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BOUND STATES OF A QUANTUM WAVEGUIDE WITH AN ARBITRARY SHAPED WINDOW

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Abstract. In this paper we prove the existence of isolated eigenvalues of finite multiplicity below the essential spectrum of a straight waveguide with a curved potential window in the three dimensional space. We give also some asymptotic results for these eigenvalues and their counting function. We illustrate our results by some numerical computations.

1. Introduction. The motion of an electron confined to a quantum waveguide is described by the Hamiltonian corresponding to the Schrödinger equation. If we consider a non-interacting electron then the associated operator is the free Laplacian with some boundary conditions. The physical properties of this system, namely the existence of localized states, can be described by the spectral properties of the operator $-\Delta$ acting on some Hilbert space and subject to some boundary conditions.

In this paper we focus on the Hamiltonian of a free quantum particle moving in a non trivial subset Ω of the three dimensional space $\mathbb{R}^3$. The considered set is $\Omega = \mathbb{R}^2 \times [0, d]$, where $d > 0$ is the width of the waveguide. We suppose

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that the waveguide has an opened window K on one of its two sides $\mathbb{R}^2 \times \{0\}$ or $\mathbb{R}^2 \times \{d\}$. The set K is a potential window and we take it a compact connected subset of $\mathbb{R}^2$ and we make only the condition that its boundary is a piecewise C^1 curve in $\mathbb{R}^2$. So it has an arbitrary shape.

The spectral properties of quantum waveguides coupled through potential windows was considered in a large set of papers. The main aim is to prove the existence of localized states, resonant states and embedded eigenvalues. Many situations were considered, depending namely on the geometry of the waveguide (see [13, 7, 12, 5, 11]), on the form of the windows (see [3, 2, 14, 16])and on the boundary conditions (see [8, 9, 1]).

The problem of a three dimensional quantum waveguide with a window was studied in the case of a circular one, so K is a disc, see [12]. In that paper, the authors proved the existence of localized states below the essential spectrum. Our aim here is to give a similar result for a general shape of the potential window K. Namely we prove that for the operator $-\Delta$ with Dirichlet conditions on one side of the waveguide and Neumann conditions on the boundary of the window, there exist isolated eigenvalues of finite multiplicities below the essential spectrum. We prove also that the counting function of these eigenvalues has an asymptotic expansion with respect to the waveguide width. As a consequence, we find that for d small enough, there exist only one localized state.

In the last section, we consider the case of a square window and construct approximate eigenfunctions associated to an isolated eigenvalue. The result can be used for numerical computation in order to illustrate the theoretical results given in the previous sections.

The paper is organized as follows: In the first section, the problem is stated. The second section is devoted to main results. In the third section, we prove the theorem on the existence of bound states. In the fourth section, we give the asymptotics of the number of eigenvalues and in the last section we compute the approximate eigenfunctions by the mode matching technique.

2. Notations and main results. In the three dimensional space $\mathbb{R}^3$, we consider the domain $\Omega = \mathbb{R}^2 \times [0, d]$ where d is a positive number. The domain Ω stands for the waveguide of a free quantum particle. Let K be a compact connected submanifold of $\mathbb{R}^2$ with boundary γ. We suppose that γ is a piecewise C^1 curve in $\mathbb{R}^2$. The set K stands for the curved potential window. See Figure 1.

Now let $\Gamma = \partial\Omega \setminus K$. The Hamiltonian of the free quantum particle confined to the waveguide is constructed by means of quadratic forms in the

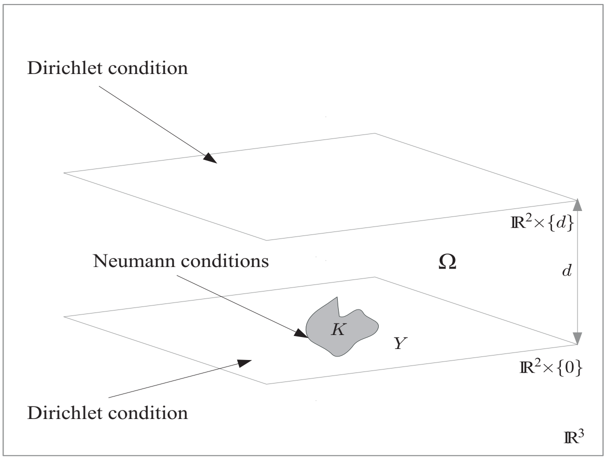

Fig. 1. The waveguide and the curved window

following way. We consider the quadratic form

$$q_0(f,g) = \int_\Omega \nabla f.\overline{\nabla g} dxdydz$$

with domain

$$Q(q_0) = \{f \in H^1(\Omega); f_{\lceil\Gamma} = 0\}.$$

The space $H^1(\Omega)$ is the classical Sobolev space. The form q_0 is symmetric, positive and closed with a dense domain. So there is an associated self adjoint operator H which has the domain

$$D(\Omega) = \left\{ f \in H^1(\Omega); -\Delta f \in L^2(\Omega), f_{\lceil\Gamma} = 0, \frac{\partial f}{\partial n}_{\lceil K} = 0 \right\}.$$

The operator H acts as $Hf = -\Delta f$, for all $f \in D(\Omega)$.
If we denote by H_0 the operator H in the case of a closed potential window, that is $K = \emptyset$, we may consider H as a compact perturbation of H_0. Therefore, the essential spectrum of H coincides with the one for H_0. It is not difficult to see that H_0 decomposes as

$$H_0 = (-\Delta_{\mathbb{R}^2} \otimes I)) \oplus \left(I \otimes (-\Delta_{[0,d]})\right)$$

on the space $L^2(\mathbb{R}^2) \otimes L^2([0,d])$. This may be used to compute the spectrum of H_0 and it is a straightforward calculus that gives

$$\sigma(H_0) = \sigma_{ess}(H_0) = \left[\left(\frac{\pi}{d}\right)^2, +\infty \right[.$$

We are firstly interested in the existence of isolated eigenvalues of finite multiplicity below the essential spectrum. So these eigenvalues will be smaller than the threshold $\left(\frac{\pi}{d}\right)^2$. The main idea is to approximate the compact K by two particular sets, a disc contained in K and a square containing K. Let a be a positive number and consider the square

$$C(a) = \{(x, y, 0); |x| \leq a, |y| \leq a\}.$$

We assume that $K \subset C(a)$, so $C(a)$ may be viewed as a squared potential window larger than K.
We also suppose that there exists $\eta > 0$ such that the disc

$$D(\eta a) = \{(x, y, 0); x^2 + y^2 < (\eta a)^2\}$$

is contained in K. This is also a potential window smaller than K with has a circular shape. The Figure 2 illustrates this configuration.

The curved window K is therefore switched between two particular potential windows: the square $C(a)$ and the disc $D(\eta a)$, so

$$D(\eta a) \subset K \subset C(a).$$

The first result is the following.

Theorem 1. *For all $a > 0$ as above and $d > 0$, the operator H has at least one isolated eigenvalue of finite multiplicity in the interval* $\left[\frac{\pi^2}{(2d)^2}, \frac{\pi^2}{d^2}\right]$.

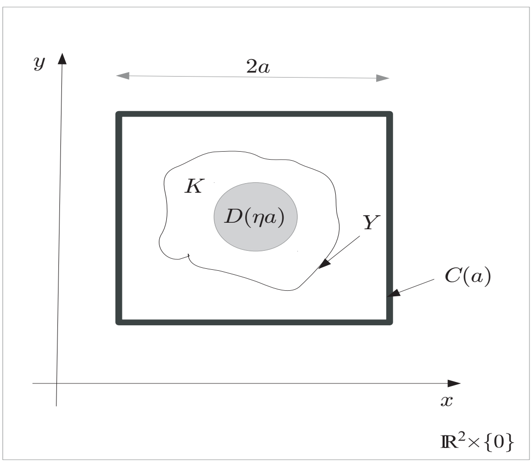

Fig. 2. The curved window switched between a disc and a square

Next we look for the number of the eigenvalues given in the previous theorem.

Theorem 2. *For $\frac{a}{d}$ large enough, the number $N(a,d)$ of eigenvalues of H below its essential spectrum has the following asymptotics:*

$$N(a,d) = \frac{3\pi}{16}\frac{a^2}{d^2} + O\left(\frac{a}{d}\right).$$

Theorem 3. *For fixed $d > 0$, there exists $a^* > 0$ such that for all $a \leq a^*$, the operator H has exactly one isolated eigenvalue less than $\frac{\pi^2}{d^2}$.*

And as a consequence of this theorem we have the following:

Corollary 1. *Let $\delta(K) = \sup_{x,y\in K} \|x-y\|$ be the diameter of K. For fixed d, there exists $a^* > 0$ such that if $\delta(K) < a^*$, the operator H has exactly one isolated eigenvalue less than $\frac{\pi^2}{d^2}$.*

3. Existence of bounded states eigenvalues. To prove that the operator H has bounded states (Theorem 1) the main idea is based on the construction of a test function φ having the following property

$$q(\varphi) := q_0(\varphi) - \frac{\pi^2}{d^2}\|\varphi\|_2^2 < 0. \tag{1}$$

We recall that $\|.\|_2$ is the L^2 norm of φ and $q_0(\varphi) = \|\nabla\varphi\|_2^2$.

The proof may be done in two steps. Firstly let χ be the transverse mode defined by:

$$\chi(z) = \begin{cases} \sqrt{\frac{2}{d}}\sin\left(\frac{\pi}{d}z\right) & \text{if} \quad z \in (0,d) \\ 0 & \text{if} \quad z \notin (0,d) \end{cases}$$

It's clear that $\|\chi\|_2 = 1$.

We consider a function φ in the Schwartz space $\mathcal{S}(\mathbb{R})$ and we put

$$\Phi(x,y,z) = \varphi(x^2+y^2)\chi(z), \quad \text{for} \quad (x,y,z) \in \mathbb{R}^3.$$

Lemma 1. *For the function Φ defined as above we have*

$$q(\Phi) = 4\pi\|\varphi'\|_{L^2([0,+\infty[,sds)}.$$

Proof. Let's compute the quadratic form q_0 for Φ.

$$\begin{aligned}
q_0(\Phi) &= \iiint_{\mathbb{R}^3} \nabla\Phi(x,y,z)\overline{\nabla\Phi}(x,y,z)dxdydz \\
&= \iiint_{\mathbb{R}^3} \left[4(x^2+y^2)(\varphi'(x^2+y^2))^2\chi^2(z) + (\varphi(x^2+y^2))^2|\chi'(z)|^2\right] dxdydz \\
&= \iint_{\mathbb{R}^2} \left(4(x^2+y^2)(\varphi'(x^2+y^2))^2 dxdy\right) \int_{\mathbb{R}} \chi^2(z)dz + \\
&+ \iint_{\mathbb{R}^2} (\varphi(x^2+y^2))^2 dxdy \int_{\mathbb{R}} |\chi'(z)|^2 dz \\
&= 2\pi \int_0^{+\infty} 4r^2(\varphi'(r^2))^2 rdr + 2\pi \int_0^{+\infty} (\varphi(r^2))^2 rdr.\frac{\pi^2}{d^2} \\
&= 8\pi \int_0^{+\infty} r^3(\varphi'(r^2))^2 dr + \frac{2\pi^3}{d^2}\int_0^{+\infty} (\varphi(r^2))^2 rdr.
\end{aligned}$$

We make the change of variable $s = r^2$ in the last two integrals so we get

$$q_0(\Phi) = 4\pi\|\varphi'\|^2_{L^2([0,+\infty[,sds)} + \frac{\pi^3}{d^2}\|\varphi\|^2_{L^2([0,+\infty[,ds)}. \tag{2}$$

Now, let's compute $q(\Phi)$.

$$\begin{aligned}
\|\Phi\|^2_{L^2(\mathbb{R}^3)} &= \int_{R^3} |\Phi(x,y,z)|^2 dxdydz \\
&= \iiint_{\mathbb{R}^3} \left|\varphi(x^2+y^2)\right|^2 \chi^2(z)dxdydz \\
&= \iint_{\mathbb{R}^2} \left|\varphi(x^2+y^2)\right|^2 dxdy \\
&= 2\pi \int_0^{+\infty} \varphi^2(r^2) rdr \\
&= \pi \int_0^{+\infty} \varphi^2(s)ds = \pi\|\varphi\|^2_{L^2([0,+\infty[,ds)}.
\end{aligned}$$

If we substitute the last identity into $q(\Phi)$ we obtain

$$\begin{aligned}
q(\Phi) &= 4\pi\|\varphi'\|_{L^2([0,+\infty[,sds)} + \frac{\pi^3}{d^2}\|\varphi\|^2_{L^2([0,+\infty[,ds)} - \frac{\pi^2}{d^2}\pi\|\varphi\|^2_{L^2[0,+\infty[)} \\
&= 4\pi\|\varphi'\|_{L^2([0,+\infty[,sds)}.
\end{aligned}$$

□

The next step in the proof is the following approximation. Recall that a is the length of the squared window in the waveguide. We take a number $b > \sqrt{2}a$ and choose $\varphi \in \mathcal{S}(\mathbb{R})$ such that $\varphi = 1$ on $[0,b]$. For $z > 0$, we put

$$\varphi_z(s) = \begin{cases} \varphi(s) & \text{if} \quad s < b \\ \varphi(b + z(Log(s) - Log(b))) & \text{otherwise.} \end{cases}$$

It's clear that $\varphi_z \in \mathcal{S}(\mathbb{R})\ \ \forall z > 0$. Indeed, we have

$$\begin{aligned}
\|\varphi_z'\|^2_{L^2([0,+\infty[,sds)} &= \int_b^{+\infty} \frac{z^2}{s^2}\left|\varphi'(b+z(Log(s)-Log(b)))\right|^2 sds \\
&= \int_b^{+\infty} \frac{z^2}{s^2}\left|\varphi'(t)\right|^2 \frac{s^2}{z}dt \\
&= z\int_b^{+\infty} \left|\varphi'(t)\right|^2 dt \\
&= z\|\varphi'\|_{L^2([0,+\infty[,dt)}.
\end{aligned}$$

We are now ready to construct a function $\Phi_{z,\varepsilon}$ that satisfies (1). We let $\varepsilon > 0$, choose a localization function $j \in C_0^\infty((0,a))$ and define

$$\Phi_{z,\varepsilon}(x,y,z) = \varphi_z(x^2+y^2)\chi(z) + \varepsilon j^2(x^2+y^2)\varphi_z(x^2+y^2)\chi(z).$$

This function belongs to the form domain Q_0. Precisely, we have

$$\Phi_{z,\varepsilon} \in \left\{f \in L^2(\Omega); \nabla f \in L^2(\Omega), f_{\lceil\Gamma} = 0\right\}.$$

$\Phi_{z,\varepsilon}$ naturally decomposes as

$$\Phi_{z,\varepsilon} = \chi\varphi_1 + \varepsilon\chi\varphi_2$$

where $\varphi_1 = \varphi_z$ and $\varphi_2 = j^2\varphi_z$.

Let's compute $q(\Phi_{\varepsilon,z})$.

$$\begin{aligned}
q(\Phi_{\varepsilon,z}) &= q(\chi\varphi_1) + \varepsilon^2 q(\chi\varphi_2) + 2\varepsilon\int_{\mathbb{R}^3}\nabla(\chi\varphi_1)\nabla(\chi\varphi_2)dxdydz - \frac{2\pi^2}{d^2}\varepsilon\langle\chi\varphi_1|\chi\varphi_2\rangle \\
&= 4\pi z\|\varphi'\|_{L^2([0,+\infty[)} + 4\pi\varepsilon^2\|2jj'\|_2^2 - \frac{2\pi^2}{d^2}\varepsilon\pi\|j^2\|_{L^2([0,+\infty[)} \\
&= 4\pi z\|\varphi'\|_{L^2([0,+\infty[)} + 16\pi\varepsilon^2\|jj'\|_2^2 - \frac{2\pi^3}{d^2}\varepsilon\|j^2\|_{L^2([0,+\infty[)}.
\end{aligned}$$

The last two terms are independent of z. Moreover, the term linear in ε is negative. So choosing ε small enough, this term will dominate the quadratic one in the sum. We fix ε equal to the corresponding value and choose z sufficiently small to make the right hand side of the last equality negative.

This ends the proof of Theorem 1.

4. Asymptotics of the counting function. In this paragraph, we are interested in the number of isolated eigenvalues created below the threshold $\frac{\pi^2}{d^2}$ of the essential spectrum . We use the Dirichlet-Neumann bracketing technique (as used in [2, 11, 13]) and we focus on the situation when the window is of a squared shape. We cut the domain Ω into two subdomains Ω^+ and $\Omega^- = \Omega \backslash \Omega^+$ where

$$\Omega^+ = \{(x, y, z) \in \Omega; |x| \leq a, |y| \leq a\}.$$

By putting Dirichlet or Neumann boundary conditions on the boundary of Ω^+ we get two new operators $H^{(N)}$ and $H^{(D)}$. These operators decompose in the following way:

$$H^{(N)} = H_t^{(N)} \oplus H_l^{(N)} \quad \text{and} \quad H^{(D)} = H_t^{(D)} \oplus H_l^{(D)}.$$

The subscripts t and l refer to transversal and longitudinal decomposition of the waveguide. Indeed, the operator H satisfies

$$H_t^{(N)} \oplus H_l^{(N)} \leq H \leq H_t^{(D)} \oplus H_l^{(D)}$$

in the sense of quadratic forms. The eigenvalues of H below the essential spectrum are squeezed between those of $H_l^{(D)}$. The operator $H_l^{(D)}$ has the following sequence of eigenvalues

$$\text{(3)} \qquad \lambda_{n,p,k}^{(H_l^{(D)})} = \left(\left(\frac{n}{a}\right)^2 + \left(\frac{p}{a}\right)^2 + \left(\frac{2k+1}{2d}\right)^2 \right) \pi^2, \quad \text{for } n, p \in \mathbb{N}^*, k \in \mathbb{N},$$

with the corresponding eigenfunctions

$$f_{n,p,k}^{(H_l^{(D)})}(x, y, z) = \sin\left(\frac{n\pi}{a}x\right) \sin\left(\frac{p\pi}{a}y\right) \cos\left(\frac{2k+1}{2d}\pi z\right).$$

The essential spectrum of H is the interval $[\left(\frac{\pi}{d}\right)^2, +\infty[$. We can approximate the number of isolated eigenvalues of H by the number N_D of eigenvalues of $H_l^{(D)}$ less than $\frac{\pi^2}{d^2}$. So we have to compute the number of $(n, p, k) \in (\mathbb{N}^*)^2 \times \mathbb{N}$ such that

$$\lambda_{n,p,k}^{(H_l^{(D)})} < \frac{\pi^2}{d^2}.$$

Using the explicit form of $\lambda_{n,p,k}^{(K)}$ given in (3), the last condition yields

$$\frac{n^2}{a^2} + \frac{p^2}{a^2} + \left(\frac{2k+1}{2d}\right)^2 < \frac{1}{d^2}.$$

This can be fulfilled only for $k = 0$.
We find therefore the following condition on (n, p)

$$\frac{n^2}{a^2} + \frac{p^2}{a^2} < \frac{3}{4d^2}.$$

The last may be written in the form

$$n^2 + p^2 < \left(\frac{\sqrt{3}}{2}\frac{a}{d}\right)^2. \tag{4}$$

Lemma 2. *Let $\alpha > 0$ be a constant and $A(\alpha)$ be the cardinal of the following set*

$$\left\{(n,p) \in \mathbb{N}^* \times \mathbb{N}^*; n^2 + p^2 < \alpha^2\right\}.$$

Then for α large enough we have

$$A(\alpha) = \frac{\pi}{4}\alpha^2 + O(\alpha).$$

Using the Weyl formula, yields

$$N_D = \frac{3\pi}{16}\frac{a^2}{d^2} + O(\frac{a}{d}).$$

This ends the proof of Theorem 2.

Proof of Lemma 2. For $\alpha > 0$, let's consider the number

$$B(\alpha) = \#\left\{(m,n) \in \mathbb{N} \times \mathbb{N}; n^2 + m^2 \le \alpha^2\right\}.$$

This counts the number of points of integer coordinates contained in the region

$$D = \left\{(x,y) \in \mathbb{R}^2; x \ge 0, y \ge 0, x^2 + y^2 \le \alpha^2\right\}.$$

We associate to each point M of D with integer coordinates the square of area 1 for which M is the left bottom extremity. Let $\mathcal{S}$ be the union of all these squares. The area of $\mathcal{S}$ is equal to $B(\alpha)$ and we have

$$\frac{\pi\alpha^2}{4} \le B(\alpha)$$

because $D \subset \mathcal{S}$ and the surface area of the set D is $\dfrac{\pi\alpha^2}{4}$.

We would like to have a more precise estimate for $B(\alpha)$. We denote by $\mathcal{T}$ the family of squares contained in D and such that the circle $\mathcal{C}$ centered at $(0,0)$ and with radius α passes through them. Let $R(\alpha)$ be the number of these squares. The set $\mathcal{S} \setminus \mathcal{T}$ is contained in D and its surface area is equal to $B(\alpha) - R(\alpha)$. So we have

$$B(\alpha) - R(\alpha) \le \frac{\pi\alpha^2}{4} \le B(\alpha). \tag{5}$$

Let's find asymptotics of $R(\alpha)$ for large α. The surface area of $\mathcal{T}$ is $R(\alpha)$. If we exclude from $T\mathcal{T}$ the two elementary squares which have common sides with the (Ox) and (Oy) axis, then we obtain a set $\mathcal{T}'$ whose surface area is equal to $\mathcal{A}(\mathcal{T}') = R(\alpha) - 2$. According to Figure 3 we denote by $S_0, \ldots, S_{k+1}$ the elements of T numbered from the left to the right and by $A_0, \ldots, A_{k+2}$ the points defined by

$$A_0 = \mathcal{C} \cap (Oy), \quad A_{k+2} = \mathcal{C} \cap (Ox), \quad A_j = \mathcal{C} \cap S_{j-1} \cap S_j \quad \text{for} \quad j = 1, \ldots, k.$$

For $j = 1, \ldots, k$, the surface area of the square S_j is less than the arc length $\widehat{A_{j-1}A_{j+1}}$. Thus we have

$$R(\alpha) - 2 \leq \sum_{j=1}^{k} \widehat{A_{j-1}A_{j+1}}. \tag{6}$$

Furthermore,

$$\begin{aligned} \sum_{j=1}^{k} \widehat{A_{j-1}A_{j+1}} &= \sum_{j=1}^{k} \widehat{A_{j-1}A_j} + \widehat{A_jA_{j+1}} \\ &= \sum_{j=0}^{k-1} \widehat{A_jA_{j+1}} + \sum_{j=1}^{k} \widehat{A_jA_{j+1}} \end{aligned}$$

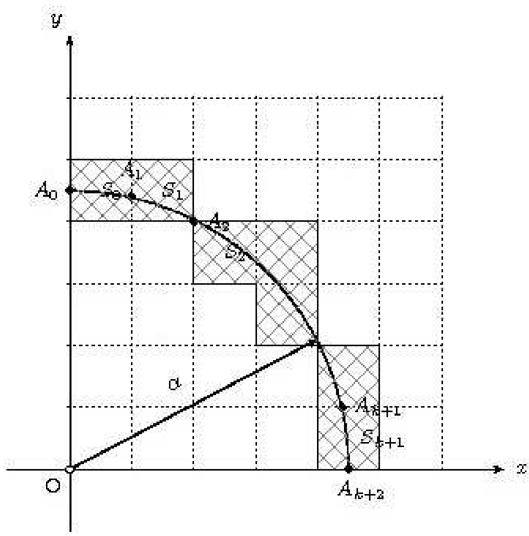

Fig. 3. Squares of integer coordinates

$$\leq \ 2\sum_{k=0}^{k+1}\widehat{A_jA_{j+1}}.$$

Indeed, the circle is of radius α, so $\displaystyle\sum_{j=0}^{k+1}\widehat{A_jA_{j+1}} = \frac{2\pi\alpha}{4} = \frac{\pi\alpha}{2}$.

The equation (6) writes then as

$$R(\alpha) \leq \pi\alpha + 2,$$

and the relation (5) gives

$$\frac{\pi}{4} \leq \frac{B(\alpha)}{\alpha^2} \leq \frac{\pi}{4} + \frac{R(\alpha)}{\alpha^2}.$$

Thus we have the asymptotics

$$\lim_{\alpha\to+\infty}\frac{B(\alpha)}{\alpha^2} = \frac{\pi}{4}$$

and

$$B(\alpha) = \frac{\pi}{4}\alpha^2 + O(\alpha)$$

for α large. To end the proof, we have just to remark that $B(\alpha) - A(\alpha) \leq 2\alpha$. $\square$

5. Approximate eigenfunctions. We give in this section some computations of approximate eigenfunctions. The results may be used to make numerical illustration of the theoretical results given in the previous sections. The operator H has its essential spectrum starting at $\dfrac{\pi^2}{d^2}$ and its whole spectrum is contained in the infinite interval $\left[\dfrac{\pi^2}{4d^2}, +\infty\right[$. So we look for eigenvalues of the form $\lambda(\varepsilon) = \varepsilon\dfrac{\pi^2}{d^2}$ where $\dfrac{1}{4} < \varepsilon < 1$.

For ε fixed, we calculate an approximate eigenfunction Ψ_ε associated to the eigenvalue $\lambda(\varepsilon)$ using the mode matching technique. For this end, we decompose the domain of the waveguide into different regions (subdomains) and we compute the corresponding approximate eigenfunction in each region. After that, we write the continuity conditions for the eigenfunction and its derivatives on the lines separating the different subdomains of the waveguide. By the mode matching technique we get a global approximate eigenfunction. For symmetry reasons, the computation will be made only in some particular regions. We restrict ourselves firstly to the quadrant $W = \left\{(x, y, z) \in \mathbb{R}^3; x > 0, y > 0, 0 \leq z \leq d\right\}$ and let's decompose W into the following three regions:

Region I: this is the region $D_I = W \cap \{(x,y,z) \in \mathbb{R}^3; x > a, y > a\}$. In this part of the waveguide we have Dirichlet boundary conditions everywhere. So we consider the transverse modes:

$$\alpha_k(z) = \begin{cases} \sqrt{\frac{2}{d}} \sin\left(\frac{k\pi}{d} z\right) & z \in [0,d] \\ 0 & \text{otherwise} \end{cases}, k \in \mathbb{N}^*$$

We look for an eigenfunction Ψ_I that decomposes into the previous transverse modes in the following way:

$$\Psi_I = \sum_{k\geq 1} \Psi_I^k \quad \text{with} \quad \Psi_I^k(x,y,z) = \varphi(x)\psi(y)\alpha_k(z).$$

If we write the eigenvalue equation $-\Delta\Psi_I = \lambda(\varepsilon)\Psi_I$, then we lead to the relation

$$\frac{\varphi''(x)}{\varphi(x)} + \frac{\psi''(y)}{\psi(y)} = (k^2 - \varepsilon)\frac{\pi^2}{d^2}, \text{ for all } x > a, y > a.$$

By the variable separation method, we know that there exists a constant $\lambda \in \mathbb{R}$ such that

$$\frac{\varphi''(x)}{\varphi(x)} = \frac{\psi''(y)}{\psi(y)} = \lambda, \text{ for all } x > a, y > a.$$

By identification we have $\lambda = (k^2 - \varepsilon)\frac{\pi^2}{2d^2}$. Let's put $\omega_k = \sqrt{(k^2 - \varepsilon)\frac{\pi^2}{d^2}}$ and recall that we look for eigenfunctions that belong to $L^2(\mathbb{R}^3)$. Therefore, we get the following solutions for ψ and φ:

$$\varphi(x) = A_k.e^{-\frac{\omega_k}{\sqrt{2}}(a-x)}, \quad \psi(y) = B_k.e^{-\frac{\omega_k}{\sqrt{2}}(a-y)}, \text{ where } A_k, B_k \text{ are constants.}$$

Then, the approximate solution Ψ_I in the subdomain D_I has the following expansion:

$$\Psi_I(x,y,z) = \sum_{k\geq 1} a_k e^{\frac{\omega_k}{\sqrt{2}}(a-x)} e^{\frac{\omega_k}{\sqrt{2}}(a-y)} \alpha_k(z), \quad \text{where} \quad a_k \quad \text{are constants.}$$

Region II: $D_I = W \cap \{(x,y,z) \in \mathbb{R}^3; 0 \leq x \leq a, 0 \leq y \leq a\}$. The transverse modes to take in this region are the functions

$$\beta_k(z) = \begin{cases} \sqrt{\frac{2}{d}} \sin\left(\frac{(2k-1)(d-z)\pi}{2d}\right) & z \in [0,d] \\ 0 & \text{otherwise} \end{cases}$$

which satisfy Dirichlet boundary conditions on the sides $\{z = 0\}$ and $\{z = d\}$ of the waveguide. We look again for an ansatz in the form $\Psi_{II}(x,y,z) =$

$\varphi(x)\psi(y)\beta_k(z)$ and satisfies $-\Delta\Psi_{II} = \lambda(\varepsilon)\Psi_{II}$. If we set $\widetilde{\omega_k} = \frac{\pi}{d}\sqrt{(k-\frac{1}{2})^2 - \varepsilon}$, then $\varphi(x)\psi(y)$ has to be a linear combination of one kind of the following functions:

$$\cosh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}x\right)\cosh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}y\right); \quad \sinh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}x\right)\sinh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}y\right);$$

$$\sinh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}x\right)\cosh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}y\right); \cosh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}x\right)\sinh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}y\right).$$

This depends on wether we take symmetric or antisymmetric solutions. Thus, the eigenfunction Ψ_{II} has one of the following expansion into the transverse modes β_k:

$$\Psi_{II}(x,y,z) = \sum_{k\geq 1} b_k \frac{\cosh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}x\right)}{\cosh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}a\right)}\frac{\cosh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}y\right)}{\cosh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}a\right)}\beta_k(z)$$

or

$$\Psi_{II}(x,y,z) = \sum_{k\geq 1} b_k \frac{\sinh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}x\right)}{\sinh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}a\right)}\frac{\sinh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}y\right)}{\sinh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}a\right)}\beta_k(z)$$

or

$$\Psi_{II}(x,y,z) = \sum_{k\geq 1} b_k \frac{\cosh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}x\right)}{\cosh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}a\right)}\frac{\sinh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}y\right)}{\sinh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}a\right)}\beta_k(z)$$

or

$$\Psi_{II}(x,y,z) = \sum_{k\geq 1} b_k \frac{\sinh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}x\right)}{\sinh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}a\right)}\frac{\cosh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}y\right)}{\cosh\left(\frac{\widetilde{\omega_k}}{\sqrt{2}}a\right)}\beta_k(z)$$

where b_k are constants.

Region III: this is the region $D_{III} = W \cap \{(x,y,z) \in \mathbb{R}^3;\ 0 \leq x \leq a,\ y > a\}$. The transverse modes are α_k and the solution takes the form

$$\sum_{k\geq 1}\Psi_{III}(x,y,z) = \sum_{k\geq 1} c_k e^{\frac{\omega_k}{\sqrt{2}}(a-y)}\varphi_{III}(y)\alpha_k(z)$$

where c_k are constants and φ_{III} is one the functions $\cosh\left(\frac{\omega_k}{\sqrt{2}}x\right)$ or $\sinh\left(\frac{\omega_k}{\sqrt{2}}x\right)$, here is again depending on symmetric or antisymmetric case.

Now let's use the mode matching technique to construct a global approximate eigenfunction. The condition for bound states is obtained by matching the approximate wave functions and their normal derivatives at the boundaries between regions. We have to write the continuity conditions for the functions Ψ_I, Ψ_{II} and Ψ_{III} and their derivatives on the boundries of the three regions I, II and III.

1) On the boundary between Region I and Region II, and taking $x = a$, we get

$$\sum_{k\geq 0} c_k e^{\frac{\omega_k}{\sqrt{2}}(a-y)}\alpha_k(z) = \sum_{k\geq 0} a_k e^{\frac{\omega_k}{\sqrt{2}}(a-y)}\alpha_k(z), \quad \forall y > a, \ 0 \leq z \leq d.$$

This gives $c_k = a_k$ for all $k \geq 0$.

2) On the boundary between Region II and Region III, and taking $x = a, y = a$, we get

$$\sum_{k\geq 0} a_k\alpha_k(z) = \sum_{k\geq 0} b_k\beta_k(z).$$

Let $j \geq 1$. Taking the scalar product of the previous terms with α_j gives

$$a_j = \sum_k b_k\langle\beta_k|\alpha_j\rangle \tag{7}$$

where

$$\langle\beta_k|\alpha_j\rangle = \frac{(-1)^{k-1}}{\pi}\frac{8j}{4j^2-(2k-1)^2}.$$

Now, let's write the continuity conditions for the derivatives. The derivative of the wavefunction with respect to y has to be continous at the points $(x = a, y = a, z)$. So

$$\frac{\partial\Psi_{II}}{\partial y}(a, a, z) = \frac{\partial\Psi_{III}}{\partial y}(a, a, z)$$

may be written as

$$-\sum_k a_k\frac{\omega_k}{\sqrt{2}}e^{\frac{\omega_k}{\sqrt{2}}(a-y)}\varphi_{III}(x)\alpha_k(z) = \sum_k a_k\frac{\widetilde{\omega_k}}{\sqrt{2}}\psi'_{II}(y)\varphi_{III}(x)\beta_k(z).$$

Therefore, for $x = a, y = a$ we have

$$-\sum_k a_k\omega_k\alpha_k(z) = \sum_k b_k\tanh^{\pm 1}\left(\widetilde{\omega_k}a\right)\beta_k(z).$$

Taking the scalar product by α_j, for $j \geq 1$ fixed, we get

$$a_j\omega_j + \sum_k b_k \tanh^{\pm 1}(\widetilde{\omega_k} a) < \beta_k|\alpha_j >= 0. \tag{8}$$

Substituting (7) into (8), we can write the equation (8) as an infinite system of linear equations like $Ca = 0$ with

$$a = (a_j)_j \quad \text{and} \quad C_{jk} = \left(\omega_j + \widetilde{\omega_k} \tanh^{\pm 1}(\widetilde{\omega_k} a)\right) < \beta_k(z)|\alpha_j > .$$

This can be solved numerically using the techniques given in [8] and [5]. The bound states are obtained by truncating the resulting expansions and solving the matrix equation. The condition for the bound state is $det(C) = 0$.

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