On the spectrum of the Schrodinger Operator with Aharonov-Bohm Magnetic Field in quantum waveguide with Neumann window

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Abstract

In a previous study [5] we investigate the bound states of the Hamiltonian describing a quantum particle living on three dimensional straight strip of width d. We impose the Neumann boundary condition on a disc window of radius a and Dirichlet boundary conditions on the remained part of the boundary of the strip. We proved that such system exhibits discrete eigenvalues below the essential spectrum for any $a > 0$. In the present work we study the effect of a magnetic filed of Aharonov-Bohm type when the magnetic field is turned on this system. Precisely we prove that in the presence of such magnetic filed there is some critical values of $a_0 > 0$, for which we have absence of the discrete spectrum for $0 < \frac{a}{d} < a_0$. We give a sufficient condition for the existence of discrete eigenvalues.

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1 Itroduction

The task of finding eigenenergies E_n and corresponding eigenfunctions $f_n(\mathbf{r})$, $n = 1, 2, ...$ of the Laplacian in the two- (2D) and three-dimensional (3D) domain Ω with mixed Dirichlet

$$f_n(\mathbf{r})|_{\partial\Omega_D} = 0 \tag{1.1}$$

and Neumann

$$\mathbf{n}\nabla f_n(\mathbf{r})|_{\partial\Omega_N} = 0, \tag{1.2}$$

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boundary conditions on its confining surface (for 3D) or line (for 2D) $\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$ ($\mathbf{n}$ is a unit normal vector to $\partial\Omega$) [9, 23, 35, 40, 47, 53] is commonly referred to as Zaremba problem [58], it is a known mathematical problem science. Apart from the purely mathematical interest, an analysis of such solutions is of a large practical significance as they describe miscellaneous physical systems. For example, the temperature T of the solid ball floating in the icewater obeys the Neumann condition on the part of the boundary which is in the air while the underwater section of the body imposes on T the Dirichlet demand [23]. Mixed boundary conditions were applied for the study of the spectral properties of the quantized barrier billiards and of the ray splitting in a variety of physical situations. The problem of the Neumann disc in the Dirichlet plane emerges naturally in electrostatics [34]. In the limit of the vanishing Dirichlet part of the border the reciprocal of the first eigenvalue describes the mean first passage time of Brownian motion to $\partial\Omega_D$. In cellular biology, the study of the diffusive motion of ions or molecules in neurobiological microstructures essentially employs the combination of these two types of the boundary coniditons on the different parts of the confinement [33].

One class of Zaremba geometries that recently received a lot of attention from mathematicians and physicists are 2D and 3D straight and bent quantum wave guides [5, 14, 16, 19, 21, 29, 39, 43, 47]. In particular, the conditions for the existence of the bound states and resonances in such classically unbound system were considered for the miscellaneous permutations of the Dirichlet and Neumann domains [21, 29, 44]. Bound states lying below the essential spectrum of the corresponding straight part were predicted to exist for the curved 2D channel if its inner and outer interfaces support the Dirichlet and Neumann requirements, respectively, and not for the opposite configuration [22, 39, 43]. This was an extension of the previous theoretical studies of the existence of the bound states for the pure Dirichlet bent wave guide [27] that were confirmed experimentally. Also, for the 2D straight Dirichlet wave guide the existence of the bound state below the essential spectrum was predicted when the Neumann window is placed on its confining surface [16, 29]. From practical point of view, such configuration can be realized in the form of the two window-coupled semiconductor channels of equal widths [29, 30] whose experimental creation and study has been made possible due to the advances of the modern growth nanotechnologies. The number of the bound states increases with the window length a and their energies are monotonically decreasing functions of a [14]. In particular, for small values of a the eigenvalue emerges from the continuous spectrum proportionally to a^4. The asymptotical estimate for small a were established in [31]. The asymptotics expansion of the emerging eigenvalue for small a was constructed formally in [50], while the rigorous results were obtained in [32]. Recently, this result was extended to the case of the 3D spatial Dirichlet duct with circular Neumann disc [5] for which a proof of the bound state existence was confirmed, the number of discrete eigenvalues as a function of the disc radius a was evaluated and their asymptotics for the large a was given. As mentioned above, such Zaremba configuration is indispensable for the investigation of the electrostatic phenomena [34]. Similar to the 2D case, it can be also considered as the equal widths limit of the two 3D coupled Dirichlet ducts of, in general, different widths with the window in their common boundary [7, 30]. Another motivation stems from the phenomenological Ginzburg-Landau theory of superconductivity [20] which states that the boundary condition for the order parameter $\Psi(\mathbf{r})$ of the superconducting electrons reads.

The study of quantum waves on quantum waveguide has gained much interest and has been intensively studied during the last years for their important physical consequences. The main reason is that they represent an interesting physical effect with important applications in nanophysical devices, but also in flat electromagnetic waveguide.
Exner et al. have done seminal works in this field. They obtained results in different contexts, we quote [24, 27, 29, 31]. Also in [37, 38, 45] research has been conducted in this area; the first is about the discrete case and the two others for deals with the random quantum waveguide.

It should be noticed that the spectral properties essentially depends on the geometry of the waveguide, in particular, the existence of a bound states induced by curvature [16, 21, 24, 27] or by coupling of straight waveguides through windows [27] were shown.

On the other hand, the results on the discrete spectrum of a magnetic Schrödinger operator in waveguide-type domains are scarce. A planar quantum waveguide with constant magnetic field and a potential well is studied in [25], where it was proved that if the potential well is purely attractive, then at least one bound state will appear for any value of the magnetic field. Stability of the bottom of the spectrum of a magnetic Schrödinger operator was also studied in [57]. Magnetic field influence on the Dirichlet-Neumann structures was analyzed in [12, 44], the first dealing with a smooth compactly supported field as well as with the Aharonov-Bohm field in a two dimensional strip and second with perpendicular homogeneous magnetic field in the quasi dimensional.

Despite numerous investigations of quantum waveguides during last few years, many questions remain to be answered, this concerns, in particulier, effects of external fields. most attention has been paid to magnitec fields, either perpendicular to the waveguides plane or threaded through the tube, while the influence of the an Aharonov-Bohm magnetic field alone remained mostly untreated.

In their celebrated 1959 paper [4] Aharonov and Bohm pointed out that while the fundamental equations of motion in classical mechanics can always be expressed in terms of field alone, in quantum mechanics the canonical formalism is necessary, and as a result, the potentials cannot be eliminated from the basic equations. They proposed several experiments and showed that an electron can be influenced by the potentials even if no fields acts upon it. More precisely, in a field-free multiply-connected region of space, the physical properties of a system depend on the potentials through the gauge-invariant quantity $\oint \mathbf{A} dl$, where $\mathbf{A}$ represents the vector potential. Moreover, the Aharonov-Bohm effect only exists in **the multiply-connected region of space**. The Aharonov-Bohm experiment allows in principle to measure the decomposition into homotopy classes of the quantum mechanical propagator.

A possible next generalization are waveguides with combined Dirichlet and Neumann boundary conditions on different parts of the boundary with a Aharonov-Bohm magnetic field with the flux $2\pi\alpha$. The presence of different boundary conditions and Aharonov-Bohm magnetic field also gives rise to nontrivial properties like the existence of bound states this question is the main objet of the paper. The rest of the paper is organized as follows, in Section 2, we define the model and recall some known results. In section 3, we present the main result of this note followed by a discussion. Section 4 is devoted for numerical computations.

2 The model

The system we are going to study is given in Fig 1. We consider a Schrödinger particle whose motion is confined to a pair of parallel plans of width d. For simplicity, we assume that they are placed at $z = 0$ and $z = d$. We shall denote this configuration space by Ω

$$\Omega_0 = \mathbb{R}^2 \times [0, d].$$

Let $\gamma(a)$ be a disc of radius a, without loss of generality we assume that the center of $\gamma(a)$ is the point $(0, 0, 0)$;

$$\gamma(a) = \{(x, y, 0) \in \mathbb{R}^3;\ x^2 + y^2 \leq a^2\}. \tag{2.3}$$

We set $\Gamma = \partial\Omega_0 \diagdown \gamma(a)$. We consider Dirichlet boundary condition on Γ and Neumann boundary condition in $\gamma(a)$.

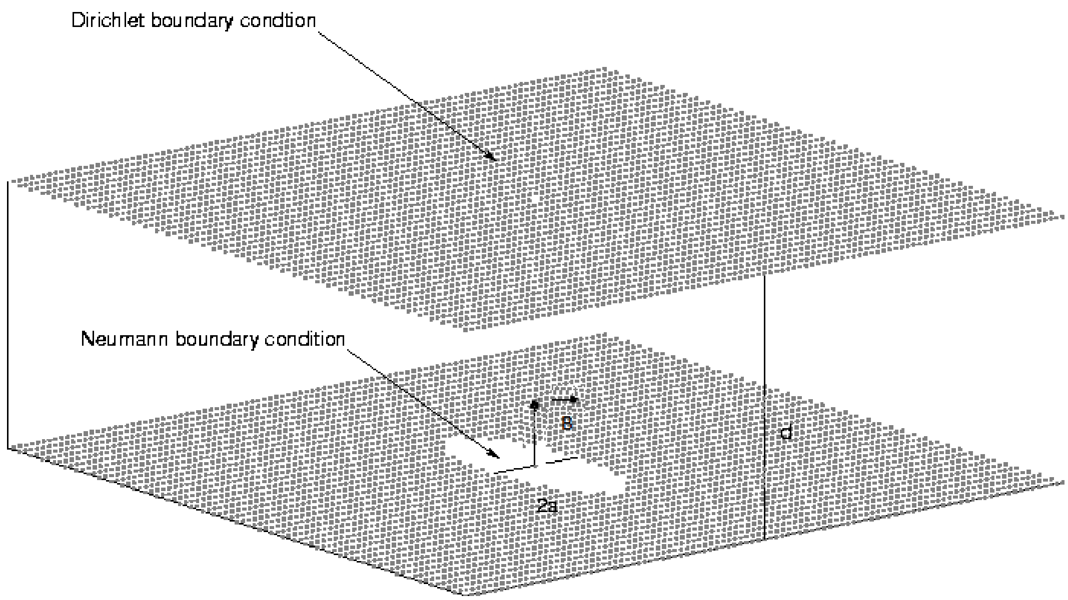

Figure 1: The waveguide with a disc window and two different boundaries conditions

2.1 The Hamiltonian

Let be the multiply-connected region $\Omega = \{(x, y, z) \in \Omega_0; \quad x^2 + y^2 > 0\}$. Let us define, now the self-adjoint operator on $\mathrm{L}^2(\Omega)$ corresponding to the particle Hamiltonian H. This is will be done by the mean of Friedrichs extension theorem. Precisely, let H_{AB} be The Aharonov-Bohm Schrödinger operator in $\mathrm{L}^2(\Omega)$, defined initially on the domain $\mathrm{C}_0^\infty(\Omega)$, and given by the expression

$$H_{AB} = (i\nabla + \mathbf{A})^2, \tag{2.4}$$

where $\mathbf{A}$ is a magnetic vector potential for the Aharonov-Bohm magnetic field $\mathbf{B}$, and given by

$$\mathbf{A}(x, y, z) = (A_1, A_2, A_3) = \alpha\left(\frac{y}{x^2 + y^2}, \frac{-x}{x^2 + y^2}, 0\right), \quad \alpha \in \mathbb{R} \setminus \mathbb{Z}. \tag{2.5}$$

The magnetic field $\mathbf{B} : \mathbb{R}^3 \to \mathbb{R}^3$ given by

$$\mathbf{B}(x, y, z) = curl\mathbf{A} = 0$$

outside the z-axis and

$$\int_\gamma \mathbf{A} = 2\pi\alpha, \tag{2.6}$$

where γ is a properly oriented closed curve which encloses the z-axis. It can be shown that H_{AB} has a four-parameter family of self-adjoint extensions which is constructed by means of von Neumanns extension theory [15]. Here we are only interested in the Friedrichs extension of H_{AB} on $\mathrm{L}^2(\Omega)$ which we now construct by means of quadratic forms.
For $\mathbf{A} = (A_1, A_2, 0)$ in (2.5), we observe that $A_1, A_2 \in \mathrm{L}^\infty_{loc}(\Omega)$. Let

$$\Omega_n = B(0, n) \times [0, d] \setminus (B(0, 1/n) \times [0, d]), \quad n \geq 2,$$

where $B(0, r)$ denotes the disk with centre 0 and radius r. We define on $\mathrm{L}^2(\Omega_n)$ (for each $n \geq 2$) the quadratic form

$$\begin{aligned} q_n[u, v] \;\; = \;\; & \int_{\Omega_n} \left(i\frac{\partial u}{\partial x} + A_1 u\right)\overline{\left(i\frac{\partial v}{\partial x} + A_1 v\right)} + \int_{\Omega_n} \left(i\frac{\partial u}{\partial y} + A_2 u\right)\overline{\left(i\frac{\partial v}{\partial y} + A_2 v\right)} \\ & + \int_{\Omega_n} \left(i\frac{\partial u}{\partial z} + A_3 u\right)\overline{\left(i\frac{\partial v}{\partial z} + A_3 v\right)}, \end{aligned}$$

on the domain

$$\mathrm{Q}(q_n) = \{u \in \mathrm{H}^1(\Omega_n); \quad u\lceil\Gamma_n = 0\},$$

where $\mathrm{H}^1(\Omega_n) = \{u \in \mathrm{L}^2(\Omega_n) | \nabla u \in \mathrm{L}^2(\Omega_n)\}$ is the standard Sobolev space, $\Gamma_n = \partial\Omega_n \setminus \gamma(a)$ and we denote by $u\lceil\Gamma_n$, the trace of the function u on Γ_n. The form q_n is closed, since $A_1, A_2 \in \mathrm{L}^\infty(\Omega_n)$.

Let the quadratic form q

$$\begin{aligned} q[u,v] &= q_n[u,v] \quad \text{if } u,v \in \mathrm{Q}(q_n), \\ \mathrm{Q}(q) &= \cup_n \mathrm{Q}(q_n). \end{aligned}$$

Lemma 2.1 *The form q is closable.*

Proof. The form q is closable if and only if any sequence, $u_n \in \mathrm{Q}(q)$, such that

$$\lim_{n\to\infty} \| u_n \| = 0 \quad \text{and} \quad \lim_{m,n\to\infty} q[u_n - u_m] = 0, \tag{2.7}$$

satisfies $\lim_{n\to\infty} q[u_n] = 0$.

Observe that (2.7) implies

$$C := \sup_n q[u_n]^{1/2} < \infty. \tag{2.8}$$

Let ba a sequence, $(u_n)_n \in \mathrm{Q}(q)$, such that (2.7) satisfies, then we take $\varepsilon > 0$ and choose n_0 such that

$$q[u_n - u_m] \leq \varepsilon \quad \text{for} \quad n,m \geq n_0, \tag{2.9}$$

and

$$\| u_n \| \leq \varepsilon \quad \text{for} \quad n \geq n_0. \tag{2.10}$$

Set, moreover, $K = \Omega_{n_0} \subset \Omega$ such that the support of u_{n_0} included in K. In view of (2.7) it follows that

$$\int_K | (i\nabla + \mathbf{A})(u_n - u_m) |^2 \leq q[u_n - u_m] \longrightarrow 0 \quad \text{as} \quad n,m \to \infty, \tag{2.11}$$

$$\int_K | u_n |^2 \longrightarrow 0 \quad \text{as} \quad n \to \infty. \tag{2.12}$$

$\mathbf{A}$ is bounded on K as

$$\| \mathbf{A} \| \leq | K | n_0, \tag{2.13}$$

we obtain that

$$\int_K | \mathbf{A} u_n |^2 \longrightarrow 0 \quad \text{as} \quad n \to \infty. \tag{2.14}$$

Since the norm in L^2 is 1-Lipschitz, then

$$\left| \left(\int_K | \mathbf{A}(u_n - u_m) |^2 \, dx \right)^{1/2} - \left(\int_K | \nabla(u_n - u_m) |^2 \, dx \right)^{1/2} \right|$$
$$\leq \left(\int_K | (i\nabla + \mathbf{A})(u_n - u_m) |^2 \, dx \right)^{1/2}.$$

According to (2.12), the first term on the left side of the latter tends to zero as $n, m \to \infty$ and, due to (2.9), the same holds for the right side. Thus,

$$\int_K | u_n - u_m |^2 + | \nabla(u_n - u_m) |^2 \quad \longrightarrow \quad 0 \quad \text{as} \quad n, m \to \infty. \tag{2.15}$$

Since the form of the classical Dirichlet-Neumann Laplacian in $\mathrm{Q}(q_{n_0})$ is closable it follows from (2.15), in conjunction with (2.11) that

$$\int_K | \nabla u_n |^2 \to 0, \quad \int_K | u_n |^2 \to 0, \quad \text{as} \quad n \to \infty. \tag{2.16}$$

Let's consider the following quadratic form

$$q[u_n] = q[u_n, u_n - u_{n_0}] + q[u_n, u_{n_0}] \leq q[u_n]^{1/2} q[u_n - u_{n_0}]^{1/2} + | q[u_n - u_{n_0}] | . \tag{2.17}$$

It follows from (2.8) and (2.9) that

$$q[u_n]^{1/2} q[u_n - u_{n_0}]^{1/2} \leq C \varepsilon^{1/2} \quad \text{when} \quad n \geq n_0. \tag{2.18}$$

Since $\mathbf{A}$ is bounded on K we infer from (2.14) and (2.16) that

$$q[u_n, u_{n_0}] = \int_K (i\nabla + \mathbf{A}) u_n \overline{(i\nabla + \mathbf{A}) u_{n_0}} \to 0 \quad \text{as} \quad n \to \infty. \tag{2.19}$$

Using (2.18)-(2.19) in (2.17) shows that $\lim_{n\to\infty} q[u_n] = 0$, this ends the proof of the lemma 2.1. ■

We denote the closure of q by $\overline{q}$ and the associated semi-bounded self-adjoint operator is the Friedrichs extension of H_{AB} is denoted by H and its domain by $D(\Omega)$. It is the hamiltonian describing our system. We conclude that the domain $D(\Omega)$ of H is

$$D(\Omega) \quad = \quad \{ u \in \mathrm{H}^1(\Omega); \quad (i\nabla + \mathbf{A})^2 u \in \mathrm{L}^2(\Omega), u \lceil \Gamma = 0, \nu . (i\nabla + \mathbf{A}) u \lceil \gamma(a) = 0 \},$$

where ν the normal vector and

$$Hu = (i\nabla + \mathbf{A})^2 u, \quad \forall u \in D(\Omega). \tag{2.20}$$

2.2 Some known facts

Let's start this subsection by recalling that in the particular case when $a = 0$, we get H^0, the magnetic Dirichlet Laplacian, and when $a = +\infty$ we get H^∞, the magnetic Dirichlet-Neumann Laplacian.

Proposition 2.2 *The spectrum of H^0 is $[(\frac{\pi}{d})^2, +\infty[$, and the spectrum of H^∞ coincides with $[(\frac{\pi}{2d})^2, +\infty[$.*

Proof. Since

$$H \;=\; (i\nabla + \widetilde{\mathbf{A}})^2 \otimes I \oplus I \otimes (-\Delta_{[0,d]}), \quad \text{on} \quad \mathrm{L}^2(\mathbb{R}^2 \setminus \{0\}) \otimes \mathrm{L}^2([0,d]).$$

where $\widetilde{\mathbf{A}} := \alpha \left(\frac{y}{x^2+y^2}, \frac{-x}{x^2+y^2} \right)$. Consider the quadratic form

$$\begin{aligned}
\widetilde{q}[u] &= \int_{\mathbb{R}^2} \mid (i\nabla + \widetilde{\mathbf{A}})u \mid^2 dxdy \\
&= \int_{\mathbb{R}^2} \left| \left(i\partial_x + \alpha \frac{y}{x^2+y^2} \right) u \right|^2 dxdy + \int_{\mathbb{R}^2} \left| \left(i\partial_y - \alpha \frac{x}{x^2+y^2} \right) u \right|^2 dxdy. \quad (2.21)
\end{aligned}$$

By introducing polar coordinates we get

$$r = \sqrt{x^2+y^2}; \qquad \frac{x}{r} = \cos\theta, \qquad \frac{y}{r} = \sin\theta,$$

and

$$\frac{\partial\theta}{\partial x} = \frac{-y}{r^2}, \quad \frac{\partial\theta}{\partial y} = \frac{x}{r^2}, \quad \partial_x = \cos\theta\frac{\partial}{\partial r} - \frac{y}{r^2}\frac{\partial}{\partial\theta}, \quad \partial_y = \sin\theta\frac{\partial}{\partial r} + \frac{x}{r^2}\frac{\partial}{\partial\theta}.$$

Hence (2.21) becomes

$$\begin{aligned}
\widetilde{q}[u] &= \int \left| \left(i\cos\theta\frac{\partial}{\partial r} - i\frac{y}{r^2}\frac{\partial}{\partial\theta} + \alpha\frac{\sin\theta}{r} \right) u \right|^2 rdrd\theta \\
&+ \int \left| \left(i\sin\theta\frac{\partial}{\partial r} + i\frac{x}{r^2}\frac{\partial}{\partial\theta} - \alpha\frac{\cos\theta}{r} \right) u \right|^2 rdrd\theta \\
&= \int \left(\cos^2\theta \mid \partial_r u \mid^2 + \frac{\sin^2\theta}{r^2} \mid (i\partial_\theta u - \alpha u) \mid^2 \right) rdrd\theta \\
&+ \int \left(\sin^2\theta \mid \partial_r u \mid^2 + \frac{\cos^2\theta}{r^2} \mid (i\partial_\theta u - \alpha u) \mid^2 \right) rdrd\theta \\
&= \int \left(\mid \partial_r u \mid^2 + \frac{1}{r^2} \mid (i\partial_\theta u - \alpha u) \mid^2 \right) rdrd\theta. \qquad (2.22)
\end{aligned}$$

Expanding u into Fourier series with respect to θ

$$u(r,\theta) = \sum_{k=-\infty}^{\infty} u_k(r)\frac{e^{ik\theta}}{\sqrt{2\pi}}.$$

enables us to rewrite (2.22) as

$$\begin{aligned}
\int\left(\mid \partial_r u \mid^2 + \frac{1}{r^2} \mid (i\partial_\theta u - \alpha u) \mid^2\right) r dr d\theta & \\
& \geq \int \frac{1}{r^2}\left|\sum_k -(k+\alpha) u_k(r) \frac{e^{ik\theta}}{\sqrt{2\pi}}\right|^2 r dr d\theta \\
& \geq \int \frac{1}{r^2} \sum_k \mid k+\alpha \mid^2 \mid u_k(r) \mid^2 r dr \\
& \geq \min_k \mid k+\alpha \mid^2 \int \frac{1}{r^2} \sum_k \mid u_k(r) \mid^2 r dr \\
& \geq \min_k \mid k+\alpha \mid^2 \int \frac{1}{r^2} \left|\sum_k u_k(r) \frac{e^{ik\theta}}{\sqrt{2\pi}}\right|^2 r dr d\theta \\
& = \min_k \mid k+\alpha \mid^2 \int \frac{1}{r^2} \mid u(r,\theta) \mid^2 r dr d\theta \\
& = \min_k \mid k+\alpha \mid^2 \int \frac{1}{x^2+y^2} \mid u(x,y) \mid^2 dx dy.
\end{aligned}$$

Hence

$$\int_{\mathbb{R}^2} \mid (i\nabla + \widetilde{\mathbf{A}}) u \mid^2 dx dy \geq \min_k \mid k+\alpha \mid^2 \int \frac{1}{x^2+y^2} \mid u(x,y) \mid^2 dx dy. \tag{2.23}$$

Here the form in the right hand side is considered on the function class $\mathrm{H}^1(\mathbb{R}^2)$, obtained by the completion of the class $\mathcal{C}_0^\infty(\mathbb{R}^2\backslash\{0\})$. Inequality (2.23) is the Hardy inequality in two dimensions with Aharonov-Bohm vector potential [3]. This yields that $\sigma\left((i\nabla + \widetilde{\mathbf{A}})^2\right) \subset [0, +\infty[$

Since $\sigma(-\Delta) = \sigma_{ess}(-\Delta) = [0, +\infty[$, then there exists a Weyl sequences $\{h_n\}_{n=1}^\infty$ for the operator $-\Delta$ in $\mathrm{L}^2(\mathbb{R}^2)$ at $\lambda \geq 0$. Construct the functions

$$\varphi_n(x,y) = \begin{cases} h_n & \text{if } x > n \text{ and } y > n, \\ 0 & \text{if not.} \end{cases}$$

$$\begin{aligned}
\parallel \left((i\nabla + \widetilde{\mathbf{A}})^2 - \lambda\right) \varphi_n \parallel & \leq \parallel (\Delta - \lambda)\varphi_n \parallel + \parallel \widetilde{\mathbf{A}}^2 \varphi_n \parallel + \parallel \widetilde{\mathbf{A}} \nabla \varphi_n \parallel \\
& \leq \parallel (\Delta - \lambda)\varphi_n \parallel + \frac{c}{n}.
\end{aligned}$$

Where c is positive real.
Therefore, the functions $\psi_n = \dfrac{\varphi_n}{\parallel \varphi_n \parallel}$ is Weyl sequence for $(i\nabla + \widetilde{\mathbf{A}})^2$ at $\lambda \geq 0$, thus

$[0,+\infty[\subset \sigma_{ess}\Big((i\nabla+\widetilde{\mathbf{A}})^2\Big)\subset \sigma\Big((i\nabla+\widetilde{\mathbf{A}})^2\Big).$

Then we get that the spectrum of $(i\nabla+\widetilde{\mathbf{A}})^2$ is $[0,+\infty[$, we know that the spectrum of $-\Delta^0_{[0,d]}$ and $-\Delta^\infty_{[0,d]}$ is $\{(\frac{j\pi}{d})^2,\quad j\in\mathbb{N}^\star\}$ and $\{(\frac{(2j+1)\pi}{2d})^2,\quad j\in\mathbb{N}\}$ respectively. Therefore we have the spectrum of H^0 is $[(\frac{\pi}{d})^2,+\infty[$. And the spectrum of H^∞ coincides with $[(\frac{\pi}{2d})^2,+\infty[$. ■

Consequently, we have

$$\Big[(\frac{\pi}{d})^2,+\infty\Big[\subset\sigma(H)\subset\Big[(\frac{\pi}{2d})^2,+\infty\Big[.$$

Using the property that the essential spectra is preserved under compact perturbation, we deduce that the essential spectrum of H is

$$\sigma_{ess}(H)=\Big[(\frac{\pi}{d})^2,+\infty\Big[.$$

2.3 Preliminary: Cylindrical coordinates

Let's notice that the system has a cylindrical symmetry, therefore, it is natural to consider the cylindrical coordinates system (r,θ,z). Indeed, we have that

$$\mathrm{L}^2(\Omega,dxdydz)\quad=\quad\mathrm{L}^2(]0,+\infty[\times[0,2\pi[\times[0,d],rdrd\theta dz).$$

Consequently, a corresponding orthonormal basis in $\mathbb{R}^3$ is given by the three vectors

$$e_r=\begin{pmatrix}\cos\theta\\ \sin\theta\\ 0\end{pmatrix},\qquad e_\theta=\begin{pmatrix}-\sin\theta\\ \cos\theta\\ 0\end{pmatrix},\qquad e_z=\begin{pmatrix}0\\ 0\\ 1\end{pmatrix}.$$

We note by $\mathbf{A}_\theta$, the Aharonov-Bohm magnetic potential vector (2.5) in cylindrical coordinates given by

$$\mathbf{A}_\theta(r,\theta,z)=\frac{\alpha}{r}(-\sin\theta,\cos\theta,0)=\frac{\alpha}{r}e_\theta.$$

We denote the gradient in cylindrical coordinates by $\nabla_{r,\theta,z}$. While the operator $i\nabla+\mathbf{A}$ in cylindrical coordinates is given by

$$i\nabla_{r,\theta,z}+\mathbf{A}_\theta=i\frac{\partial}{\partial r}e_r+\frac{1}{r}\left(i\frac{\partial}{\partial\theta}+\alpha\right)e_\theta+i\frac{\partial}{\partial z}e_z.$$

thus the Aharonov-Bohm Laplacian operator in cylindrical coordinates is given by

$$\begin{aligned}H_{r,\theta,z}\quad&:=\quad(i\nabla_{r,\theta,z}+\mathbf{A}_\theta)^2\\ &=\quad-\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial}{\partial r})+\frac{1}{r^2}(i\frac{\partial}{\partial\theta}+\alpha)^2-\frac{\partial^2}{\partial^2 z}.\end{aligned}$$

3 The result

The main result of this paper is the following:

Theorem 3.1 *Let H be the operator defined on* (2.20)*. There exist $a_0 > 0$ such that for any $0 < \frac{a}{d} < a_0$, we have*

$$\sigma_d(H) = \emptyset.$$

There exist $a_1 > 0$, such that $\frac{a}{d} > a_1$, we have

$$\sigma_d(H) \neq \emptyset.$$

Remark 3.1 *The presence of magnetic field in three dimensional straight strip of width d with the Neumann boundary condition on a disc window of radius $0 < \frac{a}{d} < a_0$ and Dirichlet boundary conditions on the remained part of the boundary, destroys the creation of discrete eigenvalues below the essential spectrum. if $\frac{a}{d} > a_1$, the effect of the magnetic field is reduced.*

Proof. As in [5], let's split $\mathrm{L}^2(\Omega, rdrd\theta dz)$ as follows, $\mathrm{L}^2(\Omega, rdrd\theta dz) = \mathrm{L}^2(\Omega_a^-, rdrd\theta dz) \oplus \mathrm{L}^2(\Omega_a^+, rdrd\theta dz)$, with

$$\begin{aligned} \Omega_a^- &= \{(r, \theta, z) \in [0, a] \times [0, 2\pi[\times[0, d]\}, \\ \Omega_a^+ &= \Omega \setminus \Omega_a^-. \end{aligned}$$

Therefore

$$H_a^{-,N} \oplus H_a^{+,N} \leq H \leq H_a^{-,D} \oplus H_a^{+,D}.$$

Here we index by D and N depending on the boundary conditions considered on the surface $r = a$. The min-max principle leads to

$$\sigma_{ess}(H) = \sigma_{ess}(H_a^{+,N}) = \sigma_{ess}(H_a^{+,D}) = [(\frac{\pi}{d})^2, +\infty[. \qquad (3.24)$$

Let us denote by $\lambda_k(H_a^{-,N})$, $\lambda_k(H_a^{-,D})$ and $\lambda_k(H)$, the k-th eigenvalue of $H_a^{-,N}$, $H_a^{-,D}$ and H respectively then, the minimax principle yields the following

$$\lambda_k(H_a^{-,N}) \leq \lambda_k(H) \leq \lambda_k(H_a^{-,D}) \qquad (3.25)$$

and for $k \geq 2$

$$\lambda_{k-1}(H_a^{-,N}) \leq \lambda_k(H) \leq \lambda_k(H_a^{-,N}); \qquad (3.26)$$

$$\lambda_{k-1}(H_a^{-,D}) \leq \lambda_k(H) \leq \lambda_k(H_a^{-,D}). \tag{3.27}$$

Thus, if $H_a^{-,N}$ does not have a discrete spectrum below $(\frac{\pi}{d})^2$, then H do not has as well. We mention that its a sufficient condition.
The eigenvalue equation is given by

$$H_a^{-,N} f(r,\theta,z) = Ef(r,\theta,z). \tag{3.28}$$

This equation is solved by separating variables and considering $f(r,\theta,z) = R(r)P(\theta)Z(z)$. Plugging the last expression in equation (3.28) and first separate Z by putting all the z dependence in one term so that $\dfrac{Z''}{Z}$ can only be constant. The constant is taken as $-k_z^2 = -(\dfrac{(2j+1)\pi}{2d})^2$ for convenience. Second, we separate the term $\dfrac{1}{P}(i\dfrac{\partial}{\partial\theta} + \alpha)^2 P$ which has all the θ dependance. Using the fact that the problem has an axial symmetry and the solution has to be 2π periodic and single value in θ, we obtain $\dfrac{1}{P}(i\dfrac{\partial}{\partial\theta} + \alpha)^2 P$ should be a constant $-(m-\alpha)^2 = -\nu^2$ for $m \in \mathbb{Z}$. Finally, we get the following equation for R

$$R''(r) + \frac{1}{r}R'(r) + [E - k_z^2 - \frac{\nu^2}{r^2}]R(r) = 0. \tag{3.29}$$

We notice that the equation (3.29), is the Bessel equation and its solutions could be expressed in terms of Bessel functions. More explicit solutions could be given by considering boundary conditions. The solution of the equation (3.29) is given by $R(r) = cJ_\nu(\beta r)$, with $c \in \mathbb{R}$, $\beta^2 = E - k_z^2$ and J_ν is the Bessel function of first kind of order ν. We assume that $R'(a) = 0$. So we get the condition $a\beta = x'_{\nu,n}$, with $x'_{\nu,n}$ are the positive zeros of the Bessel function J'_n. Thus $H_a^{-,N}$ has a sequence of eigenvalues given by

$$\begin{aligned} \lambda_{j,\nu,n} &= \frac{x'^2_{\nu,n}}{a^2} + k_z^2 \\ &= \frac{x'^2_{\nu,n}}{a^2} + \left(\frac{(2j+1)\pi}{2d}\right)^2. \end{aligned}$$

As we are interested for discrete eigenvalues which belongs to $[\left(\dfrac{\pi}{2d}\right)^2, \left(\dfrac{\pi}{d}\right)^2)$ only $\lambda_{0,\nu,n}$ intervenes.
If

$$\left(\frac{\pi}{d}\right)^2 \leq \lambda_{0,\nu,n}, \tag{3.30}$$

then there H does not have a discrete spectrum. We recall that $\nu^2 = (m-\alpha)^2$ and it is related to magnetic flux, also recall that $x'_{\nu,n}$ are the positive zeros of the Bessel function

J'_n and $\forall \nu > 0$, $\forall n \in \mathbb{N}^\star$; $0 < x'_{\nu,n} < x'_{\nu,n+1}$ (see [54]). So, for any eigenvalue of $H_a^{-,N}$,

$$\frac{x'^2_{\nu,1}}{a^2} + \left(\frac{\pi}{2d}\right)^2 < \frac{x'^2_{\nu,n}}{a^2} + \left(\frac{\pi}{2d}\right)^2 = \lambda_{0,\nu,n}.$$

An immediate consequence of the last inequality is that to satisfy (3.30) it is sufficient to have

$$3\left(\frac{\pi}{2d}\right)^2 < \frac{x'^2_{\nu,1}}{a^2},$$

therefore

$$\frac{\sqrt{3}\pi}{2d} < \frac{x'_{\nu,1}}{a},$$

then

$$\frac{a}{d} < \frac{2x'_{\nu,1}}{\sqrt{3}\pi}.$$

Or (see [17, 41, 49, 54]), we have

$$\nu + \alpha_n \nu^{1/3} < x'_{\nu,n},$$

where $\alpha_n = 2^{-1/3}\beta_n$ and β_n is the n-th positive root of the equation

$$J_{\frac{2}{3}}\left(\frac{2}{3}x^{3/2}\right) - J_{\frac{-2}{3}}\left(\frac{2}{3}x^{3/2}\right) = 0.$$

For $n = 1$, we have

$$c_0 := 0.6538 + \alpha < 0.6538 + \nu < x'_{\nu,1}. \tag{3.31}$$

Then we get that for d and a positives such that $\dfrac{a}{d} < a_0 := \dfrac{2c_0}{\sqrt{3}\pi}$,

$$\sigma_d(H) = \emptyset.$$

This ends the proof of the first result of the theorem 3.1.

By the min-max principle and (3.27), we know that if $H_a^{-,D}$ exhibits a discrete spectrum below $(\frac{\pi}{d})^2$, then H do as well.

$H_a^{-,D}$ has a sequence of eigenvalues [5, 56], given by

$$\lambda_{j,\nu,n} \quad = \quad \left(\frac{x_{\nu,n}}{a}\right)^2 + \left(\frac{(2j+1)\pi}{2d}\right)^2.$$

Where $x_{\nu,n}$ is is the $n-$th positive zero of Bessel function of order ν (see [5]). As we are interested for discrete eigenvalues which belongs to $[(\dfrac{\pi}{2d})^2, (\dfrac{\pi}{d})^2)$ only for $\lambda_{0,\nu,n}$.

If we is satisfied the condition

$$\lambda_{0,\nu,n} < \left(\frac{\pi}{d}\right)^2, \tag{3.32}$$

then H have a discrete spectrum.

We recall that $0 < x_{\nu,n} < x_{\nu,n+1}$ for any $\nu > 0$ and any $n \in \mathbb{N}^\star$ (see [54]). So, for any eigenvalue of $H_a^{-,D}$,

$$\frac{x_{\nu,1}^2}{a^2} + \left(\frac{\pi}{2d}\right)^2 < \frac{x_{\nu,n}^2}{a^2} + \left(\frac{\pi}{2d}\right)^2 = \lambda_{0,\nu,n}.$$

An immediate consequence of the last inequality is that to satisfy (3.32) it is sufficient to set then

$$\frac{2x_{\nu,1}}{\sqrt{3}\pi} < \frac{a}{d}$$

Or (see [17, 54]), we have

$$\sqrt{\left(n - \frac{1}{4}\right)^2 \pi^2 + \nu^2} < x_{\nu,n},$$

For $n = 1$, we have

$$c_1 := \sqrt{\left(\frac{3\pi}{4}\right)^2 + \alpha^2} < \sqrt{\left(\frac{3\pi}{4}\right)^2 + \nu^2} < x_{\nu,1}. \tag{3.33}$$

Then we get that for d and a positives such that $\frac{a}{d} > a_1 := \frac{2c_1}{\sqrt{3}\pi}$,

$$\sigma_d(H) \neq \emptyset.$$

■

4 Numerical computations

This section is devoted to some numerical computations. We represent the radius values $a_0 : \alpha \mapsto \frac{2x'_{\alpha,1}}{\sqrt{3}\pi}$ and $a_1 : \alpha \mapsto \frac{2x_{\alpha,1}}{\sqrt{3}\pi}$, where $x'_{\alpha,1}$ and $x_{\alpha,1}$ is the first positive zero of Bessel function J'_α and J_α respectively, a function of the flux magnetic α, which makes it possible to exist or not discrete eigenvalues of H.

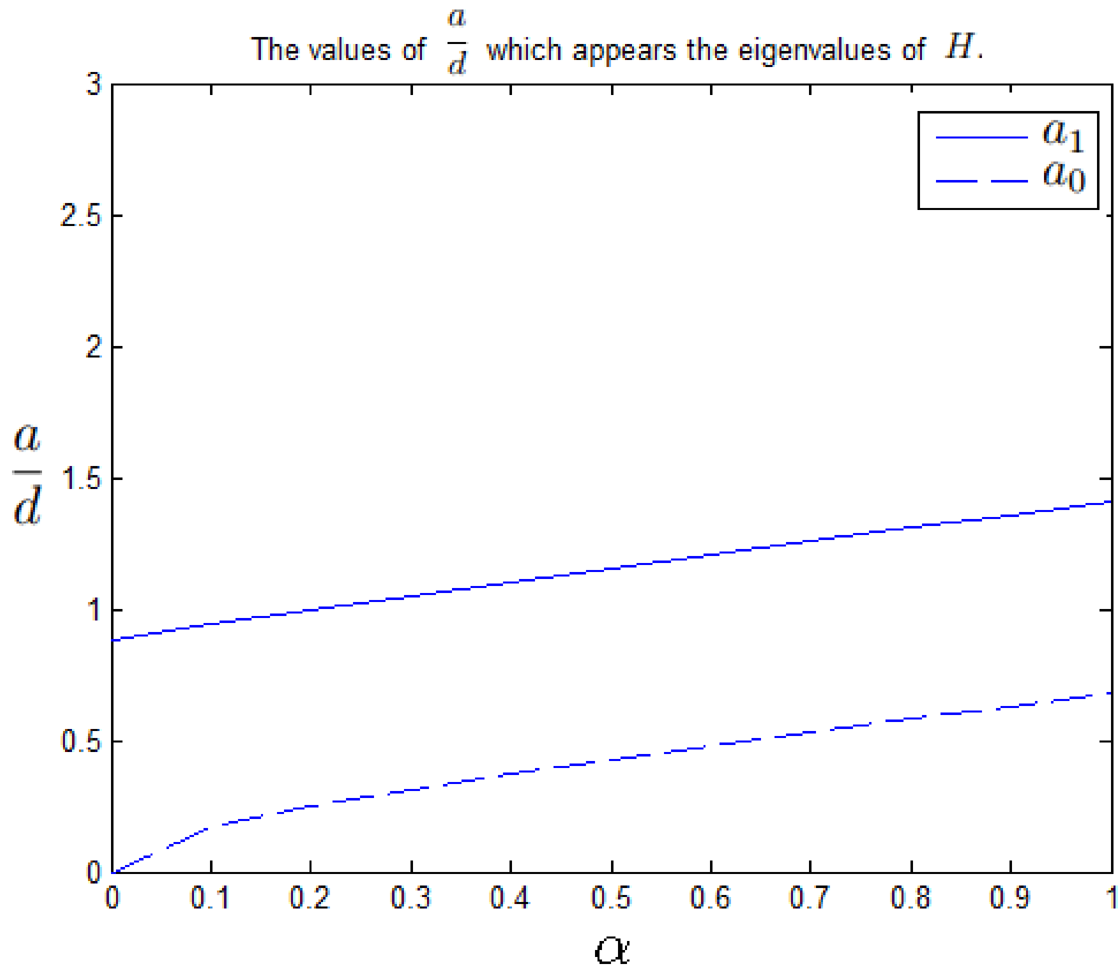

Figure 2: We represent $a_0 : \alpha \mapsto \frac{2x'_{\alpha,1}}{\sqrt{3}\pi}$ where $x'_{\alpha,1}$ and $a_1 : \alpha \mapsto \frac{2x_{\alpha,1}}{\sqrt{3}\pi}$.

In the neighborhood to zeros, we do to zoom the figure 2, when $d \to 0$, we observe that the discrete eigenvalues of H exists, contrary when $a \to 0$.

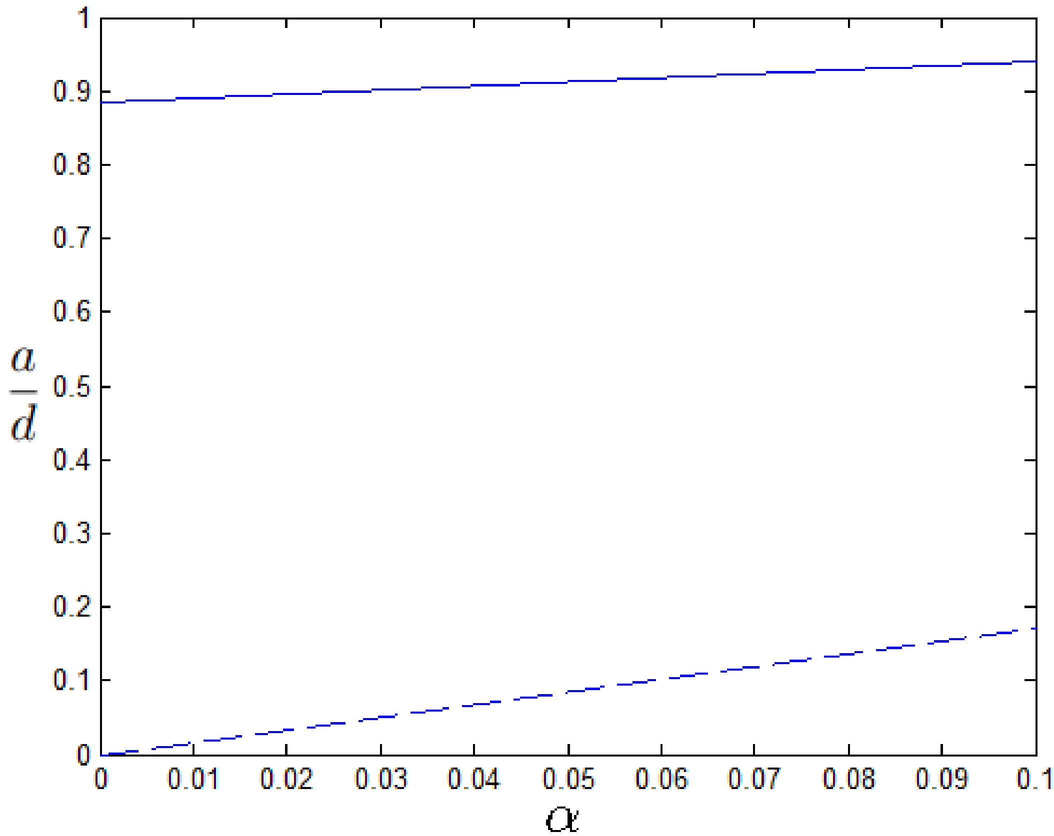

Figure 3: Zoom of figure 2 in the neighborhood to zeros.

We analyse a dependence of the first eigenfunction on the flux magnetic α in the whole range of their variation. We chose a more natural method: the finite element method. Consider a triangulation τ_h of Ω. We will construct the matrices of mass M and of assemblage A associated to the mesh and to the operator. We consider two elements u, V of $D(\Omega)$. Note U, V vector whose i-th coordinate gives the value of u, v at i-th point of the mesh. Denote by ϕ_i the basis functions for the finite element element $\mathbb{P}_k$ considered, the matrices M and A are given by their coefficients $M_{i,j}$ and $A_{i,j}$ are numerical approximations of integrals:

$$\begin{aligned} M_{i,j} &\approx \int_\Omega \phi_i \overline{\phi_j}. \\ A_{i,j} &\approx \int_\Omega (i\nabla + \mathbf{A})\phi_i \overline{(i\nabla + \mathbf{A})\phi_j}. \end{aligned}$$

Matrices M and A satisfied then:

$$\begin{aligned} \int_\Omega u\overline{v} &\approx {}^t\overline{V}MU, \\ a(u,v) &\approx {}^t\overline{V}AU. \end{aligned}$$

From calculation of the two matrices M and A, we wish to determine the eigenvector of the operator H. We can draw a parallel between the initial theoretical problem and the numerical problem that we solve:

• find $u \in D(\Omega)$, $\mu \in \mathbb{R}$ such that $\forall v \in D(\Omega)$, $a(u,v) = \mu < u, v >$.

• find $U \in \mathbb{P}_k$, $\mu \in \mathbb{R}$ such that $\forall V \in \mathbb{P}_k$, ${}^t\overline{V}AU = \mu {}^t\overline{V}MA$.

The approximate problem is to determine the eigenvectors of the matrix A for the matrix M, that is to say, to find $U \in \mathbb{P}_k$, such as: $AU = \lambda MU$.

We represent the first eigenfunction of H for the Neumann radius a=3, $d = \pi$ and $\alpha = 0.5$.

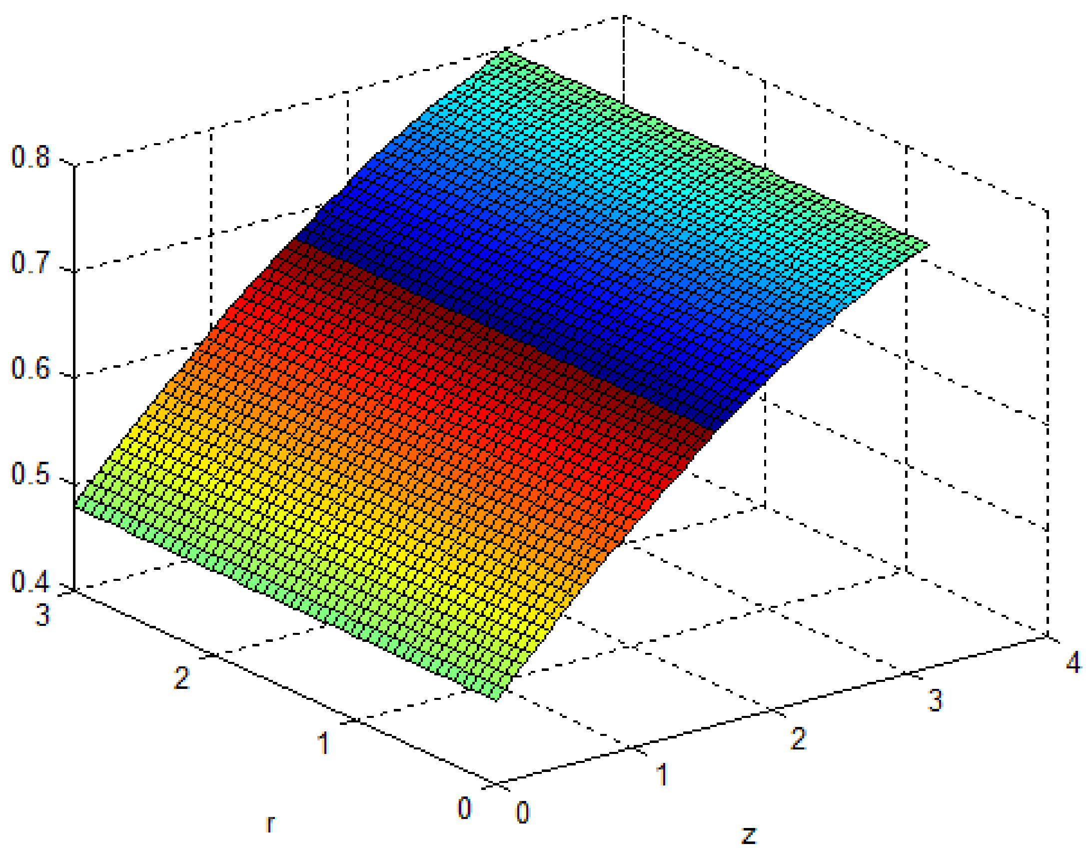

Figure 4: the first eigenfunction of H for the Neumann radius a=3, $d = \pi$ and $\alpha = 0.5$.

We represent the first eigenfunction of H for the Neumann radius a=3, $d = \pi$ and $\alpha = 1$.

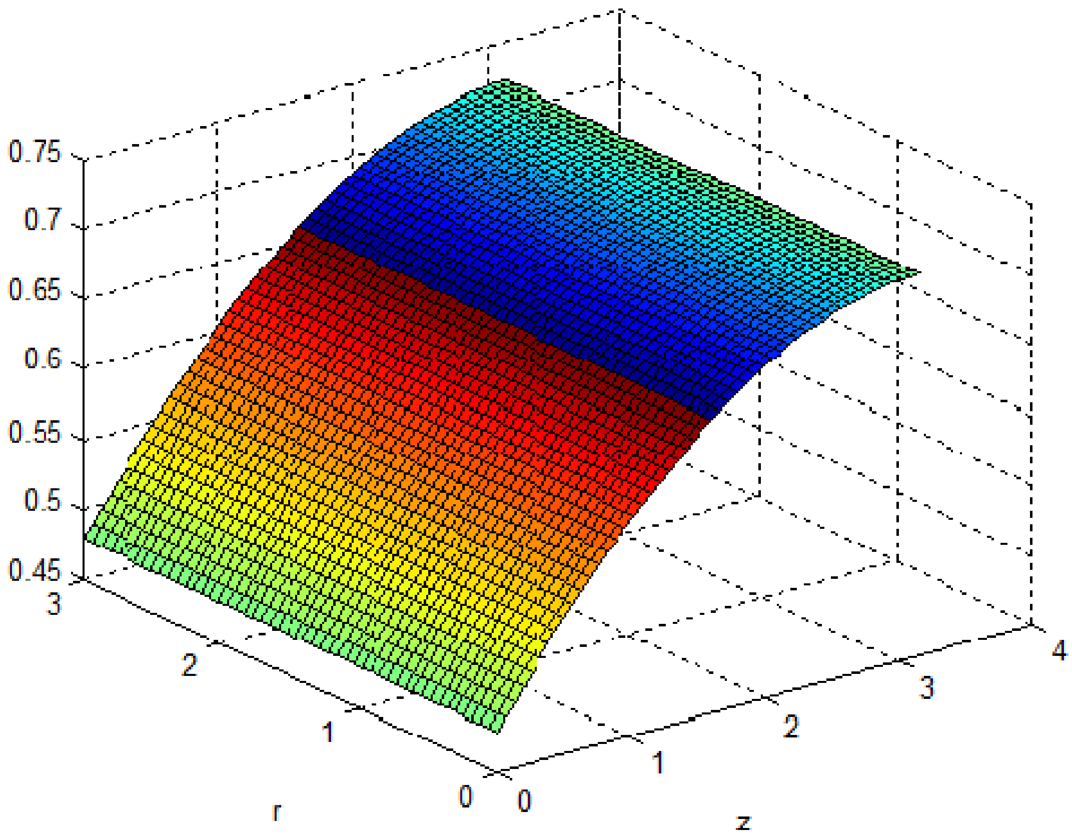

Figure 5: the first eigenfunction of H for $d = \pi$ and $\alpha = 0.75$.

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