

On the discrete spectrum of a spatial quantum waveguide with a disc window

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Abstract

In this study 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 prove that such system exhibits discrete eigenvalues below the essential spectrum for any $a > 0$. We give also a numeric estimation of the number of discrete eigenvalue as a function of $\frac{a}{d}$. When a tends to the infinity, the asymptotic of the eigenvalue is given.

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1 Introduction

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. See the monograph [10] and the references therein.

Exner et al. have done seminal works in this field. They obtained results in different contexts, we quote [2, 6, 8, 9]. Also in [12, 13, 14] 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.

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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 [3, 6, 7, 8] or by coupling of straight waveguides through windows [8, 10] were shown. The waveguide with Neumann boundary condition were also investigated in several papers [15, 17]. A possible next generalization are waveguides with combined Dirichlet and Neumann boundary conditions on different parts of the boundary. The presence of different boundary conditions also gives rise to nontrivial properties like the existence of bound states. 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 experiments.

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

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

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

$$\gamma(a) = \{(x, y, 0) \in \mathbb{R}^3; x^2 + y^2 \leq a^2\}. \quad (2.1)$$

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

2.1 The Hamiltonian

Let us define the self-adjoint operator on $L^2(\Omega)$ corresponding to the particle Hamiltonian H . This is will be done by the mean of quadratic forms. Precisely, let q_0 be the quadratic form

$$q_0(f, g) = \int_{\Omega} \nabla f \cdot \overline{\nabla g} d^3x, \text{ with domain } \mathcal{Q}(q_0) = \{f \in H^1(\Omega); f|_{\Gamma} = 0\}, \quad (2.2)$$

where $H^1(\Omega) = \{f \in L^2(\Omega) | \nabla f \in L^2(\Omega)\}$ is the standard Sobolev space and we denote by $f|_{\Gamma}$, the trace of the function f on Γ . It follows that q_0 is a densely defined, symmetric,

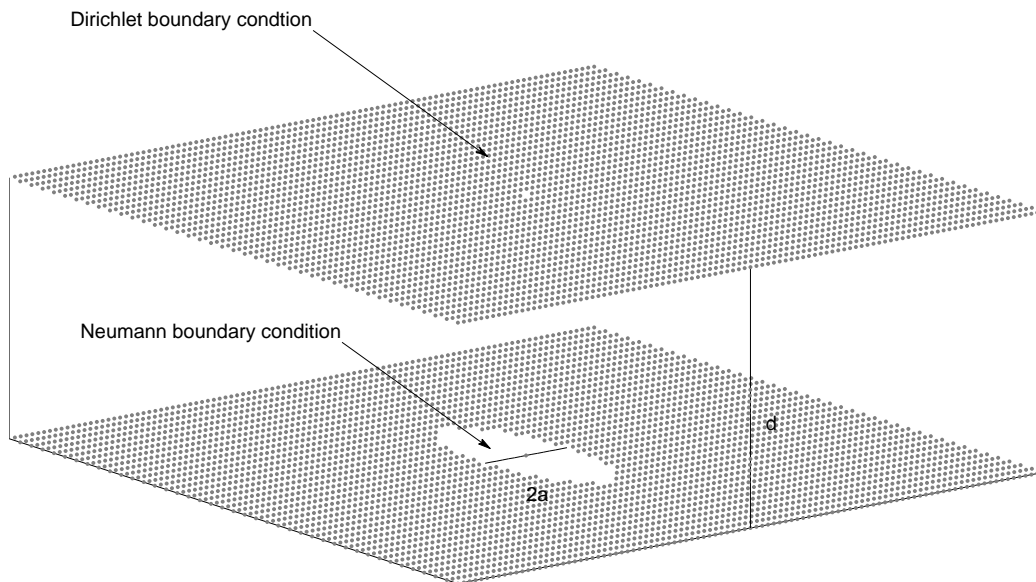


Figure 1: The waveguide with a disc window and two different boundaries conditions

positive and closed quadratic form. We denote the unique self-adjoint operator associated to q_0 by H and its domain by $D(\Omega)$. It is the hamiltonian describing our system. From [18] (page 276), we infer that the domain $D(\Omega)$ of H is

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

and

$$Hf = -\Delta f, \quad \forall f \in D(\Omega).$$

2.2 Some known facts

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

$$H = (-\Delta_{\mathbb{R}^2}) \otimes I \oplus I \otimes (-\Delta_{[0,d]}), \text{ on } L^2(\mathbb{R}^2) \otimes L^2([0, d]),$$

(see [18]) we get that the spectrum of H^0 is $[(\frac{\pi}{2d})^2, +\infty[$. Consequently, we have

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

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

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

An immediate consequence is the discrete spectrum lies in $\left[\left(\frac{\pi}{2d} \right)^2, \left(\frac{\pi}{d} \right)^2 \right]$.

2.3 Preliminary: Cylindrical coordinates

Let us 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

$$L^2(\Omega, dx dy dz) = L^2([0, +\infty[\times [0, 2\pi[\times [0, d], r dr d\theta dz),$$

We note by $\langle \cdot, \cdot \rangle_r$, the scalar product in $L^2(\Omega, dx dy dz) = L^2([0, +\infty[\times [0, 2\pi[\times [0, d], r dr d\theta dz)$ given by

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

We denote the gradient in cylindrical coordinates by ∇_r . While the Laplacian operator in cylindrical coordinates is given by

$$\Delta_{r,\theta,z} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + \frac{d^2}{dz^2}. \quad (2.3)$$

Therefore, the eigenvalue equation is given by

$$-\Delta_{r,\theta,z} f(r, \theta, z) = E f(r, \theta, z). \quad (2.4)$$

Since the operator is positive, we set $E = k^2$. The equation (2.4) is solved by separating variables and considering $f(r, \theta, z) = \varphi(r) \cdot \psi(\theta) \chi(z)$. Plugging the last expression in equation (2.4) and first separate χ by putting all the z dependence in one term so that $\frac{\chi''}{\chi}$ can only be constant. The constant is taken as $-s^2$ for convenience. Second, we separate the term $\frac{\psi''}{\psi}$ 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 $\frac{\psi''}{\psi}$ should be a constant $-n^2$ for $n \in \mathbb{Z}$. Finally, we get the following equation for φ

$$\varphi''(r) + \frac{1}{r} \varphi'(r) + \left[k^2 - s^2 - \frac{n^2}{r^2} \right] \varphi(r) = 0. \quad (2.5)$$

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.

3 The result

The main result of this note is the following Theorem.

Theorem 3.1 *The operator H has at least one isolated eigenvalue in $[(\frac{\pi}{2d})^2, (\frac{\pi}{d})^2]$ for any $a > 0$.*

Moreover for a big enough, if $\lambda(a)$ is an eigenvalue of H less than $\frac{\pi^2}{d^2}$, then we have.

$$\lambda(a) = \left(\frac{\pi}{2d}\right)^2 + o\left(\frac{1}{a^2}\right). \quad (3.6)$$

Proof. Let us start by proving the first claim of the Theorem. To do so, we define the quadratic form \mathcal{Q}_0 ,

$$\mathcal{Q}_0(f, g) = \langle \nabla f, \nabla g \rangle_r = \int_{]0, +\infty[\times]0, 2\pi[\times]0, d[} (\partial_r f \overline{\partial_r g} + \frac{1}{r^2} \partial_\theta f \overline{\partial_\theta g} + \partial_z f \overline{\partial_z g}) r dr d\theta dz, \quad (3.7)$$

with domain

$$\mathcal{D}_0(\Omega) = \{f \in L^2(\Omega, r dr d\theta dz); \nabla_r f \in L^2(\Omega, r dr d\theta dz); f|_{\Gamma} = 0\}.$$

Consider the functional q defined by

$$q[\Phi] = \mathcal{Q}_0[\Phi] - \left(\frac{\pi}{d}\right)^2 \|\Phi\|_{L^2(\Omega, r dr d\theta dz)}^2. \quad (3.8)$$

Since the essential spectrum of H starts at $(\frac{\pi}{d})^2$, if we construct a trial function $\Phi \in \mathcal{D}_0(\Omega)$ such that $q[\Phi]$ has a negative value then the task is achieved. Using the quadratic form domain, Φ must be continuous inside Ω but not necessarily smooth. Let χ be the first transverse mode, i.e.

$$\chi(z) = \begin{cases} \sqrt{\frac{2}{d}} \sin(\frac{\pi}{d}z) & \text{if } z \in (0, d) \\ 0 & \text{otherwise.} \end{cases} \quad (3.9)$$

For $\Phi(r, \theta, z) = \varphi(r)\chi(z)$, we compute

$$\begin{aligned} q[\Phi] &= \langle \nabla_r \varphi \chi, \nabla_r \varphi \chi \rangle - \left(\frac{\pi}{d}\right)^2 \|\varphi \chi\|_{L^2(\Omega, r dr d\theta dz)}^2, \\ &= \int_{]0, +\infty[\times]0, 2\pi[\times]0, d[} (|\chi(z)|^2 |\varphi'(r)|^2 + |\varphi(r)| |\chi'(z)|^2) r dr d\theta dz - \left(\frac{\pi}{d}\right)^2 \|\varphi \chi\|_{L^2(\Omega, r dr d\theta)}^2 \\ &= 2\pi \|\varphi'\|_{L^2([0, +\infty[, r dr)}^2 \end{aligned}$$

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

$$\varphi_\tau(r) = \begin{cases} \varphi(r) & \text{if } r \in (0, b) \\ \varphi(b + \tau(\ln r - \ln b)) & \text{if } r \geq b. \end{cases} \quad (3.10)$$

Let us write

$$\begin{aligned} \|\varphi'_\tau\|_{L^2((0,+\infty),rdr)} &= \int_{(0,\infty)} |\varphi'_\tau(r)|^2 r dr, \\ &= \int_{(b,+\infty)} \tau^2 |\varphi'(b + \tau(\ln r - \ln b))|^2 r dr, \\ &= \int_{(b,+\infty)} \frac{\tau^2}{r^2} |\varphi'(b + \tau(\ln r - \ln b))|^2 r dr, \\ &= \tau \int_{(b,+\infty)} \frac{\tau}{r} |\varphi'(b + \tau(\ln r - \ln b))|^2 dr, \\ &= \tau \int_{(0,+\infty)} |\varphi'(s)|^2 ds = \tau \|\varphi'\|_{L^2((0,+\infty))}^2. \end{aligned} \quad (3.11)$$

Let j be a localization function from $C_0^\infty(0, a)$ and for $\tau, \varepsilon > 0$ we define

$$\Phi_{\tau,\varepsilon}(r, z) = \varphi_\tau(r)[\chi(z) + \varepsilon j(r)^2] = \varphi_\tau(r)\chi(z) + \varphi_\tau\varepsilon j^2(r) = \Phi_{1,\tau,\varepsilon}(r, z) + \Phi_{2,\tau,\varepsilon}(r). \quad (3.12)$$

$$\begin{aligned} q[\Phi] &= q[\Phi_{1,\tau,\varepsilon} + \Phi_{2,\tau,\varepsilon}] \\ &= \mathcal{Q}_0[\Phi_{1,\tau,\varepsilon} + \Phi_{2,\tau,\varepsilon}] - \left(\frac{\pi}{d}\right)^2 \|\Phi_{1,\tau,\varepsilon} + \Phi_{2,\tau,\varepsilon}\|_{L^2(\Omega, r dr d\theta dz)}^2 \\ &= \mathcal{Q}_0[\Phi_{1,\tau,\varepsilon}] - \left(\frac{\pi}{d}\right)^2 \|\Phi_{1,\tau,\varepsilon}\|_{L^2(\Omega, r dr d\theta dz)}^2 + \mathcal{Q}_0[\Phi_{2,\tau,\varepsilon}] - \left(\frac{\pi}{d}\right)^2 \|\Phi_{2,\tau,\varepsilon}\|_{L^2(\Omega, r dr d\theta dz)}^2 \\ &\quad + 2\langle \nabla_r \Phi_{1,\tau,\varepsilon}, \nabla_r \Phi_{2,\tau,\varepsilon} \rangle_r - \left(\frac{\pi}{d}\right)^2 \langle \Phi_{1,\tau,\varepsilon}, \Phi_{2,\tau,\varepsilon} \rangle_r. \end{aligned}$$

Using the properties of χ , noting that the supports of φ and j are disjoint and taking into account equation (3.11), we get

$$q[\Phi] = 2\pi\tau \|\varphi'\|_{L^2(0,+\infty)}^2 - 8\pi d\varepsilon \|j^2\|_{L^2(0,+\infty)}^2 + 2\varepsilon^2\pi \{2\|jj'\|_{L^2(0,\infty),rdr}^2 - \left(\frac{\pi}{d}\right)^2 \|j^2\|_{L^2(0,\infty),rdr}^2\}. \quad (3.13)$$

Firstly, we notice that only the first term of the last equation depends on τ . Secondly, 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 the right hand side of (3.13) is negative. This ends the proof of the first claim.

The proof of the second claim is based on bracketing argument. Let us split $L^2(\Omega, r dr d\theta dz)$

as follows, $L^2(\Omega, r dr d\theta dz) = L^2(\Omega_a^-, r dr d\theta dz) \oplus L^2(\Omega_a^+, r dr d\theta dz)$, 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

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

Hence if $H_r^{-,D}$ exhibits a discrete spectrum below $\frac{\pi^2}{d^2}$, then H do as well. We mention that this is not a necessary condition. If we denote by $\lambda_j(H_a^{-,D})$, $\lambda_j(H_a^{-,N})$ and $\lambda_j(H)$, the j -th eigenvalue of $H_a^{-,D}$, $H_a^{-,N}$ and H respectively then, again the minimax principle yields the following

$$\lambda_j(H_a^{-,N}) \leq \lambda_j(H) \leq \lambda_j(H_a^{-,D}) \quad (3.14)$$

and for $2 \geq j$

$$\lambda_{j-1}(H_a^{-,D}) \leq \lambda_j(H) \leq \lambda_j(H_a^{-,D}). \quad (3.15)$$

$H_a^{-,D}$ has a sequence of eigenvalues [1, 19], given by

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

Where $x_{n,l}$ is the l -th positive zero of Bessel function of order n (see [1, 19]). The condition

$$\lambda_{k,n,l} < \frac{\pi^2}{d^2}, \quad (3.16)$$

yields that $k = 0$, so we get

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

This yields that the condition (3.16) to be fulfilled, will depends on the value of $\left(\frac{x_{n,l}}{a} \right)^2$. We recall that $x_{n,l}$ are the positive zeros of the Bessel function J_n . So, for any $\lambda(a)$, eigenvalue of H , there exists, $n, l, n', l' \in \mathbb{N}$, such that

$$\frac{\pi^2}{4d^2} + \frac{x_{n,l}^2}{a^2} \leq \lambda(a) \leq \frac{\pi^2}{4d^2} + \frac{x_{n',l'}^2}{a^2}. \quad (3.17)$$

The proof of (3.6) is completed by observing by that $x_{n,l}$ and $x_{n',l'}$ are independent from a . In Figure 2, the domain of existence of $\lambda_1(H)$, $\lambda_2(H)$ and $\lambda_3(H)$ are represented. \square

4 Numerical computations

This section is devoted to some numerical computations. In [11] and [16], the number of positive zeros of Bessel functions less than λ is estimated by $\frac{\lambda^2}{\pi^2}$ which is based on the approximate formula for the roots of Bessel functions for large l is

$$x_{n,l} \sim (n + 2l - \frac{1}{2}) \frac{\pi}{2}. \quad (4.18)$$

taking into account (3.14), we get that for, d and a positives such that $\frac{a^2}{d^2} < \lambda^* = 1,9276$, H has a unique discrete eigenvalue.

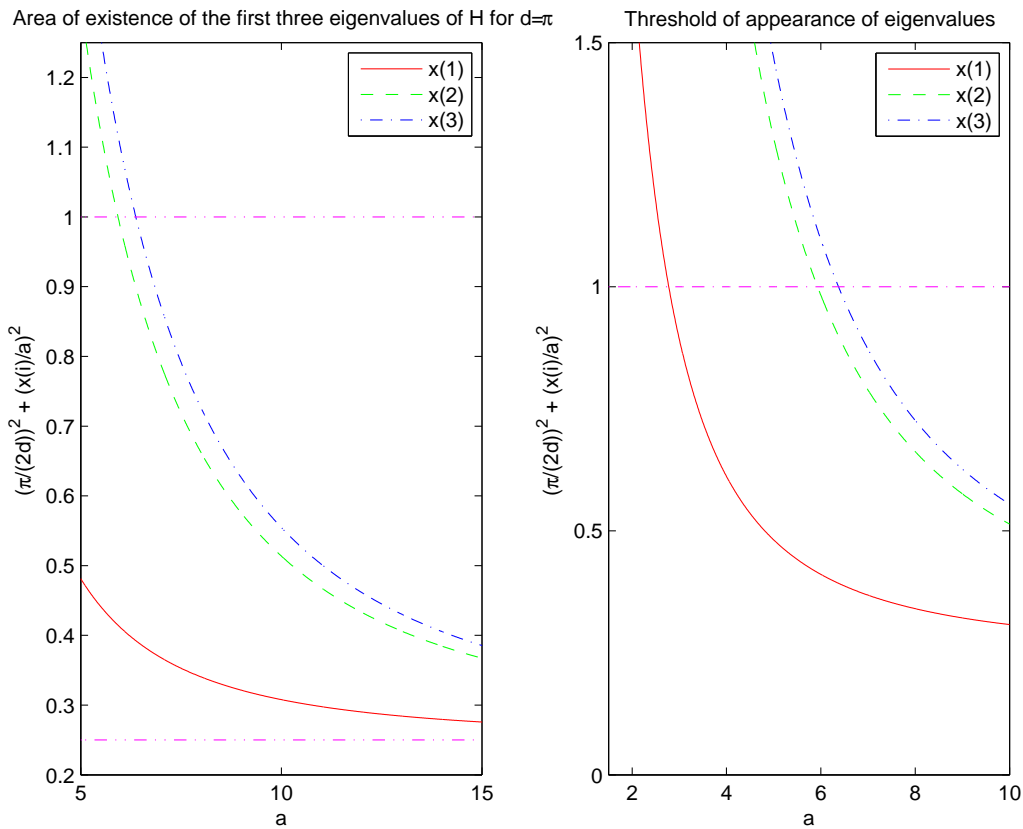


Figure 2: We represent $a \mapsto (\frac{\pi}{2d})^2 + (\frac{x(i)}{a})^2$ where $x(1), x(2), x(3)$ are the first three zeros of the bessel functions increasingly ordered.

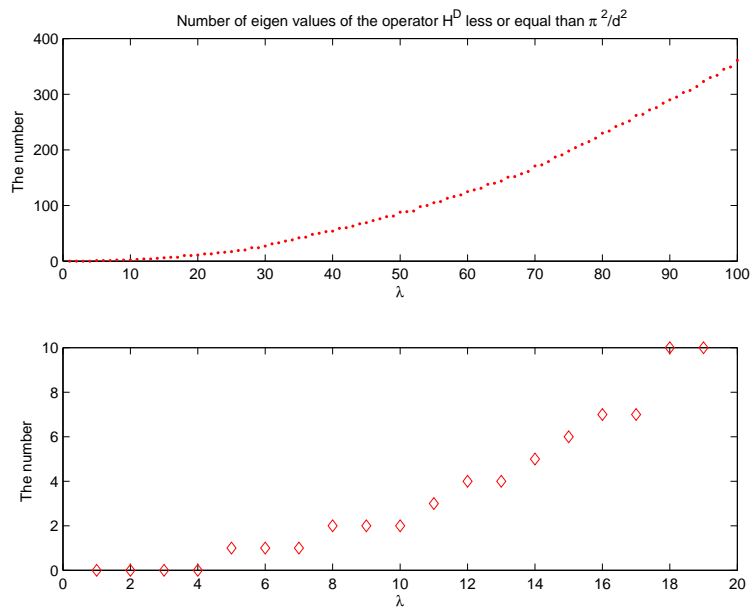


Figure 3: The number of the eigenvalues of the operator H^D function of $\lambda \equiv a/d$.

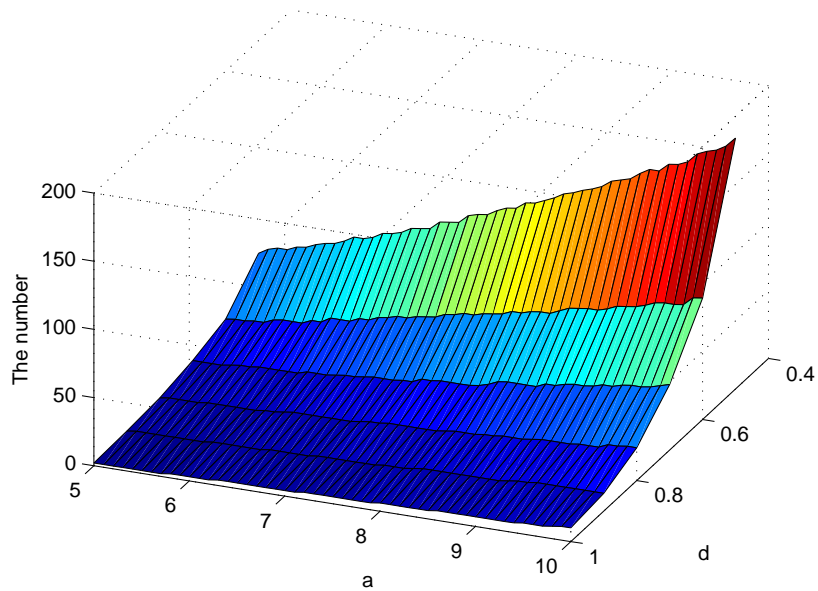


Figure 4: The number of the eigenvalues of the operator H^D function of d and a .

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