0$, thus coefficients A_j, B_j should satisfy

$$\frac{A_j}{B_j} = -\frac{Y_j(\sqrt{\nu_j}r_0)}{J_j(\sqrt{\nu_j}r_0)} = -\frac{Y_j(\sqrt{\nu_j}r_1)}{J_j(\sqrt{\nu_j}r_1)}. \tag{3.15}$$

This equation also imposes extra conditions on the energy ν_j which was arbitrary so far but now we have a set of discrete roots of (3.15) $\nu_j = \{\nu_{jk}\}_{k=0}^{\infty}$ for each j. It is evident that the energy is doubly degenerate for each index $j \geq 1$, for both $Ce^{+ij\varphi}$, $Ce^{-ij\varphi}$ give the same contribution. Assuming we have proper coefficient A_{jk}, B_{jk} and energies ν_{jk}, the wave functions in polar coordinates can be written:

$$\psi_{jk}(r,\varphi) = Ce^{\pm ij\varphi}\left(A_{jk}J_j(\sqrt{\nu_{jk}}r) + B_{jk}Y_j(\sqrt{\nu_{jk}}r)\right). \tag{3.16}$$

3.2 Circle

We have a circle described with radius R. The course of solution is very similar to the annulus and we will follow [8]. The only distinction is that there is no inner boundary, just $\psi(R,\varphi) = 0$. We noticed that the Bessel functions of second order Y_m converges to infinity when r approaches zero and thus the question arises whether Y_m belongs to the domain of the Dirichlet Laplacian, i.e. if it is quadratic integrable on the circle. We can check that it isn't and hence the normalized $\psi_{jk}(r,\varphi)$ looks

$$\psi_{jk}(r,\varphi) = \frac{1}{R\sqrt{\pi}J_{j+1}(R\sqrt{\mu_{jk}})}e^{\pm ij\varphi}J_j(\sqrt{\mu_{jk}}r) \tag{3.17}$$

where the energy μ_{jk} is the (k+1)-th root of the equation

$$J_j(R\sqrt{\mu}) = 0. \tag{3.18}$$

4 Wave function for the cone layer

In the part about the annulus we discovered that the wave functions of the annulus with infinitely high walls

$$\psi_{mj}(r,\varphi) = Ce^{\pm im\varphi}\left(A_{mj}J_m(\sqrt{\nu_{mj}}r) + B_{mj}Y_m(\sqrt{\nu_{mj}}r)\right). \tag{4.1}$$

depend on radii $r_0(z)$, $r_1(z)$ and the energies are discrete $\nu = \{\nu_{mj}\}_{m,j=0}^{\infty}$. Our goal is to find the smallest possible energies and we assume that these energies correspond to a wave function with fixed angular momentum $m = 0$. The decomposition in the area with annular cross-sections looks

$$\psi(r,z) = \sum_{j=0}^{\infty} f_j(z)\chi_j(r,z), \quad \chi_j(r,z) = A_j J_0(\sqrt{\nu_{0j}}r) + B_j Y_0(\sqrt{\nu_{0j}}r). \tag{4.2}$$

Substituting this Ansatz into the equation

$$-\triangle_D\psi = \left(-\frac{\partial^2}{\partial z^2} - \triangle_D^{annulus}\right)\psi = \epsilon\psi \tag{4.3}$$

and using $-\triangle_D^{annulus}\chi_j = \nu_j\chi_j$ we obtain

$$\sum_{j=0}^{\infty}\left(-f_j''(z)\chi_j(r,z) - 2f_j'(z)\chi_{j,z}(r,z) - f_j(z)\chi_{j,zz}(r,z)\right) - \\ - \sum_{j=0}^{\infty} f_j(z)\nu_j(z)\chi_j(r,z) = \epsilon\sum_{j=0}^{\infty} f_j(z)\chi_j(r,z). \tag{4.4}$$

Here we will use the orthogonality of $\chi_j(r,z)$ on the annulus: $\int_{r_0}^{r_1}\int_0^{2\pi} r\chi_j(r,z)\chi_k(r,z) = \delta_{jk}$, what is surely true because minus the Dirichlet

Laplacian is a self-adjoint operator with a discrete spectrum and therefore its eigenfunctions belonging to different eigenvalues are orthogonal. Apply $\int_{r_0}^{r_1}\int_0^{2\pi} r\chi_k(r,z)$ on the equation (4.4)

$$-f_k''(z) - \sum_{j=0}^{\infty}\Big[2f_j'(z)\Big(\chi_k(.,z),\chi_{j,z}(.,z)\Big) + f_j\Big(\chi_k(.,z),\chi_{j,zz}(.,z)\Big)\Big] + \\ + \nu_k f_k(z) = \epsilon f_k(z), \quad (4.5)$$

where $\Big(\chi_j(.,z),\chi_k(.,z)\Big)$ means $\int_{r_0}^{r_1}\int_0^{2\pi} r\chi_j(r,z)\chi_k(r,z)$. The equation can be rewritten into the form

$$-f_k''(z) - 2\sum_{j=0}^{\infty}\Big(\chi_k(.,z),\chi_{j,z}(.,z)\Big)f_j'(z) + \\ + \sum_{j=0}^{\infty}\Big[(\nu_j(z)-\epsilon)\delta_{jk} - \Big(\chi_k(.,z),\chi_{j,zz}(.,z)\Big)\Big]f_j(z) = 0 \qquad (4.6)$$

In the area of circle cross-sections the wave function can be similarly decomposed into the basis of eigenfunction of the circle and we can perform the same operations as above. The orthogonality for these eigenfunctions also holds, thus equation (4.6) is valid for all z in $(0,\infty)$.

5 Numerical solution

As was said before, our approach to the solution of Dirichlet Laplacian in the cone layer is to dismantle the wave function into the basis of transverse sections. Therefore we would like to know how these eigenfunctions look like. Energies $\{\nu_j(z)\}_{j=0}^{\infty}$ of the annulus can be enumerated as roots of the equation

$$-Y_0(\sqrt{\nu_j}r_0)J_0(\sqrt{\nu_j}r_1) + Y_0(\sqrt{\nu_j}r_1)J_0(\sqrt{\nu_j}r_0) = 0 \tag{5.1}$$

and unnormalized wave functions with zero z-component of the angular momentum can be written as

$$\psi_j = J_0(\sqrt{\nu_j}r) + C_j Y_0(\sqrt{\nu_j}r), \quad C_j = \frac{B_j}{A_j} = -\frac{J_0(\sqrt{\nu_j}r_0)}{Y_0(\sqrt{\nu_j}r_0)}. \tag{5.2}$$

These functions we want to derive because the first and second derivative according to z appears in the differential equations (4.6). These derivations are performed numerically by the formulas

$$\begin{aligned}\frac{\partial\psi_j(r,z)}{\partial z} &= \frac{\psi_j(r,z+h) - \psi(r,z-h)}{2h}\\ \frac{\partial^2\psi_j(r,z)}{\partial z^2} &= \frac{\psi_j(r,z+h) - 2\psi_j(r,z) + \psi_j(r,z-h)}{h^2},\end{aligned}$$

where h is a small positive number. As a next step we integrate $\psi_k\psi_{j,z}$ and $\psi_k\psi_{j,zz}$ on the annulus with the help of function QUAD8 in the program MATLAB. Equations (4.6) are of the second order but can be rewritten into the system of equations of the first order. When we define

$$\vec{\xi} = \begin{pmatrix} \vec{f} \\ \vec{g} \end{pmatrix}, \quad \vec{f} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \end{pmatrix}, \quad \vec{g} = \begin{pmatrix} f_1' \\ f_2' \\ f_3' \\ \vdots \end{pmatrix},$$

the equation in matrix notation looks

$$\vec{\xi} = \begin{pmatrix} 0 & 1 \\ B - C & -2A \end{pmatrix} \vec{\xi},$$

where $A(z)$, $B(z)$ and $C(z)$ are defined

$$A_{kj} = \Big(\chi_k(.,z), \chi_{j,z}(.,z)\Big), \quad C_{kj} = \Big(\chi_k(.,z), \chi_{j,zz}(.,z)\Big)$$

$$B = \begin{pmatrix} \nu_1 - \epsilon & 0 & 0 & \cdots \\ 0 & \nu_2 - \epsilon & 0 & \cdots \\ 0 & 0 & \nu_3 - \epsilon & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

On this system of equations we would use the function ODE45. We would integrate from some distant point z_0 with the initial conditions at z_0

$$\vec{f} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \quad \vec{g} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}$$

and we would demand that the longitudinal function vanish at the outer vertex. Unfortunately, the longitudinal functions behave at the inner vertex very badly, that is they have a great jump, and are not calculable by means of this method. This property is probably caused by the insufficiently smooth behavior of transversal energies as shown in the Fig. (5.1), so we had to find another procedure to enumerate the energies. Finite element method seemed to the be a suitable method and accordingly we used it.

The finite element method[10] is a numerical method which rephrases the original differential equation in its weak form and this weak form is discretized in a finite dimensional space, which is usually the space of piecewise functions. This approximating function can be resolved into a basis and the differential equation becomes a system of linear equations. No matter how extended the system is, the solution is very good accessible. As a basis we usually choose functions with small support and hence most of the base vectors are orthogonal and the matrix describing the system is sparse and hence easier invertible.

We have chosen the specialized program COMSOL MultiPhysics to perform our calculations on. After inputting proper parameters of the layer

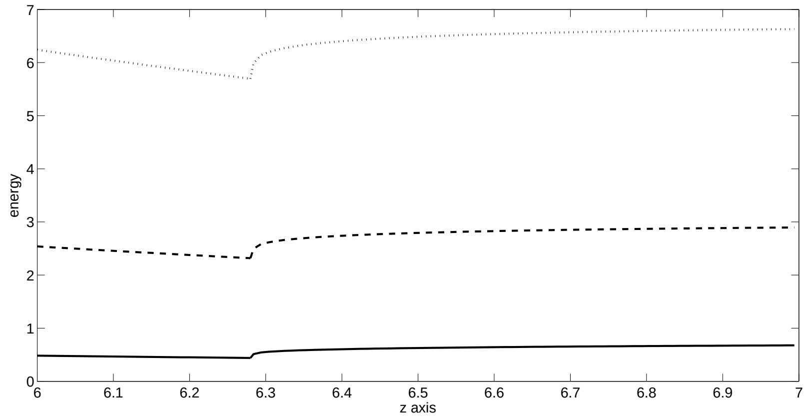

Figure 5.1: Energies of transversal modes for angle 30^o

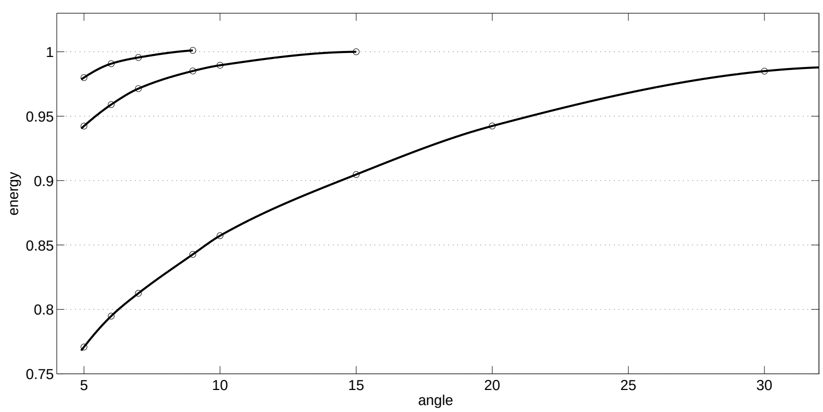

Figure 5.2: Energies of bound states depending on the angle

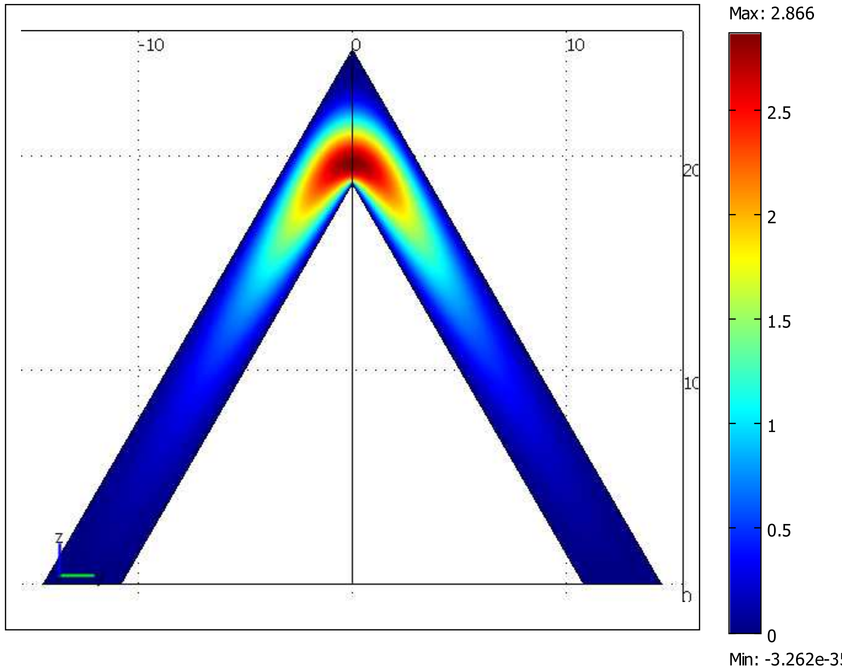

Figure 5.3: Wave function of the first bound state - slice

and accuracy we got energies shown in the Figure (5.2). As you can see the figure confirms all our theoretical conclusions. Energy of the first bound state seems to converge to the beginning of the essential spectrum when the angle φ approaches 90^o and the bound state always exists. In the area of small angles φ the number of bound states begins to increase, in the graph we have plotted only the first three. Figures (5.3) and (5.4) show how the wave function of the first bound state look like when the angle φ equals 30^o.

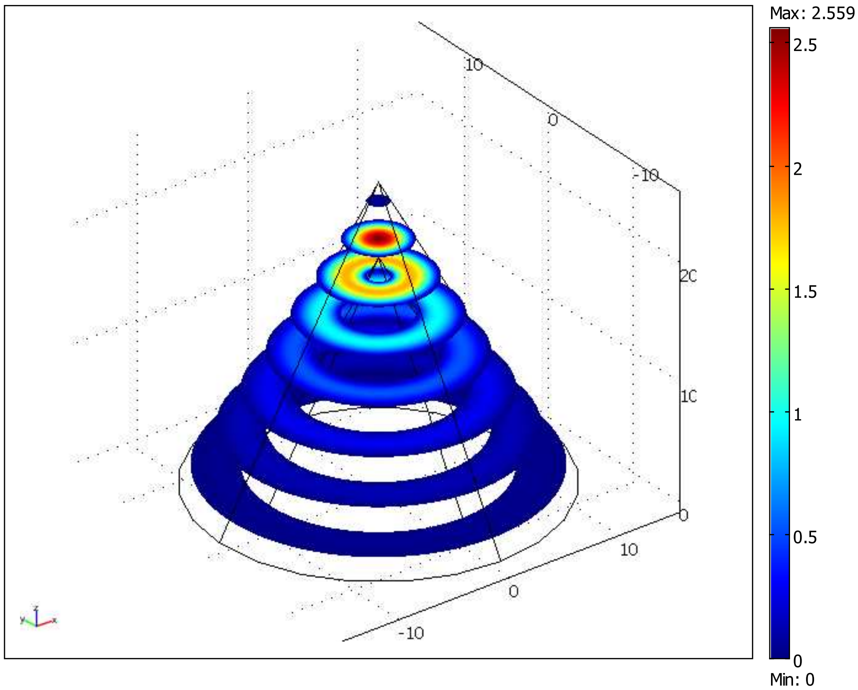

Figure 5.4: Wave function of the first bound state

6 Conclusion

Our main aim in this work was the study of geometrically induced bound states in a cone layer. We have theoretically surveyed the layer in Chapter 2 and with the help of previous papers we have proved the existence of at least one bound state for any cone. Besides we have found out an interesting property of the cone layer for small angles φ, which is the arbitrary number of bound states. In Chapters 3 and 4 we tried to transform the stationary Schrödinger equation into the system of differential equations of one variable. During the numerical solution an impassible problem occured in the form of the behavior of transverse functions f_i, which aren't analytical, so we were forced to use an alternative method of finite elements and the program COMSOL. Figure (5.2) shows the dependence of bound state energies on the angle φ and it is the chief result of this work because it contains all theoretical conclusions too.

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