NUMERICAL RESULTS A QUANTUM WAVEGUIDE WITH MIXED BOUNDARY CONDITIONS

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ABSTRACT. This article is devoted to the numerical study of the existence of the eigenvalues of the Hamiltonian describing a quantum particle living on three dimensional straight strip of width \(d\) in the presence of an electric field of constant intensity \(F\) in the direction perpendicular to the electron plane. We impose Neumann boundary conditions on a disc window of radius \(a\) and Dirichlet boundary conditions on the remaining part of the boundary of the strip.

1. Introduction and the model

The system we are going to study is given in Figure 1. This system is based on the work of Najar et al. [2] where it is proved that such system admits a discrete spectrum below its essential spectrum we are interested on numerical results of some of untreated cases in the mentioned reference. Here we our computation are based on Mathlab and Maple.

We consider a quantum particle, this leads to the study of an Hamiltonian which we denote by \(H_a(F)\), 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 \(\Omega\)

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

We suppose that the particle is a fermion of a nonzero charge \(q\). We also assume that it is under influence of a homogeneous electric field of an intensity \(E\), we denote \(F := Eq\). Without loss of generality we shall suppose in the following that \(F \geq 0\) and that the electric field is perpendicular to the electron plane.

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

\[\gamma(a) = \{(x, y, 0) \in \mathbb{R}^3; \ x^2 + y^2 \leq a^2\}.\] (1.1)

We set \(\Gamma = \partial \Omega \setminus \gamma(a)\). We consider Dirichlet boundary condition on \(\Gamma\) and Neumann boundary condition on \(\gamma(a)\).

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Figure 1. The waveguide with a disc window and two different boundary conditions with orthogonal electric field.

1.1. The Hamiltonian. Let us define the self-adjoint operator on $L^2(\Omega)$ corresponding to the particle Hamiltonian $H_a(F)$. This will be done by the mean of quadratic forms. Precisely, let $q_a$ be the quadratic form

$$q_a[u, v] = \int_{\Omega} \nabla u \nabla v + Fzu \, dx \, dy \, dz \quad u, v \in D(q_a),$$

where $D(q_a) := \{ u \in H^1(\Omega), u|\Gamma = 0 \}$ and $H^1(\Omega)$ is the standard Sobolev space and $u|\Gamma$ is the trace of the function $u$ on $\Gamma$. It follows that $q_a$ is a densely defined, symmetric, positive and closed quadratic form [5]. We denote the unique self-adjoint operator associated to $q_a$ by $H_a(F)$ and its domain by $D$. It is the hamiltonian describing our system. From [5] (page 276), we infer that the domain $D$ of $H_a(F)$ is

$$D = \{ u \in H^1(\Omega); \quad -\Delta u \in L^2(\Omega), u|\Gamma = 0, \frac{\partial u}{\partial z}|_{\gamma(a) = 0} \},$$

and

$$H_a(F)u = (-\Delta + Fz)u, \quad \forall u \in D. \quad (1.2)$$

2. Numerical computations

This section is devoted to some numerical computations. Let us start this section by giving some notations that we will use in the rest of this work: $\lambda_k(H_a^{-N}(F))$, $\lambda_k(H_a^{-D}(F))$ and $\lambda_k(H_a(F))$, the $k$-th eigenvalue of $H_a^{-N}(F)$,
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$H_{a}^{-D}(F)$ and $H_{a}(F)$, respectively. Then, the min-max principle yields the following

$$\lambda_k(H_{a}^{-N}(F)) \leq \lambda_k(H_{a}(F)) \leq \lambda_k(H_{a}^{-D}(F))$$

(2.1)

and for $2 \geq k$

$$\lambda_{k-1}(H_{a}^{-D}(F)) \leq \lambda_k(H_{a}(F)) \leq \lambda_k(H_{a}^{-D}(F)).$$

(2.2)

Thus, if $H_{a}^{-D}(F)$ exhibits a discrete spectrum below $\lambda_1^0$, then $H_{a}(F)$ do as well.

We mention that its a sufficient condition.

Let us consider the eigenvalue equation is given by

$$H_{a}^{-D}(F)f(r,\theta,z) = \lambda f(r,\theta,z).$$

(2.3)

This equation is solved by separating variables and considering $f(r,\theta,z) = R(r)P(\theta)Z(z)$.

We divide the equation (2.3) by $f$, we obtain

$$\frac{1}{R}(R'' + \frac{1}{r}R') + \frac{1}{r^2} \frac{P''}{P} + \frac{Z''}{Z} - Fz = -\lambda.$$  

(2.4)

Plugging the last expression in equation (2.4) and first separate the term $\frac{P''}{P}$ which has all the $\theta$ dependance. Using the fact that the problem has an axial symmetry and the solution has to be $2\pi$ periodic and single value in $\theta$, we obtain $\frac{P''}{P}$ should be a constant $-m^2$ for $m \in \mathbb{Z}$.

Second, we separate $Z$ by putting all the $z$ dependence in one term so that $\frac{Z''}{Z} - Fz$ can only be constant. The constant is taken as $\lambda_\infty^n$ for $n \in \mathbb{N}$.

Finally, we write the equation (2.4) as a function of $R$

$$R''(r) + \frac{1}{r}R'(r) + [\lambda - \lambda_\infty^n - \frac{m^2}{r^2}]R(r) = 0.$$  

(2.5)

We notice that the equation (2.5), 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 (2.5) is given by $R(r) = c J_m(\eta r)$, where $c \in \mathbb{R}^*$, $\eta^2 = \lambda - \lambda_\infty^n$ and $J_m$ is the Bessel function of first kind of order $m$.

We assume that

$$R(a) = 0 \iff J_m(\eta a) = 0 \iff a\eta = x_{m,k}.$$  

(2.6)

Where $x_{m,k}$ is the $k$–th positive zero of the Bessel function $J_m$ (see [1]).

Then $H_{a}^{-D}(F)$ has a sequence of eigenvalues [1, 7], given by

$$\lambda_{n,m,k} = \left(\frac{x_{m,k}}{a}\right)^2 + \lambda_\infty^n.$$  

the condition

$$\lambda_{n,m,k} < \lambda_0^1,$$  

(2.7)
yields that \( n = 1 \), so we get
\[
\lambda_{1,m,k} = \left( \frac{x_{m,k}}{a} \right)^2 + \lambda_1^1. \tag{2.8}
\]
This yields that the condition (2.7) to be fulfilled, will depends on the value of \( \left( \frac{x_{m,k}}{a} \right)^2 \). We recall that \( x_{m,k} \) are the positive zeros of the Bessel function \( J_m \).

So, for any \( \lambda_a \) eigenvalue of \( H_a(F) \), there exists \( m, k, m', k' \in \mathbb{N} \), such that
\[
\left( \frac{x_{m',k'}}{a} \right)^2 + \lambda_1^1 \leq \lambda_a \leq \left( \frac{x_{m,k}}{a} \right)^2 + \lambda_1^1. \tag{2.9}
\]
Using the boundary conditions, we obtain that the operators \( h_0(F) \) and \( h_\infty(F) \) have a sequence of eigenvalues

- in the case of weak electric field respectively given by:
  \[
  \lambda_0^n = \left( \frac{n\pi + \sqrt{n^2\pi^2 + d^2 F^2}}{2d} \right)^2 + o(F); \quad n \in \mathbb{N}^*.
  \]
  \[
  \lambda_\infty^n = \left( \frac{(2n+1)\pi + \sqrt{(2n+1)^2(\frac{\pi}{2})^2 + d^2 F^2}}{2d} \right)^2 + o(F); \quad n \in \mathbb{N}.
  \]

- in the case of strong electric field respectively given by:
  \[
  \lambda_0^n = -\alpha_n F_\frac{2}{3}, \quad n \in \mathbb{N}^*.
  \]
  \[
  \lambda_\infty^n = -\alpha'_n F_\frac{2}{3}, \quad n \in \mathbb{N}^*.
  \]
Where \( \alpha_n \) and \( \alpha'_n \) are the \( n \)-th negative zeros of the Airy functions \( Ai \) and \( Ai' \) respectively. Consequently, we have

- in the case of weak electric field respectively given by:
  \[
  \lambda_0^1 = \left( \frac{\pi + \sqrt{\pi^2 + d^2 F^2}}{2d} \right)^2 + o(F).
  \]

- in the case of strong electric field respectively given by:
  \[
  \lambda_0^1 = -\alpha_1 F_\frac{2}{3} \simeq 2.3381 F_\frac{2}{3}.
  \]

**Remark 2.1.** Using the inequality (2.9), for \( a \) big enough, if \( \lambda_a \) is an eigenvalue of the operator \( H_a(F) \) less then \( \lambda_0^1 \) then we have
\[
\lambda_a = \lambda_\infty^1 + o\left( \frac{1}{a^2} \right).
\]

In the following of this section, we represent the area of existence of the first three eigenvalues of \( H_a(F) \) \( \lambda_0^1, \lambda_0^2 \) and \( \lambda_0^3 \) and the threshold of appearance of eigenvalues, for the electric field of constant weak intensity \( F \) in Figure 2, and for \( F \) strong enough in Figure 3.

We observe that the area of existence of the eigenvalues of \( H_a(F) \) is proportional to the intensity \( F \).
Figure 2. We represent
\[
\lambda_\infty + \left( \frac{x(i)}{a} \right)^2
\]
where \(x(1), x(2), x(3)\) are the first three zeros of the Bessel functions increasingly ordered.
Area of existence of the first three eigenvalues of $H_a(F)$ for $d = 1$ and $F = 10$. 

$$\lambda^1_{\infty} + \left(x(1)/a\right)^2$$

$$\lambda^1_{\infty} + \left(x(2)/a\right)^2$$

$$\lambda^1_{\infty} + \left(x(3)/a\right)^2$$
In the Figure 4, we set the $F$ intensity of the electric field by a low value 0.1. We represent the curve of the number of eigenvalues of the operator $H_a^D(F)$ a function of the quotient of the radius value $a$ by the width of the strip $d$.

**Figure 4.** The number of eigenvalues of the operator $H_a^D(F)$ a function of $a/d$. 
In the Figure 5, Similarly we set the intensity $F$ of the electric field $l’\text{intensit du champ lectrique}$ by a great value 10. We represent the curve of the number of eigenvalues of the operator $H_a^{D}(F)$ a function of the quotient of the radius value $a$ by the width of the strip $d$.

**Figure 5.** The number of eigenvalues of the operator $H_a^{D}(F)$ a function of $a/d$. 
In Figures 6 and 7, we set the quotient of the radius value \( a \) by the width of the strip \( d \) by real 10. We represent the curve of the number of eigenvalues of the operator \( H_a^D(F) \) a function of the intensity \( F \) of the electric field.

**Figure 6.** The number of eigenvalues of the operator \( H_a^D(F) \) a function of the intensity \( F \).
Figure 7. The number of eigenvalues of the operator $H^D_a(F)$ a function of the intensity $F$.

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