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Original article

On the discrete spectrum of a quantum waveguide with Neumann windows in presence of exterior field

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ABSTRACT The discrete spectrum of the Hamiltonian describing a quantum particle living in three dimensional straight layer of width d in the presence of a constant electric field of strength F is studied. The Neumann boundary conditions are imposed on a finite set of bounded domains (windows) posed at one of the boundary planes and the Dirichlet boundary conditions on the remaining part of the boundary (it is a reduced problem for two identical coupled layers with symmetric electric field). It is proved that such system has eigenvalues below the lower bound of the essential spectrum for any $F \geq 0$. Then we closer examine a dependence of bound state energies on F and window's parameters, using numerical methods.

KEYWORDS quantum waveguide, Schrödinger operator, discrete spectrum.

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1. Introduction

The study of quantum waveguides is an active field of research since 1990th, when replication of nanoelectronic devices on the scale of nanometres became possible. On these scales, wave nature of an electron becomes vital and modelling the system by one-particle Schrödinger equation with various boundary conditions, becomes acceptable. In this context, boundary conditions are imposed on various surfaces in 2D and 3D, restricting the waveguide, such as infinite planar layers, strips or cylinders, usually, with introducing of a perturbation, which affects the spectrum. There are results for a number of different types of perturbations, including deformations of geometry [1–8], addition of a potential [5] or magnetic field [9, 10]. The Laplace operator can be perturbed by differential operator [11], or, for more general case of operator perturbation, see [12]. A multi-particle problem for such systems was also considered in a number of works ([13–16]).

In the present work, the perturbation by changing the type of the boundary condition on a part of the boundary is considered. Let E_j and $f_j(\mathbf{r})$, $j = 1, 2, ...$ be eigenvalues and the corresponding eigenfunctions of the Laplacian with the following conditions: a 3D layer, confined between two planes, with the Dirichlet boundary conditions imposed on them:

$$f_j(\mathbf{r})|_{\partial\Omega_D} = 0. \tag{1}$$

One of the planes contains a finite domain, there are a finite number of regions, on which the boundary condition is replaced by the Neumann one:

$$\mathbf{n}\nabla f_j(\mathbf{r})|_{\partial\Omega_N} = 0, \tag{2}$$

where $\mathbf{n}$ is a unit vector normal to the surface. The Neumann part of the boundary is referred to as "window(s)". The problems of this type are called Zaremba problems [17].

In this context, we refer to the main results in [12, 18–25] and references therein. For the case of 2D strip, where there is a Neumann condition on a part of boundary, representing a window, existence of bound states was proven in [26, 27], and in [21], it was shown that with the increase of window width, the number of bound states rises and their energies fall. For the case of 3D straight strip with circular Neumann windows, see [28, 29], where the existence of bound states is proven and asymptotics of energies for large window radii were given.

An additional magnetic field in a waveguide with the Neumann window is considered in [9, 30]. In [30], for a $3D$ waveguide with the Aharonov-Bohm magnetic field, the authors proved existence of threshold window length $a_0 > 0$, such that for $a < a_0$, the discrete spectrum is empty, and obtained a condition for bound state existence.

For systems of a type studied in this paper, but with uniform electric field in both layers, there are results in [31], where dependence on window's parameters was calculated numerically. Analogous numerical results for similar system is in [32]. Further results, concerning existence of bound states and their classification, extended to the multi-particle case were received in [13].

In general, the investigations of the quantum waveguides mostly cover the case of external magnetic field [9, 10, 30, 33], while there are many unanswered questions concerning waveguides in electric field alone. In [34], the case of bent tubes with non-linear electrostatic potential was investigated. In this case it was shown that Stark effect is non-trivial due to perturbations. Generally, mixed boundary conditions or curvature, affect propagation of waves, creating a situation analogous to the shock wave picture.

The paper is organized as follows. In section 2, we define the model of the quantum waveguide, give properly the functional domain, and study the self-adjointness of the operator. Then we show the stability of the essential spectrum when we consider perturbation by varying boundary condition from Dirichlet to Neumann. Section 3 is devoted to the main result and its proof. It deals with the effect of the electric field on our system. Precisely, we prove that such system exhibits discrete eigenvalues below the essential spectrum for any $F \geq 0$. The last section is devoted to numerical results for specifying the dependence of eigenvalues on system parameters.

2. The model

2.1. Geometry of the system

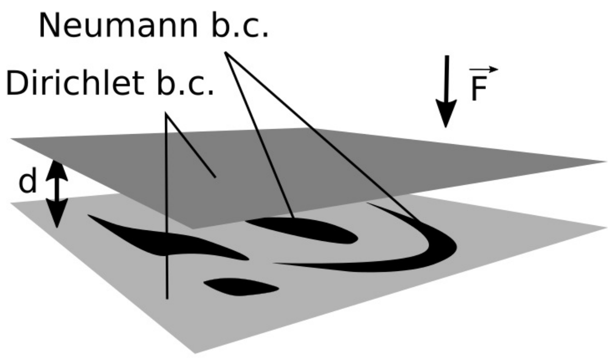

FIG. 1. The waveguide with a family of windows and two different boundary conditions with orthogonal electric field

The system we are going to study is given in Fig. 1. We consider a quantum particle confined inside two parallel layers coupled through a system of windows. We assume the Dirichlet condition at the layer boundaries. We simulate windows as regions at the boundary where the Neumann boundary conditions are imposed. This model is appropriate if the layers have identical widths and the electric field is symmetric in respect to the plane separating the layers. In this case, it is sufficient to deal with the Hamiltonian $H(F)$ for one layer between the planes $z = 0$ and $z = d$. We shall denote this configuration space by Ω,

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

We assume that the considered particle is under the influence of a homogeneous electric field of intensity E orthogonal to the layers. We denote $F := Eq$, where q is the particle charge. We assume that $F \geq 0$. Let $(\gamma_i)_{1 \leq i \leq p}$ be a finite family of bounded and open sets lying on the boundary of Ω at $z = 0$.

We set $\Gamma = \partial\Omega \setminus (\cup_{i=1}^{p} \gamma_i)$. We consider the Dirichlet boundary conditions on Γ and the Neumann boundary conditions on $\cup_{i=1}^{p} \gamma_i$. The black surface in Fig. 1 corresponds to the Neumann boundary condition, while the grey surfaces correspond to the Dirichlet condition.

2.2. The Hamiltonian

Let us define the self-adjoint operator on $L^2(\Omega)$ corresponding to the particle Hamiltonian $H(F)$. For this purpose we use quadratic forms. Precisely, let $q(F)$ be the quadratic form

$$q(F)[u, v] \;=\; \int_\Omega \big(\nabla u \overline{\nabla v} + F z u \overline{v}\big) dx dy dz, \quad u, v \in \mathcal{D}(q(F)), \tag{3}$$

where $\mathcal{D}(q(F)) := \big\{u \in \mathrm{H}^1(\Omega), u\lceil\Gamma = 0\big\}$, $\mathrm{H}^1(\Omega)$ is the standard Sobolev space and $u\lceil\Gamma$ is the trace of the function u on Γ. It follows that $q(F)$ is a densely defined, symmetric, positive and closed quadratic form [35]. We denote the unique self-adjoint operator associated with $q(F)$ by $H(F)$ and its domain by $\mathcal{D}$. It is the Hamiltonian describing our system (we will use the atomic units $2m = h = q = 1$ to simplify the equation). From [36] (page 276) and [35](page 263), one infers that the domain $\mathcal{D}$ of $H(F)$ is as follows

$$\mathcal{D} = \{u \in \mathrm{H}^1(\Omega);\ -\Delta u \in \mathrm{L}^2(\Omega), u\lceil\Gamma = 0, \frac{\partial u}{\partial z}\lceil\cup_{i=1}^p \gamma_i = 0\} \tag{4}$$

and

$$H(F)u = (-\Delta + Fz)u, \quad \forall u \in \mathcal{D}. \tag{5}$$

2.3. Preliminary: Cylindrical coordinates

As γ_i are open sets, they contain a small disc of radius a, $a > 0$. Let us mark this disc on the plane $z = 0$ as $\gamma(a)$. Without loss of generality, we assume that the center of $\gamma(a)$ is the point $(0, 0, 0)$ and $\gamma(a) \subset \gamma_{i_0}$ for some $1 \le i_0 \le p$;

$$\gamma(a) = \{(x, y, 0) \in \mathbb{R}^3;\ x^2 + y^2 \le a^2\}. \tag{6}$$

There exists b, $0 < a < b$ such that for all i, $1 \le i \le p$, one has $\gamma_i \subset \gamma(b)$. We denote, respectively, by $H_b(F)$ and $H_a(F)$ the operator (5) with unique disc window with radius b and a, respectively. For $i \in \{a, b\}$, we denote the domain of $H_i(F)$ by

$$\mathcal{D}(i) = \{u \in \mathrm{H}^1(\Omega); \quad -\Delta u \in \mathrm{L}^2(\Omega), u\lceil\Gamma = 0, \frac{\partial u}{\partial z}\lceil\gamma(i) = 0\}.$$

Using the inclusion for the domains;

$$\mathcal{D}(b) \subseteq \mathcal{D} \subseteq \mathcal{D}(a),$$

one obtains the following bracketing [35]

$$H_b(F) \le H(F) \le H_a(F). \tag{7}$$

Let us notice that the new domains $\mathcal{D}(a)$ and $\mathcal{D}(b)$ have a cylindrical symmetry. Therefore, it is natural to consider the cylindrical coordinates system (r, θ, z). Indeed, we have that

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

We denote by $\langle\cdot,\cdot\rangle_r$, the scalar product in $L^2(\Omega, dxdydz) = L^2((0, +\infty) \times [0, 2\pi[\times[0, d], rdrd\theta dz)$ given by the formula

$$\langle f, g\rangle_r = \int_{(0,+\infty)\times[0,2\pi[\times[0,d]} fgrdrd\theta dz.$$

We denote the gradient in cylindrical coordinates by ∇_r. The Laplace operator in cylindrical coordinates is given by the following expression

$$\Delta_{r,\theta,z} = \frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial}{\partial r}) + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{d^2}{dz^2}. \tag{8}$$

2.4. A few known facts

Let us start this subsection by recalling that in the particular case when $a = 0$, one has $H_0(F)$, the Dirichlet Stark operator, and $b = +\infty$ one has $H_\infty(F)$, the Dirichlet-Neumann Stark operator. For $\bullet \in \{0, \infty\}$, let

$$H_\bullet(F) = (-\Delta_{\mathbb{R}^2}) \otimes I_d \oplus I_d \otimes (h_\bullet(F)), \text{on } L^2(\mathbb{R}^2) \otimes L^2([0, d]),$$

where the transverse operator $h_\bullet(F) := -\Delta_{[0,d]} + Fz$ defined on $L^2([0, d])$ with the Dirichlet boundary conditions at d and 0 for $\bullet = 0$ and Neumann boundary at 0 for $\bullet = \infty$. The operator $h_\bullet(F)$ has purely discrete spectrum. We denote by $\lambda_\bullet^1$ the lowest transverse mode. Using Dirichlet Neumann bracketing, (see [35]), one obtains that

$$[\lambda_0^1, +\infty) = \sigma(H_0(F)) \subseteq \sigma(H_a(F)) \subseteq \sigma(H(F)) \subseteq \sigma(H_b(F)) \subseteq \sigma(H_\infty) = [\lambda_\infty^1, +\infty). \tag{9}$$

2.5. Stability of the essential spectrum

Using the property that the essential spectrum is preserved under compact perturbations, we are going to obtain its stability. We recall that the essential spectrum of an operator A which we denote by $\sigma_{ess}(A)$ consists of the point λ at which $\Re(\lambda I - A)$, the range of $\lambda I - A$ is not closed and of eigenvalues of infinite multiplicity. The discrete spectrum is the set of isolated eigenvalues with finite multiplicities. It is denoted by $\sigma_{dis}(A)$.

Theorem 2.1. *Let $H(F)$ be the operator given by (5). Then,*

$$\sigma_{ess}(H(F)) = [\lambda_0^1, +\infty[. \tag{10}$$

Proof.

First, let us note that an equation analogous to (9) also holds for the essential spectrum. Let $\Omega^{-,a}$ be the cylinder $\gamma(a) \times [0, d]$ and $\Omega^{+,a}$ the outside part of $\Omega^{-,a}$ in Ω. So

$$L^2(\Omega) = L^2(\Omega^{+,a}) \oplus L^2(\Omega^{-,a}). \tag{11}$$

Let H be, formally, the operator analogous to $H_a(F)$ but with imposing an extra Dirichlet condition on both sides of the lateral surface of the cylinder $\Omega^{-,a}$. The decomposition (11) yields that $H = H_1 \oplus H_2$. The operator H_2 defined on bounded domain $\Omega^{-,a}$ is known to have a discrete spectrum and $\sigma_{ess}(H_2)$ is empty. So $\sigma_{ess}(H) = \sigma_{ess}(H_1)$.

Using Wolf result [37] for operators of the form

$$A = -\sum_i \frac{\partial^2}{\partial x_i^2} + \sum_i a_i(x)\frac{\partial}{\partial x_i} + b(x), \tag{12}$$

one obtains that for $\lambda < 0$, the difference of resolvents,

$$(\lambda I - H_a(F))^{-1} - (\lambda I - H)^{-1}, \tag{13}$$

is a compact operator. It follows that $(\lambda I - H)^{-1}$ is a compact perturbation of $(\lambda I - H_a(F))^{-1}$. By Weyl Theorem, it immediately follows that the essential spectrum of $(\lambda I - H)^{-1}$ and $(\lambda I - H_a(F))^{-1}$ are the same and by the spectral mapping theorem one concludes that

$$\sigma_{ess}(H) = \sigma_{ess}(H_a(F)). \tag{14}$$

As the steps in the previous study are independent of a, we get

$$\sigma_{ess}(H) = \sigma_{ess}(H_1) = \sigma_{ess}(H_b(F)) = \sigma_{ess}(H(F)) = \sigma_{ess}(H_a(F)). \tag{15}$$

Using cylindrical symmetry once more, we consider H as acting on

$$L^2((a, +\infty) \times [0, 2\pi] \times [0, d], rdrd\theta dz).$$

One can write

$$H_1 = -\Delta_{(a,+\infty)\times[0,2\pi]} \otimes I_{d_{[0,d]}} \oplus I_{d_{(a,+\infty)}\times[0,2\pi]} \otimes h_0(F).$$

So

$$\sigma_{ess}(H_1) = [\lambda_0^1, +\infty).$$

By (15), one ends the proof.

□

3. Existence of eigenvalues for one-particle Hamiltonian

In the last subsection, we have proved that

$$\sigma_{ess}\big(H(F)\big) = [\lambda_0^1, +\infty[. \tag{16}$$

So, by this and the min-max principle [35] we conclude that if the discrete spectrum exists, it lies below λ_0^1. The main result of the paper is the following:

Theorem 3.1. *For any $F \geq 0$, the operator $H(F)$ has at least one isolated eigenvalue below λ_0^1 i.e*

$$\sigma_{dis}\big(H(F)\big) \neq \emptyset.$$

As it was already mentioned earlier, the result differs from one, corresponding to two-dimensional waveguides considered in [34], which shows that the existence of the discrete spectrum depends on the values of F. The absence of eigenvalues for some F in [34] is due to the fact that the field in the waveguide has a tilt, which gives one two parts of the operator with different essential spectra. In the present paper we deal with electric field symmetric in respect to the plane separating the layers.

It is important to notice that electric and magnetic fields have different effects on the spectrum of our system. Indeed, it was proved in [30] that in the case of magnetic filed, there is some critical values of window radius to get existence of discrete spectrum.

The proof is based on the Goldstone and Jaffe trick [38], boosting the trial function by a deformation in the Neumann region. First we note that due to the fact that

$$\sigma(H(F)) \subseteq \sigma(H_a(F)); \quad \sigma_{ess}(H_a(F)) = \sigma_{ess}(H(F)),$$

one obtains

$$\sigma_{dis}(H_a(F)) \neq \emptyset \Rightarrow \sigma_{dis}(H(F)) \neq \emptyset. \tag{17}$$

Let us consider the quadratic form Q_r

$$Q_r[f, g] \quad = \quad \int_{(0,+\infty)\times[0,2\pi[\times[0,d]} \nabla_r f\overline{\nabla_r g} + Fzf\overline{g}rdrd\theta dz,$$

with the domain

$$\mathcal{D}_r \quad = \quad \big\{f \in L^2(\Omega, rdrd\theta dz); \nabla_r f \in L^2(\Omega, rdrd\theta dz); f\lceil\Gamma = 0\big\}.$$

Consider the quadratic function Q defined by

$$Q[\Phi] \quad = \quad Q_r[\Phi] - \lambda_0^1 \|\Phi\|^2_{L^2(\Omega, rdrd\theta dz)}. \tag{18}$$

Since the essential spectrum of $H_a(F)$ starts at λ_0^1, if we construct a trial function $\Phi \in \mathcal{D}_r$ such that $Q[\Phi]$ has a negative value then the task is achieved. Using the quadratic form domain, Φ must be continuous inside, but not necessarily smooth. Let χ_1 be the positive eigenfunction associated to λ_0^1 of the operator $h_0(F)$ $(ie. -\chi_1'' = (\lambda_0^1 - Fz)\chi_1)$, with $\|\chi_1\| = 1$ (see [36]).
For $\Phi(r, \theta, z) = \varphi(r)\chi_1(z)$, we compute

$$\begin{aligned}
Q[\Phi] &= Q_r[\Phi] - \lambda_0^1 \|\Phi\|^2_{L^2(\Omega, rdrd\theta dz)} \\
&= \int_{(0,+\infty)\times[0,2\pi[\times[0,d]} \Big(|\chi_1(z)|^2 |\varphi'(r)|^2 + |\chi_1'(z)|^2 |\varphi(r)|^2 \\
&+ Fz|\chi_1(z)|^2 |\varphi(r)|^2 \Big) rdrd\theta dz - \lambda_0^1 \|\varphi\chi_1\|^2_{L^2(\Omega, rdrd\theta dz)} \\
&= 2\pi \|\varphi'\|^2_{L^2((0,+\infty), rdr)} \\
&+ \int_{(0,+\infty)\times[0,2\pi[\times[0,d]} \Big(\big(\lambda_0^1 - Fz\big) |\chi_1(z)|^2 |\varphi(r)|^2 \Big) rdrd\theta dz \\
&+ \int_{(0,+\infty)\times[0,2\pi[\times[0,d]} Fz|\chi_1(z)|^2 |\varphi(r)|^2 rdrd\theta dz - \lambda_0^1 \|\varphi\chi_1\|^2_{L^2(\Omega, rdrd\theta dz)} \\
&= 2\pi \|\varphi'\|^2_{L^2((0,+\infty), rdr)}.
\end{aligned} \tag{19}$$

Now, let us consider an interval $I = [0, b]$ for a positive b, $b > a$, and a function $\varphi \in \mathcal{S}([0, +\infty[)$ such that $\varphi(r) = 1$ for $r \in I$. We also define a family $\{\varphi_\tau : \tau > 0\}$ by

$$\varphi_\tau(r) = \begin{cases} \varphi(r) & \text{if } r \in (0, b) \\ \varphi(b + \tau(\ln r - \ln b)) & \text{if } r \geq b. \end{cases} \tag{20}$$

We have,

$$\begin{aligned}
\|\varphi_\tau'\|_{L^2([0,+\infty[, rdr)} &= \int_{(0,+\infty)} |\varphi_\tau'(r)|^2 rdr \\
&= \int_{[b,+\infty[} \frac{\tau^2}{r^2} |\varphi'(b + \tau(\ln r - \ln b))|^2 rdr \\
&= \tau \int_{[b,+\infty[} \frac{\tau}{r} |\varphi'(b + \tau(\ln r - \ln b))|^2 dr \\
&= \tau \int_{(0,+\infty)} |\varphi'(s)|^2 ds \\
&= \tau \|\varphi'\|^2_{L^2([0,+\infty[)}.
\end{aligned} \tag{21}$$

We set

$$\begin{aligned}
\Phi_{\tau,\varepsilon}(r, z) &= \varphi_\tau(r)[\chi_1(z) + \varepsilon\chi_1(z)\phi^2(r)] \\
&= \varphi_\tau(r)\chi_1(z) + \varepsilon\varphi_\tau(r)\chi_1(z)\phi^2(r) \\
&= \Phi_{1,\tau}(r, z) + \Phi_{2,\tau,\varepsilon}(r, z).
\end{aligned} \tag{22}$$

Then,

$$\begin{aligned}
Q[\Phi_{\tau,\varepsilon}] &= Q[\Phi_{1,\tau} + \Phi_{2,\tau,\varepsilon}] \\
&= Q_r[\Phi_{1,\tau} + \Phi_{2,\tau,\varepsilon}] - \lambda_0^1 \|\Phi_{1,\tau} + \Phi_{2,\tau,\varepsilon}\|^2_{L^2(\Omega, rdrd\theta dz)} \\
&= Q_r[\Phi_{1,\tau}] - \lambda_0^1 \|\Phi_{1,\tau}\|^2_{L^2(\Omega, rdrd\theta dz)} + Q_r[\Phi_{2,\tau,\varepsilon}] - \lambda_0^1 \|\Phi_{2,\tau,\varepsilon}\|^2_{L^2(\Omega, rdrd\theta dz)} \\
&+ 2\langle \nabla_r \Phi_{1,\tau}, \nabla_r \Phi_{2,\tau,\varepsilon} \rangle_r + 2F\langle z\Phi_{1,\tau}, \Phi_{2,\tau,\varepsilon} \rangle_r - 2\lambda_0^1 \langle \Phi_{1,\tau}, \Phi_{2,\tau,\varepsilon} \rangle_r.
\end{aligned}$$

Using the properties of χ_1 and taking into account (19) and (21), one obtains

$$\begin{aligned}
Q_r[\Phi_{1,\tau}] - \lambda_0^1 \|\Phi_{1,\tau}\|^2_{L^2(\Omega, rdrd\theta dz)} &= Q[\varphi_\tau \chi_1] \\
&= 2\pi \|\varphi_\tau'\|^2_{L^2((0,+\infty), rdr)} \\
&= 2\pi\tau \|\varphi'\|^2_{L^2((0,+\infty))}.
\end{aligned}$$

As the supports of φ and ϕ are disjoint, one gets

$$\begin{aligned}
& Q_r[\Phi_{2,\tau,\varepsilon}] - \lambda_0^1 \|\Phi_{2,\tau,\varepsilon}\|^2 \\
= & \int_{(0,+\infty)\times[0,2\pi[\times[0,d]} \left(\left| \nabla_r \left(\varepsilon \varphi_\tau(r) \chi_1(z) \phi(r)^2 \right) \right|^2 \right. \\
+ & \left. \varepsilon^2 F z |\varphi_\tau(r)|^2 |\chi_1(z)|^2 \left|\phi^2(r)\right|^2 \right) r dr d\theta dz - \varepsilon^2 \lambda_0^1 \|\varphi_\tau \chi_1 \phi^2\|^2_{\mathrm{L}^2(\Omega, r dr d\theta dz)} \\
= & \int_{(0,+\infty)\times[0,2\pi[\times[0,d]} 4\varepsilon^2 |\chi_1(z)|^2 |\phi'(r)\phi(r)\varphi(r)|^2 + \varepsilon^2 |\chi_1'(z)|^2 |\varphi_\tau(r)\phi^2(r)|^2 \\
+ & \varepsilon^2 F z |\varphi_\tau(r)\chi_1(z)\phi^2(r)|^2 r dr d\theta dz - \varepsilon^2 \lambda_0^1 \|\varphi_\tau \chi_1 \phi^2\|^2_{\mathrm{L}^2(\Omega, r dr d\theta dz)} \\
\le & \varepsilon^2 d 2\pi \Big(4 \|\phi\phi'\varphi_\tau(r)\|^2_{\mathrm{L}^2([0,+\infty[, r dr)} + F d \|\varphi_\tau(r)\phi^2\|^2_{\mathrm{L}^2([0,+\infty[, r dr)} \\
+ & \|\chi_1'(z)\varphi_\tau(r)\phi^2(r)\|^2_{\mathrm{L}^2([0,+\infty[\times[0,d], r dr dz)} - \lambda_0^1 \|\phi^2\|^2_{\mathrm{L}^2([0,+\infty[, r dr)} \Big).
\end{aligned}$$

As the supports of φ_τ and ϕ are disjoint, one obtains

$$\langle \nabla_r \Phi_{1,\tau}, \nabla_r \Phi_{2,\tau,\varepsilon} \rangle_r = \langle \nabla_r (\varphi_\tau \chi_1), \nabla_r (\varepsilon \varphi_\tau \chi \phi^2) \rangle_r = 0.$$

Using the fact that $-\chi_1'' = (\lambda_0^1 - Fz)\chi_1$ and properties of φ_τ and ϕ one gets to the following estimation:

$$\begin{aligned}
\langle (Fz - \lambda_0^1)\Phi_{1,\tau}, \Phi_{2,\tau,\varepsilon} \rangle_r &= \langle (Fz - \lambda_0^1)\varphi_\tau \chi_1, \varepsilon \varphi_\tau \chi_1 \phi^2 \rangle_r \\
&= \varepsilon \langle (Fz - \lambda_0^1)\chi_1, \chi_1 \phi^2 \rangle_r \\
&= \varepsilon \langle \chi_1'', \chi_1 \phi^2 \rangle_r \\
&= -\varepsilon \Big(2\pi \|\phi\|^2_{\mathrm{L}^2([0,+\infty[, r dr)} \int_0^d |\chi_1'(z)|^2 dz \Big) < 0.
\end{aligned}$$

Therefore, one has

$$\begin{aligned}
& Q[\Phi_{\tau,\varepsilon}] \le 2\pi\tau \|\varphi'\|^2_{L^2([0,+\infty[)} \\
& + \varepsilon^2 d 2\pi \Big(4\|\phi\phi'\|^2_{L^2([0,+\infty[, r dr)} + F d \|\varphi_\tau(r)\phi^2\|^2_{L^2([0,+\infty[, r dr)} \\
& + \|\chi_1'(z)\varphi_\tau(r)\phi^2(r)\|^2_{L^2([0,+\infty[\times[0,d], r dr dz)} - \lambda_0^1 \|\phi^2\|^2_{L^2((0,+\infty), r dr)} \Big) \\
& - \varepsilon \Big(2\pi \|\phi\|^2_{L^2((0,+\infty), r dr)} \int_0^d |\chi_1'(z)|^2 dz \Big). \qquad (23)
\end{aligned}$$

We notice that only the first term of the last equation depends on τ. The linear term in ε is negative and could be chosen sufficiently small so that it dominates over the quadratic one. Fixing this ε and then choosing τ sufficiently small, one makes the right hand side of (23) negative. So, $\sigma_{dis}(H_a(F)) \neq \emptyset$ by (17). This ends the proof of the Theorem. □

4. Numerical results and conclusion

In this section, we study the dependence of the discrete spectrum on system's parameters, to build an intuition about a system and suggest directions for further research. We use a finite element method and consider a case of a single circular window, with varying area (and elliptical window for the last result). In all calculations, we use atomic system of units, with $\hbar = e = 1$, $m = 0.5$ (e, m are the electron charge and mass, correspondingly). The colors of energy levels are consistent between all plots. Across all plots, the black line represents a lowest boundary of the essential spectrum.

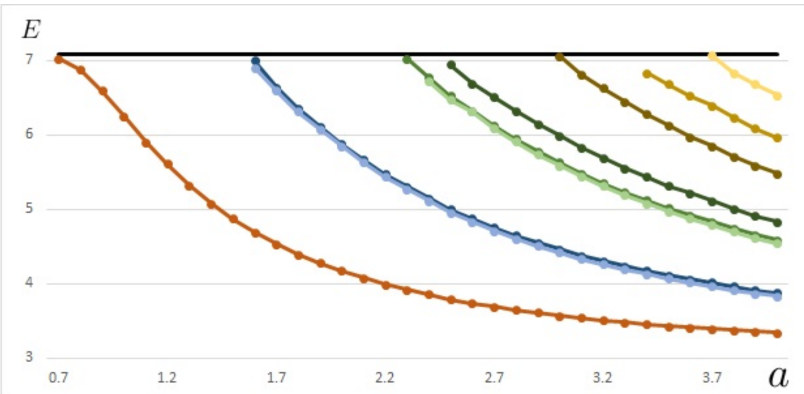

FIG. 2. Energies of bound states as functions of window radius a. Electric field intensity is fixed $F = 5$

First, we study dependence of the discrete spectrum on window's area, shown in Fig. 2. Here a field intensity is fixed, $F = 5$(which corresponds to middle value from the second plot). The essential spectrum is independent of window's parameters (Th. 2.1). Each bound state as a function of window's area is monotonically decreasing and a number of bound states is increasing. In accordance with the main theorem, the first bound state is lower then the boundary for all positive radii, and merges with the essential spectrum boundary as radius goes to zero.

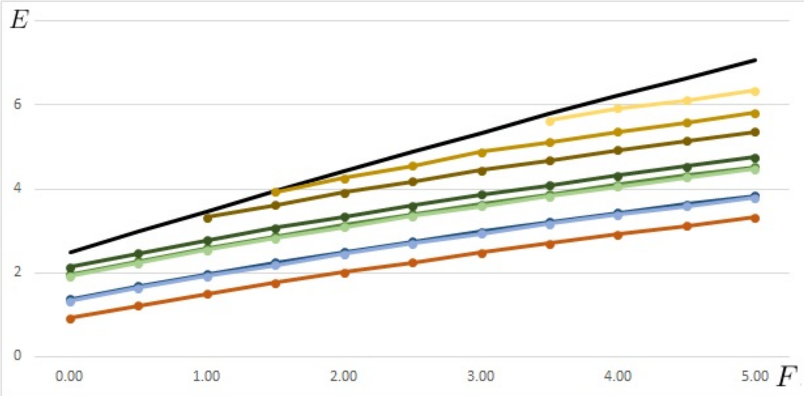

FIG. 3. Energies of bound states as functions of electric field intensity F. Window radius is fixed $a = 4$

Now we investigate the dependence of spectrum on the electric field intensity (Fig. 3). The window radius is fixed, $a = 4$ (which is the maximum radius from Fig. 2) An electric field isn't a local perturbation of a system, so it changes the essential spectrum, as well as discrete. Both spectra are increasing functions of F, but essential spectrum boundary grows faster, allowing more bound states to emerge, as field intensity increases.

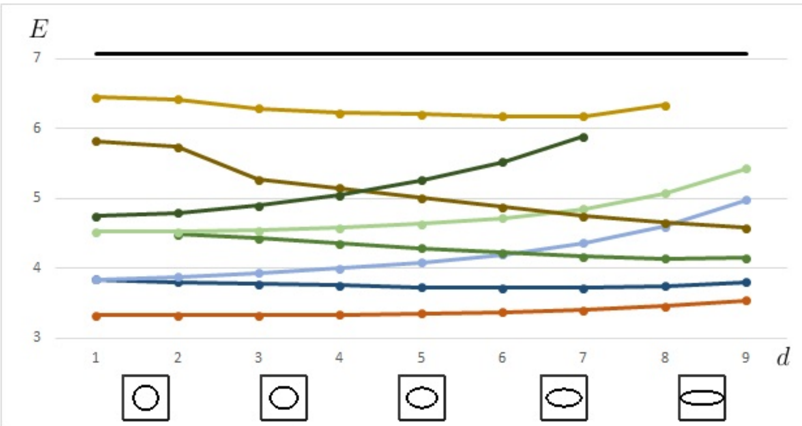

FIG. 4. Energies of bound states as functions of distance between foci of elliptical window. Window's area is constant (16π) and electric field intensity is fixed $F = 5$

Naturally, the question arises, about which parameters of the window are important. Particularly, how the discrete spectrum depends on window's area, perimeter and shape. These questions are considered in more detail for a similar system (same geometry, but homogeneous electrical field), in [13]. Here we consider influence of window's shape, particularly, we change an eccentricity of elliptical window, tracking different bound states, see Fig. 4. Area is fixed and corresponds to area of a circle with $a = 4$. Field intensity is fixed, $F = 5$. Here we can see different dynamics for different types of bound states (see [13] for more details of the classification).

To summarize, we considered a quantum system of parallel 3D layers of the same width, connected through a set of windows in a bounded region, with symmetrical external electrical field (Fig. 1). For such a system we have proven existence of at least one discrete eigenvalue below essential spectrum, for any size of windows. Then, numerically, we more closely examined a number of bound states, and their particular dependence on area of a window, different intensities of external field and shapes of a window. The results show a monotonic growth of bound states number with the increase of area or field intensity, for a circular opening. For the case of window shape's deformation, bound states form several distinct types, with consistent and predictable behaviour. The latter results suggest a number of directions for further research, such as getting bounds on number of bound states for certain types of windows and determining vital parameters of window's shape, when considering any particular bound state type.

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