UDC 517.938

# VARIATIONAL ESTIMATIONS OF THE EIGENVALUES FOR 3D QUANTUM WAVEGUIDES IN A TRANSVERSE ELECTRIC FIELD

D. G. Matveev<sup>1</sup>, I. Yu. Popov<sup>2</sup>

<sup>1</sup>Microsoft, Redmond, WA, USA <sup>2</sup>Saint Petersburg National Research University of Information Technologies, Mechanics and Optics, Russia

d.g.matveev@gmail.com, popov1955@gmail.com

## PACS 05.45.Df, 61.43.Hv, 83.10.Rs

It is shown that an eigenvalue of the Laplacian exists below the continuous spectrum for a system of threedimensional quantum waveguides laterally coupled via a small window and placed in a transverse electric field, and the estimation for the eigenvalue is obtained. A field induced shift of the eigenvalue is estimated by using a variation.

Keywords: variational method, spectrum estimations, quantum waveguides, external field.

# 1. Introduction

The properties of electron transport in small conductors are related to the relevant length scales. In the diffusive transport regime, in which the elastic mean free path  $l_e$  is much smaller than the dimension of the conductor, quantum interference effects can produce deviations from the from the prediction of classical transport theory. These interference effects result from phase differences acquired by an electron wave in travelling between two points in the sample along different possible trajectories. Many different trajectories can arise from scattering at impurities, resulting in phenomena like one-dimensional weak localization and universal conductance fluctuations.

Modern technologies permit the fabrication of structures in which  $l_e$  is smaller than the length but larger than the width of the sample. In this quasi-ballistic regime, scattering at the boundary of the conductor is important. If the irregularities in the boundary are much smaller than the Fermi wavelength  $\lambda_F$ , the scattering at the boundary is beleived to be specular. For larger irregularities the scattering at the boundary becomes diffusive.

At present the fabrication of the structures in which  $l_e$  is much greater than the length and the width of the sample is possible. It is the fully ballistic regime. Elastic scattering of electrons, which can give rise to resistance, occurs only at the boundary of the conductor. To study quantum confinement effects,  $\lambda_F$  must be of order of the width of the conductor. Currently it is not possible to satisfy this conditions for metals, where  $\lambda_F = 0.1$  nm. Due to the much lower electron density in semiconductors,  $\lambda_F$  is typically equal to 50 nm, which is feasible dimension for fabricating small conductors. In the present paper we deal with quantum transport in such ballistic conductors.

A lot of the papers contain the methods to obtain the nanostructures of this kind, for example, metalorganic vapor phase epitaxy and molecular beam epitaxy [1]. The same is about doping - the organic monolayers with thermal annealing can be used [2]. By this way it is possible to produce the nanostructures with the desired characteristics and, as a result, to create the new



Fig. 1. Schematic diagram of the laterally coupled waveguides: d is the waveguide thickness; 2a – the length and the width of the coupling window; 2l – the waveguides width; E – the electric field

nano-devices. In the present paper we deal with nanostructures called as quantum waveguide (quantum wire). Particularly, we study a system of two quantum waveguides coupled through small window (see Fig. 1). An impotent question is how to control the electronic transport in the device. The conventional way is to use the external fields [3]. From the mathematical standpoint, an analysis of the properties for this kind of the systems leads to the solving waveguide problem with the external fields. This question is investigated in the present paper.

The problem is to prove the existence of the bound electron state (eigenvalue of the corresponding Laplacian) and to estimate the shift of this state from the continuous spectrum. The boundary conditions play crucial role in the spectral problem. The choice of the condition is related with the physical motivation. Namely, for semiconductor nanostructures the Dirichlet conditions are the most natural. As for metallic structures, both the Dirichlet and Neumann conditions take places in the different situations [4,5]. Particularly, for the layered sandwich structure of magnetic and non-magnetic layers it depends on the electron spin and the magnetic moment of the layers [6]. It will be shown below that different conditions can be used for side and vertical surfaces, including the coupling surface for the waveguides. For example, Neumann is for upper and bottom boundaries and Dirichlet is for coupling surface and side boundaries, or just Neumann is for all boundaries except coupling one. Surely, during the proof both conditions will never be used for the one boundary together.

Sequence of papers describes the spectral problems for two-dimensional waveguide systems with the identical or different sizes for the coupled wires. It was shown that the window coupling leads to the appearance of the eigenvalues below the continuous spectrum. Variational estimations for the eigenvalues are obtained [7, 8, 9]. As for three-dimensional case, there were no analogous results for the system in the electric field. In the present paper we consider three-dimensional structure (See Figure 1) of two identical waveguides (width 21, thickness d) coupled through the square window (width 2a) in the transverse electric field (E). It is proved that there exists an eigenvalue below the continuous spectrum and the estimation for the eigenvalue is obtained. We use the variational way of proving analogous to that in [10]. As for other approaches, e.g. the asymptotic one, a reader can see, for example, [11, 12]. The described system is interesting for many physical applications (see, e.g., [13] and references therein).

## 2. Preliminary notes

To start the variational proof we investigate the behavior of the system without the coupling window in transverse electric field. Let's consider transverse homogenous electric field and solve Schrodinger equation for the function of the transverse coordinate (after separation of variables):

$$\varphi'' + \frac{2m}{\hbar^2} \left(\lambda + Ey\right) \varphi = 0.$$
$$\left(y + \frac{\lambda}{2}\right) n^{\frac{1}{3}} n = \frac{2mE}{2mE} \text{ one } q$$

After the replacement  $z = (y + \frac{\lambda}{E}) p^{\frac{1}{3}}$ ,  $p = \frac{2mE}{\hbar^2}$ , one obtains the Airy equation:  $\varphi'' + z\varphi = 0$ .

Here y is the transverse coordinate, m is the effective electron mass,  $\hbar$  is the Planck constant,  $\lambda$  is the spectral parameter. The solutions are the Airy functions Ai(z), Bi(z). In our case the electric field is small (i.e. |z| is large) one can use the asymptotic expressions for the functions:

$$Ai(-z) = z^{-\frac{1}{4}} \left( \sin\left(\frac{2}{3}z^{\frac{3}{2}} + \frac{\pi}{4}\right) + o\left(z^{-\frac{3}{2}}\right) \right),$$
  
$$Bi(-z) = z^{-\frac{1}{4}} \left( \cos\left(\frac{2}{3}z^{\frac{3}{2}} + \frac{\pi}{4}\right) + o\left(z^{-\frac{3}{2}}\right) \right).$$

Hence, the asymptotic expression for the general solution is as follows

$$\varphi(z) = Cz^{-\frac{1}{4}} \left( \sin\left(\frac{2}{3}z^{\frac{3}{2}} + \frac{\pi}{4}\right) + o\left(z^{-\frac{3}{2}}\right) \right) + Dz^{-\frac{1}{4}} \left( \cos\left(\frac{2}{3}z^{\frac{3}{2}} + \frac{\pi}{4}\right) + o\left(z^{-\frac{3}{2}}\right) \right).$$

For the Neumann conditions  $\varphi'(0) = \varphi'(d) = 0$  we have the following bottom  $\lambda_0$  of the continuous spectrum:  $\sqrt{\lambda_0} = \sqrt{\Lambda} - \frac{1}{4} \frac{dE}{\sqrt{\Lambda}}$ , where  $\Lambda = \frac{\pi^2 \hbar^2}{2md^2}$  is the spectrum boundary in the case of the electric field absence. One can note that the expression for  $\lambda_0$  doesn't change in the case of the Dirichlet conditions  $\varphi(0) = \varphi(d) = 0$  (it is shown in [8]).

Let's note that in the case of the weak electric field and the small limited y one has:

$$\left(\frac{yE+\lambda}{E}\right)p^{\frac{1}{3}}\xrightarrow[E\to 0]{}\frac{\lambda}{E}p^{\frac{1}{3}}$$

and, consequently,

$$-\varphi'' = \frac{\lambda}{E} p^{\frac{1}{3}} \varphi.$$

According to the variational principle, in order to prove the existence of the eigenvalue below the threshold of the continuous spectrum, it is sufficient to find a trial function  $\psi$  such that the ratio  $\frac{M(\psi)}{\|\psi\|^2}$  acquires a negative value, where:

$$M(\psi) = (H\psi, \psi) - \frac{\lambda}{E} p^{\frac{1}{3}} \|\psi\|^2, \quad H = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2}.$$

#### 3. Trial function constructing

Trial function should satisfy the boundary conditions. Also the function can contain some free parameters. It allows one to choose the function in a proper way to ensure the inequality. Let's try to find a trial function in the following form [10]:

$$\psi(x, y, z) = F(x, y, z) + G(x, y, z).$$

Here the first term F(x, y, z) is used to describe the electron behavior in the waveguide outside the window neighbourhood. The second term G(x, y, z) is used to describe the electron behavior in the domain containing coupling window. Functions F(x, y, z) and G(x, y, z) are presented in the form:

$$F(x, y, z) = \alpha U(x)V(y)Z(z), G(x, y, z) = \eta P(x)R(y)T(z).$$

 $\alpha$  and  $\eta$  are parameters we can change in accordance with our goals. The functions U(x) and P(x) are the same as in [8]:

$$U(x) = \min\{1, e^{-k(|x|-a)}\},\$$
$$P(x) = \cos\frac{\pi x}{2a}\chi_{[-a,a]}(x).$$

U(x) provides the attenuation on the infinity while P(x) describes the garmonic behavior. Here k is one more free parameter to use in the variations,  $\chi_{[-a,a]}(x)$  is the characteristic function of the window. In the preliminary notes we described the electron behavior along the transverse coordinate, so the results (the asymptotic expressions for the Airy functions) can be used for the corresponding trial function component V(y):

$$V(y) = C\left(y + \frac{\lambda}{E}\right)^{-\frac{1}{4}} p^{-\frac{1}{12}} \sin\left(\frac{2}{3}\left(y + \frac{\lambda}{E}\right)^{\frac{3}{2}} p^{\frac{1}{2}} + \frac{\pi}{4}\right) + D\left(y + \frac{\lambda}{E}\right)^{-\frac{1}{4}} p^{-\frac{1}{12}} \cos\left(\frac{2}{3}\left(y + \frac{\lambda}{E}\right)^{\frac{3}{2}} p^{\frac{1}{2}} + \frac{\pi}{4}\right).$$

One can consider V(y) as the even function due to the choice of C, D. We choose R(y) in the following form:

$$R(y) = \begin{cases} e^{-\frac{\pi y}{2a}}, \ y \in \left[0, \frac{d}{2}\right]; \\ 4\left(1 - \frac{y}{d}\right)^2 e^{-\frac{\pi d}{4a}}, \ y \in \left[\frac{d}{2}, d\right]. \end{cases}$$

The evenness is reachable by the even continuing of this function to the bottom waveguide. V(y) obeys as well Neumann as Dirichlet conditions at the ends of the segments outside the window (-d, 0) and (0, d), and R(y) obeys as Neumann as Dirichlet conditions at the ends of segments for the window domain (-d, d). To follow the chosen behavior for the longitudinal axis (U(x)) - let's choose Z(z) in the form:

$$Z(z) = \min\left(1, \frac{(l-|z|)^2}{(l-a)^2} e^{-k(|z|-a)}\right).$$

Parameter k is the same as for U(x) to keep the identical exponential behavior on the OXZ plane. Note that this function also obeys any desired boundary conditions at the ends on segment (-l, l). With the same argumentation we introduce the last function as follows:

$$T(z) = \cos\frac{\pi z}{2a}\chi_z[-a,a](z).$$

It is similar to P(x) because of the identical parameters of the coupling window in OXZ plane and of central symmetry regarding O. The trial function terms are now looking like:

$$\begin{split} F(x,y,z) &= \alpha \min\left\{1, \ e^{-k(|x|-a)}\right\} \left(C\left(y+\frac{\lambda}{E}\right)^{-\frac{1}{4}} p^{-\frac{1}{12}} \sin\left(\frac{2}{3}\left(y+\frac{\lambda}{E}\right)^{\frac{3}{2}} p^{\frac{1}{2}} + \frac{\pi}{4}\right) + \\ &+ D\left(y+\frac{\lambda}{E}\right)^{-\frac{1}{4}} p^{-\frac{1}{12}} \cos\left(\frac{2}{3}\left(y+\frac{\lambda}{E}\right)^{\frac{3}{2}} p^{\frac{1}{2}} + \frac{\pi}{4}\right)\right) \min\left(1, \frac{(l-|z|)^2}{(l-a)^2} e^{-k(|z|-a)}\right), \\ &G(x,y,z) = \eta \cos\frac{\pi x}{2a} \chi_{[-a,a]}(x) \times \\ &\times \begin{cases} e^{-\frac{\pi y}{2a}}, \ y \in [0, \frac{d}{2}]; \\ 4\left(1-\frac{y}{d}\right)^2 e^{-\frac{\pi d}{4a}}, \ y \in [\frac{d}{2}, d]; \end{cases} \\ &\times \cos\frac{\pi z}{2a} \chi_{z}[-a, a](z). \end{split}$$

## 4. Lemmas

**Lemma 1.**  $M(\psi)$  for the function  $\psi(x, y, z)$  results in the following expression:

$$\begin{split} M(\psi) &= \|F'_x\|^2 + \|G'_x\|^2 + \|F'_z\|^2 + \|G'_z\|^2 + \|G'_y\|^2 - \\ &- \frac{\lambda}{E} p^{\frac{1}{3}} \|G\|^2 - 2 \int_{-a}^{a} \int_{-l}^{l} \left(\overline{G}F'_y + \overline{F'_y}G\right)|_{y=0} dz dx. \end{split}$$

*Proof.* Let's consider  $H(\psi, \psi)$  expression:

$$(H\psi,\psi) = \int_{-\infty}^{+\infty} \int_{-d}^{d} \int_{-l}^{l} \left( -\psi_{xx}'\overline{\psi} - \psi_{yy}'\overline{\psi} - \psi_{zz}'\overline{\psi} \right) dz dy dx = -\int_{-d}^{d} \int_{-\infty}^{l} \left( \psi_{x}'\overline{\psi} \mid_{-\infty}^{\infty} - \int_{-\infty}^{+\infty} \psi_{x}'\overline{\psi_{x}'} dx \right) dz dy - \int_{-\infty}^{+\infty} \int_{-l}^{l} \left( \psi_{y}'\overline{\psi} \mid_{-d}^{d} - \int_{-d}^{d} \psi_{y}'\overline{\psi_{y}'} dy \right) dz dx - -\int_{-\infty}^{+\infty} \int_{-\infty}^{d} \left( \psi_{z}'\overline{\psi} \mid_{-l}^{l} - \int_{-l}^{l} \psi_{z}'\overline{\psi_{z}'} dz \right) dy dx = \|\psi_{x}'\|^{2} + \|\psi_{y}'\|^{2} + \|\psi_{z}'\|^{2}.$$

To annihilate the terms outside of integral it is sufficient to use the one of the suggested boundary conditions but not the both - either the function or the derivative will have null values at -d, d, -l, l. We get:  $(H\psi, \psi) = \|\psi'_x\|^2 + \|\psi'_y\|^2 + \|\psi'_z\|^2 - \frac{\lambda}{E}p^{\frac{1}{3}}\|\psi\|^2$  Let's compute the received norms of the functions.

$$\begin{aligned} \|\psi_x'\|^2 &= \int_{-\infty}^{+\infty} \int_{-d}^d \int_{-l}^l \psi_x' \overline{\psi_x'} dz dy dx = \int_{-\infty}^{+\infty} \int_{-d}^d \int_{-l}^l \left(F_x' + G_x'\right) \left(\overline{F_x'} + \overline{G_x'}\right) dz dy dx = \\ &= \int_{-\infty}^{+\infty} \int_{-d}^d \int_{-l}^l F_x' \overline{F_x'} dy dx + \int_{-a}^a \int_{-a}^d \int_{-a}^a G_x' \overline{G_x'} dz dy dx + \int_{-a}^a \int_{-d}^d \int_{-a}^a \left(F_x' \overline{G_x'} + G_x' \overline{F_x'}\right) dz dy dx = \\ &= \|F_x'\|^2 + \|G_x'\|^2, \end{aligned}$$

that's possible because  $F'_x = \alpha U'_x(x)V(y) = 0$  on the interval [-a, a] given the fact that  $U(x)|_{|x| \leq a} = const$  (as constructed).

Variational estimations of the eigenvalues for 3D quantum waveguides

$$\begin{split} \|\psi'_{y}\|^{2} &= \int_{-\infty}^{+\infty} \int_{-d}^{d} \int_{-l}^{l} \psi'_{y} \overline{\psi'_{y}} dz dy dx = \int_{-\infty}^{+\infty} \int_{-d}^{d} \int_{-l}^{l} \left(F'_{y} + G'_{y}\right) \left(\overline{F'_{y}} + \overline{G'_{y}}\right) dz dy dx = \\ &= \int_{-\infty}^{+\infty} \int_{-d}^{d} \int_{-l}^{l} F'_{y} \overline{F'_{y}} dz dy dx + \int_{-a}^{a} \int_{-d}^{d} \int_{-a}^{a} G'_{y} \overline{G'_{y}} dz dy dx + \int_{-a}^{a} \int_{-d}^{d} \int_{-a}^{a} \left(F'_{y} \overline{G'_{y}} + G'_{y} \overline{F'_{y}}\right) dz dy dx = \\ &= \|F'_{y}\|^{2} + \|G'_{y}\|^{2} + \int_{-a}^{a} \int_{-a}^{d} \int_{-a}^{a} \left(F'_{y} \overline{G'_{y}} + G'_{y} \overline{F'_{y}}\right) dz dy dx. \end{split}$$

It makes sense to simplify the expression above to look for the another suitable representation of the triple integral:

$$\int_{-a}^{a} \int_{-a}^{d} \int_{-a}^{a} \left(F'_{y}\overline{G'_{y}} + G'_{y}\overline{F'_{y}}\right) dz dy dx =$$

$$= 2 \int_{-a}^{a} \int_{0}^{d} \int_{-a}^{a} F'_{y}\overline{G'_{y}} dz dy dx + \int_{-a}^{a} \int_{0}^{d} \int_{-a}^{a} G'_{y}\overline{F'_{y}} dz dy dx =$$

$$= 2 \int_{-a}^{a} \int_{0}^{a} \int_{-a}^{d} F''_{y}\overline{G} dy dx + \int_{-a}^{a} \int_{-a}^{a} \int_{-a}^{d} G'_{y}\overline{F'_{y}} dz dy dx =$$

$$= \int_{-a}^{a} \int_{-a}^{d} \int_{-a}^{d} F''_{y}\overline{G} dy dx + \int_{-a}^{a} \int_{-a}^{a} \int_{-a}^{d} \left(\overline{F'_{y}}G_{0}^{d} - \int_{0}^{d} \overline{F''_{y}}\overline{G} dy\right) dz dx =$$

$$= \int_{-a}^{a} \int_{-a}^{d} \int_{-a}^{a} \left(F''_{yy}\overline{G} + \overline{F''_{yy}}G\right) dz dy dx - 2 \int_{-a}^{a} \int_{-a}^{a} \left(\overline{G}F'_{y} + \overline{G}\overline{F''_{y}}\right) \Big|_{y=0} dz dx.$$

It is the correct transition because of the absence of the separating surface on the interval [-a, a] - the window between the waveguides is placed here. Taking into account that  $F''_{yy}(x, y) = \frac{\lambda}{E}p^{\frac{1}{3}}F(x, y)$ , one receives:

$$\int_{-a}^{a} \int_{-a}^{d} \int_{-a}^{a} \left(F_{yy}''\overline{G} + \overline{F_{yy}''}G\right) dz dy dx =$$

$$= -\int_{-a}^{a} \int_{-a}^{d} \int_{-a}^{a} \left(y + \frac{\lambda}{E}\right) p^{\frac{1}{3}} \left(\overline{G}F + G\overline{F}\right) dz dy dx =$$

$$= -\int_{-a}^{a} \int_{-a}^{d} \int_{-a}^{a} y p^{\frac{1}{3}} \left(\overline{G}F + G\overline{F}\right) dz dy dx - \frac{\lambda}{E} p^{\frac{1}{3}} \int_{-a}^{a} \int_{-a}^{d} \int_{-a}^{a} \left(\overline{G}F + G\overline{F}\right) dz dy dx =$$

$$= -\frac{\lambda}{E} p^{\frac{1}{3}} \int_{-a}^{a} \int_{-a}^{d} \int_{-a}^{a} \left(\overline{G}F + G\overline{F}\right) dz dy dx.$$

One can consider the first integral to be zero because of the symmetric interval for the integral while the odd function is used in calculation (F, G are the even functions, but y is the

odd one). So, consequently

$$\left\|\psi_{y}'\right\|^{2} = \left\|F_{y}'\right\|^{2} + \left\|G_{y}'\right\|^{2} + \frac{\lambda}{E}p^{\frac{1}{3}}\int_{-a}^{a}\int_{-a}^{d}\int_{-a}^{a}\left(\overline{G}F + G\overline{F}\right)dzdydx - 2\int_{-a}^{a}\int_{-a}^{a}\left(\overline{G}F_{y}' + G\overline{F_{y}'}\right)|_{y=0}dzdx,$$

where one can calculate the norm  $\left\|F_y'\right\|^2$  using the integration by parts

$$\begin{split} \left\|F'_{y}\right\|^{2} &= \int_{-\infty}^{+\infty} \int_{-l}^{d} \int_{-l}^{l} F'_{y} \overline{F'_{y}} dz dy dx = \int_{-\infty}^{+\infty} \int_{-l}^{l} \left(F\overline{F'_{y}}\Big|_{-d}^{d} - \int_{-d}^{d} F\overline{F''_{yy}} dy\right) dz dx = \\ &= \int_{-\infty}^{+\infty} \int_{-d}^{d} \int_{-l}^{l} F'_{y} \overline{F''_{yy}} dz dy dx = \frac{\lambda}{E} p^{\frac{1}{3}} \int_{-a}^{a} \int_{-a}^{d} \int_{-a}^{a} F\overline{F} dz dy dx = \frac{\lambda}{E} p^{\frac{1}{3}} \|F\|^{2} \,. \end{split}$$

The norm of the last term in  $(H\psi,\psi)$  expression could be simplified like:

$$\begin{aligned} \|\psi_z'\|^2 &= \int_{-\infty}^{+\infty} \int_{-d}^d \int_{-l}^l \psi_z' \overline{\psi_z'} dy dx = \int_{-\infty}^{+\infty} \int_{-d}^d \int_{-l}^l \left(F_z' + G_z'\right) \left(\overline{F_z'} + \overline{G_z'}\right) dy dx = \\ &= \int_{-\infty}^{+\infty} \int_{-d}^d \int_{-l}^l F_z' \overline{F_z'} dy dx + \int_{-a}^a \int_{-d}^d \int_{-a}^a G_z' \overline{G_z'} dz dy dx + \int_{-a}^a \int_{-a}^d \int_{-a}^a \left(F_z' \overline{G_z'} + G_z' \overline{F_z'}\right) dz dy dx = \\ &= \|F_z'\|^2 + \|G_z'\|^2. \end{aligned}$$

Let's note that the third integral in the previous expression is zero due to constant behavior of Z on the coupling window:  $Z(z)|_{|z| \leq a} = const$ . In a similar manner we compute norm of the main function:

$$\begin{aligned} \left\|\psi\right\|^{2} &= \int_{-\infty}^{+\infty} \int_{-d}^{d} \int_{-l}^{l} \left(F+G\right) \left(\overline{F}+\overline{G}\right) dz dy dx = \\ &= \left\|F\right\|^{2} + \left\|G\right\|^{2} + \int_{-\infty}^{+\infty} \int_{-d}^{d} \int_{-l}^{l} \left(\overline{G}F+G\overline{F}\right) dz dy dx. \end{aligned}$$

If one collects all the norms being considered in the lemma together - it will give us the required proof:

$$\begin{split} M(\psi) &= \|\psi'_x\|^2 + \|\psi'_y\|^2 + \|\psi'_z\|^2 - \frac{\lambda}{E} p^{\frac{1}{3}} \|\psi\|^2 = \\ &= \|F'_x\|^2 + \|G'_x\|^2 + \|F'_z\|^2 + \|G'_z\|^2 + \frac{\lambda}{E} p^{\frac{1}{3}} \|F\|^2 + \|G'_y\|^2 + \\ &+ \frac{\lambda}{E} p^{\frac{1}{3}} \int_{-a}^{a} \int_{-a}^{d} \int_{-a}^{a} \left(\overline{G}F + \overline{GF}\right) dz dy dx - 2 \int_{-a}^{a} \int_{-a}^{a} \left(\overline{G}F'_y + \overline{GF'_y}\right) \Big|_{y=0} dz dx - \frac{\lambda}{E} p^{\frac{1}{3}} \|F\|^2 - \\ &- \frac{\lambda}{E} p^{\frac{1}{3}} \|G\|^2 - \frac{\lambda}{E} p^{\frac{1}{3}} \int_{-\infty}^{+\infty} \int_{-d}^{d} \int_{-1}^{l} \left(\overline{G}F + \overline{GF}\right) dz dy dx = \\ \|F'_x\|^2 + \|G'_x\|^2 + \|F'_z\|^2 + \|G'_z\|^2 + \|G'_y\|^2 - \frac{\lambda}{E} p^{\frac{1}{3}} \|G\|^2 - 2 \int_{-a}^{a} \int_{-a}^{a} \left(\overline{G}F'_y + \overline{GF'_y}\right) \Big|_{y=0} dz dx. \end{split}$$

		L
		L
		L
		L
		L

**Lemma 2.**  $M(\psi)$  has the following upper estimation for the trial function  $\psi$ :

$$M(\psi) < \eta^{2} \frac{\pi}{2} a \left(3 + 2\varepsilon_{1}\right) + \alpha^{2} k \left\|V\right\|^{2} \left\|Z\right\|^{2} + \left(\frac{\alpha^{2}}{k} + 2\alpha^{2} a\right) \left\|V\right\|^{2} \left\|Z'\right\|^{2} - 64\eta \frac{a^{2}}{\pi^{2}} \alpha p^{-\frac{1}{12}} \left(\frac{\lambda}{E}\right)^{-\frac{5}{4}} \sqrt{C^{2} + D^{2}} \sqrt{p \left(\frac{\lambda}{E}\right)^{3} + \frac{1}{16}} \cos\gamma,$$

where  $\gamma$  could be represented as follows:

$$\gamma = \frac{2}{3} \left(\frac{\lambda}{E}\right)^{\frac{3}{2}} p^{\frac{1}{2}} + \frac{\pi}{4} + \operatorname{arctg} \frac{\frac{1}{4}C(\frac{E}{\lambda})^{\frac{3}{2}} + Dp^{\frac{1}{2}}}{Cp^{\frac{1}{2}} - \frac{1}{4}D(\frac{E}{\lambda})^{\frac{3}{2}}}.$$

*Proof.* Let's estimate all the expressions from the previous lemma. We can skip the negative terms because of the upper estimation. We'll apply it for  $-\frac{\lambda}{E}p^{\frac{1}{3}} ||G||^2$ .

$$\begin{split} \|F'_x\|^2 &= \int_{-\infty}^a \int_{0}^d \int_{-l}^l \alpha^2 k^2 e^{2k(x+a)} V^2(y) Z^2(z) dz dy dx + \\ &+ \int_{a}^{+\infty} \int_{0}^d \int_{-l}^l \alpha^2 k^2 e^{-2k(x+a)} V^2(y) Z^2(z) dz dy dx = \\ &= \alpha^2 k^2 \frac{1}{2k} e^{2k(x+a)} \Big|_{-\infty}^{-a} \int_{0}^d \int_{-l}^l V^2(y) Z^2(z) dz dy + \\ &+ \alpha^2 k^2 \left( -\frac{1}{2k} \right) e^{-2k(x-a)} \Big|_{a}^{+\infty} \int_{0}^d \int_{-l}^l V^2(y) Z^2(z) dz dy = \\ &= \alpha^2 k \int_{0}^d V^2(y) dy \int_{-l}^l Z^2(z) dz = \alpha^2 k \|V\|^2 \|Z\|^2. \end{split}$$

We'll not compute the expressions with V and Z at this stage, it is sufficient to know about their positive values as squares.

$$\begin{split} \|F_{z}'\|^{2} &= \int_{-\infty}^{a} \int_{0}^{d} \int_{-l}^{l} \alpha^{2} e^{2k(x+a)} V^{2}\left(y\right) Z'^{2}(z) dz dy dx + \\ &+ \int_{a}^{+\infty} \int_{0}^{d} \int_{-l}^{l} \alpha^{2} e^{-2k(x+a)} V^{2}\left(y\right) Z'^{2}(z) dz dy dx + 2\alpha^{2}a \int_{0}^{d} \int_{-l}^{l} V^{2}\left(y\right) Z'^{2}(z) dz dy = \\ &= \alpha^{2} \frac{1}{2k} e^{2k(x+a)} \Big|_{-\infty}^{-a} \int_{0}^{d} \int_{-l}^{l} V^{2}\left(y\right) Z'^{2}(z) dz dy + \\ &+ \alpha^{2} \left(-\frac{1}{2k}\right) e^{-2k(x-a)} \Big|_{a}^{+\infty} \int_{0}^{d} \int_{-l}^{l} V^{2}\left(y\right) Z'^{2}(z) dz dy + \\ &+ 2\alpha^{2}a \int_{0}^{d} \int_{-l}^{l} V^{2}\left(y\right) Z'^{2}(z) dz dy = \\ &= \frac{\alpha^{2}}{k} \int_{0}^{d} V^{2}\left(y\right) dy \int_{-l}^{l} Z'^{2}(z) dz + 2\alpha^{2}a \int_{0}^{d} V^{2}\left(y\right) dy \int_{-l}^{l} Z'^{2}(z) dz = \\ &= \left(\frac{\alpha^{2}}{k} + 2\alpha^{2}a\right) \int_{0}^{d} V^{2}\left(y\right) dy \int_{-l}^{l} Z'^{2}(z) dz = \left(\frac{\alpha^{2}}{k} + 2\alpha^{2}a\right) \|V\|^{2} \|Z'\|^{2}. \end{split}$$

Calculation for  $\int_{-l}^{l} Z'^{2}(z) dz$  could be skipped using the same argumentation as one has for the case with positive value of  $||F'_{x}||^{2}$ . Simplification for the norm of  $G'_{x}$  can be achieved in the next way:

$$\|G'_x\|^2 = \int_{-a}^{a} \int_{-a}^{d} \int_{-a}^{a} \eta^2 R^2(y) \cdot \cos^2 \frac{\pi z}{2a} \sin^2 \frac{\pi x}{2a} \cdot \left(\frac{\pi}{2a}\right)^2 dz dy dx =$$
  
=  $\int_{-a}^{a} \sin^2 \frac{\pi x}{2a} dx \int_{-d}^{d} \eta^2 R^2(y) \left(\frac{\pi}{2a}\right)^2 dy \int_{-a}^{a} \cos^2 \frac{\pi z}{2a} dz =$   
=  $\eta^2 \frac{\pi^2}{4} \int_{-d}^{d} R^2(y) dy = \eta^2 \frac{\pi^2}{4} \|R\|^2.$ 

For  $G'_y$  one will have:

$$\left\|G'_{y}\right\|^{2} = \int_{-a}^{a} \int_{-a}^{d} \int_{-a}^{a} \eta^{2} R'_{y}^{2}(y) \cdot \cos^{2} \frac{\pi x}{2a} \cos^{2} \frac{\pi z}{2a} dz dy dx =$$
$$= \eta^{2} \left\|R'\right\|^{2} \cdot \int_{-a}^{a} \cos^{2} \frac{\pi x}{2a} dx \cdot \int_{-a}^{a} \cos^{2} \frac{\pi z}{2a} dz = \eta^{2} a^{2} \left\|R'\right\|^{2}.$$

And, finally  $G'_z$ :

$$\|G'_{z}\|^{2} = \int_{-a}^{a} \int_{-a}^{d} \int_{-a}^{a} \eta^{2} R^{2}(y) \cdot \cos^{2} \frac{\pi x}{2a} \sin^{2} \frac{\pi z}{2a} \cdot \left(\frac{\pi}{2a}\right)^{2} dz dy dx =$$
$$= \int_{-a}^{a} \cos^{2} \frac{\pi x}{2a} dx \int_{-d}^{d} \eta^{2} R^{2}(y) \left(\frac{\pi}{2a}\right)^{2} dy \int_{-a}^{a} \sin^{2} \frac{\pi z}{2a} dz =$$
$$= \eta^{2} \frac{\pi^{2}}{4} \int_{-d}^{d} R^{2}(y) dy = \eta^{2} \frac{\pi^{2}}{4} ||R||^{2}.$$

Estimates for  $||R||^2$ ,  $||R'||^2$  are not known at the moment, one can find them using the expressions we have chosen for R:

$$||R||^{2} = 2 \cdot \int_{0}^{\frac{d}{2}} \left(e^{-\frac{\pi y}{2a}}\right)^{2} dy + \int_{\frac{d}{2}}^{d} \left(4\left(1-\frac{y}{d}\right)^{2}e^{-\frac{\pi d}{4a}}\right)^{2} dy =$$
$$= 2\frac{a}{\pi} \left(1+\frac{\pi}{a}e^{-\frac{\pi d}{2a}}\left(\frac{\pi d}{10a}-1\right)\right) < 2\frac{a}{\pi}\left(1+\varepsilon_{1}\right).$$

We got:

$$\left\|R\right\|^{2} < 2\frac{a}{\pi}\left(1+\varepsilon_{1}\right),$$

where  $\varepsilon_1$  is the positive constant which depends on the parameters of the structure. For the derivative of R the estimation is:

$$\begin{aligned} \|R'\|^2 &= 2 \cdot \int_0^{\frac{a}{2}} \frac{\pi^2}{4a^2} e^{-\frac{\pi y}{a}} dy + 2 \int_{\frac{d}{2}}^d \frac{64}{d^2} \left(1 - \frac{y}{d}\right)^2 e^{-\frac{\pi d}{2a}} dy = \\ &= \frac{\pi}{2a} + \left(\frac{16}{3d} - \frac{\pi}{2a}\right) e^{-\frac{\pi d}{2a}} < \frac{\pi}{2a}, \end{aligned}$$

if  $\frac{\pi}{2a} > \frac{16}{3d}$ ,  $a < \frac{3\pi d}{32}$ , i.e.  $a < \frac{3\pi d}{32}$ . The result is the estimation  $||R'||^2 < \frac{\pi}{2a}$ . Let's note that we have received a limitation for the coupling window measurements - the window width should not be greater than approximately 0.3 of the waveguide thickness (simplification for  $\frac{3}{32}$ ). In sum we have:

$$\|G'_x\|^2 + \|G'_y\|^2 + \|G'_z\|^2 < 2\frac{a}{\pi}(1+\varepsilon_1)\cdot\eta^2\frac{\pi^2}{4} + \frac{\pi}{2a}\cdot\eta^2a^2 + 2\frac{a}{\pi}(1+\varepsilon_1)\cdot\eta^2\frac{\pi^2}{4} = \eta^2\frac{\pi}{2}a(3+\varepsilon_1).$$

Constructed functions have no complex terms.

So,  $\int_{-a}^{a} \int_{-a}^{a} \left(\overline{G}F'_{y} + G\overline{F'_{y}}\right) \Big|_{y=0} dz dx$  could be written as  $\int_{-a}^{a} \int_{-a}^{a} 2 \cdot GF'_{y} \Big|_{y=0} dz dx$ . Using the sions for  $CF'_{y}$  one obtains

expressions for  $GF'_{y}\Big|_{y=0}$  one obtains

$$\int_{-a}^{a} \int_{-a}^{a} 2 \cdot GF'_{y} \Big|_{y=0} dz dx =$$

$$= 2\eta \alpha p^{-\frac{1}{12}} \left(\frac{\lambda}{E}\right)^{-\frac{5}{4}} \sqrt{C^{2} + D^{2}} \sqrt{p\left(\frac{\lambda}{E}\right)^{3} + \frac{1}{16}} \cos \gamma \int_{-a}^{a} \int_{-a}^{a} \cos \frac{\pi nx}{2a} \cos \frac{\pi nz}{2a} dz dx =$$

$$= 32\eta \frac{a^{2}}{\pi^{2}} \alpha p^{-\frac{1}{12}} \left(\frac{\lambda}{E}\right)^{-\frac{5}{4}} \sqrt{C^{2} + D^{2}} \sqrt{p\left(\frac{\lambda}{E}\right)^{3} + \frac{1}{16}} \cos \gamma.$$

Overall, the result could be stated like:

$$M(\psi) < \alpha^{2} k \|V\|^{2} \|Z\|^{2} + \left(\frac{\alpha^{2}}{k} + 2\alpha^{2} a\right) \|V\|^{2} \|Z'\|^{2} + \eta^{2} \frac{\pi}{2} a(3 + \varepsilon_{1}) - 64\eta \frac{a^{2}}{\pi^{2}} \alpha p^{\frac{-1}{12}} \left(\frac{\lambda}{E}\right)^{\frac{-5}{4}} \sqrt{C^{2} + D^{2}} \sqrt{p\left(\frac{\lambda}{E}\right)^{3} + \frac{1}{16}} \cos \gamma.$$

**Lemma 3.** Trial function  $\psi(x, y, z)$  has the next upper estimate:

$$\|\psi\|^{2} \leq \left(\frac{\alpha^{2}}{k} + 2\alpha^{2}a\right) \|V\|^{2} \|Z\|^{2} (2 + \varepsilon_{2}).$$

*Proof.* It is known that the function norm can be estimated as  $\|\Phi(M, N)\| \leq 2 \|M\| + 2 \|N\|$ . Let's apply this inequality for the norm of  $\psi$ :

$$\|\psi\|^{2} \leq 2 \|F\|^{2} \Big|_{|x|>a} + 2 \|F\|^{2} \Big|_{|x|\leq a} + 2 \|G\|^{2}.$$

Now, it is required to estimate the corresponding terms. Let's start with the norm of F:

$$\begin{split} \|F\|^{2} \Big|_{|x|>a} &= \int_{-\infty}^{-a} \int_{0}^{d} \int_{-l}^{l} F\bar{F}dzdydx + \int_{a}^{+\infty} \int_{0}^{d} \int_{-l}^{l} F\bar{F}dzdydx = \\ &= \alpha^{2} \int_{-\infty}^{-a} e^{2k(x+a)}dx \int_{0}^{d} V^{2}(y)dy \int_{-l}^{l} Z^{2}(z)dz + \\ &+ \alpha^{2} \int_{a}^{+\infty} e^{-2k(x-a)}dx \int_{0}^{d} V^{2}(y)dy \int_{-l}^{l} Z^{2}(z)dz = \\ &= \frac{\alpha^{2}}{k} \int_{0}^{d} V^{2}(y)dy \int_{-l}^{l} Z^{2}(z)dz = \frac{\alpha^{2}}{k} \|V\|^{2} \|Z\|^{2}, \end{split}$$

If one uses the same approach for the norm of G, the estimation will be the next:

$$||G||^{2} = \int_{-a}^{a} \int_{-a}^{d} \int_{-a}^{a} \eta^{2} R^{2}(y) \cdot \cos^{2} \frac{\pi x}{2a} \cos^{2} \frac{\pi z}{2a} dz dy dx =$$
$$= \eta^{2} a^{2} ||R||^{2} = \eta^{2} a^{2} \cdot 2 \frac{a}{\pi} (1 + \varepsilon_{1}) = 2\eta^{2} \frac{a^{3}}{\pi} (1 + \varepsilon_{1}).$$

Calculation of the norm F on the window interval could be performed like:

$$2 \|F\|_{|x|\leq a}^{2} = 2 \int_{-a}^{a} \int_{-d}^{d} \int_{-l}^{l} \alpha^{2} V^{2}(y) Z^{2}(z) dz dy dx =$$
$$= 2\alpha^{2} \cdot 2a \cdot \|V\|^{2} \|Z\|^{2} = 4a\alpha^{2} \|V\|^{2} \|Z\|^{2}.$$

Overall, norm of  $\psi$  results in:

$$\begin{split} \|\psi\|_{|x|\leqslant a}^{2} &\leqslant 2\frac{\alpha^{2}}{k} \left\|V\right\|^{2} \|Z\|^{2} + 2\eta^{2}\frac{a^{3}}{\pi}\left(1+\varepsilon_{1}\right) + 4a\alpha^{2} \left\|V\right\|^{2} \|Z\|^{2} = \\ &= 2\left(\frac{\alpha^{2}}{k} + 2\alpha^{2}a\right) \left\|V\right\|^{2} \|Z\|^{2} + 2\eta^{2}\frac{a^{3}}{\pi}\left(1+\varepsilon_{1}\right) = \\ &= \left(\frac{\alpha^{2}}{k} + 2\alpha^{2}a\right) \left\|V\right\|^{2} \|Z\|^{2} \times \left(2 + \frac{\eta^{2}\frac{a^{3}}{\pi}\left(1+\varepsilon_{1}\right)}{\left(\frac{\alpha^{2}}{k} + 2\alpha^{2}a\right) \left\|V\right\|^{2} \|Z\|^{2}}\right) = \\ &= \left(\frac{\alpha^{2}}{k} + 2\alpha^{2}a\right) \left\|V\right\|^{2} \|Z\|^{2} \left(2+\varepsilon_{2}\right), \end{split}$$

where  $\varepsilon_2$  is the positive "constant" which depends on the varied parameters of the trial function. Also, the trial function can be estimated as follows:

$$\begin{aligned} \|\psi\|_{|x|\leqslant a}^{2} &\leqslant 2\frac{\alpha^{2}}{k} \|V\|^{2} \|Z\|^{2} + 2\eta^{2}a2\frac{a}{\pi} (1+\varepsilon_{1}) + 8\alpha^{2}a \|V\|^{2} \|Z\|^{2} = \\ &= \frac{\alpha^{2}}{k} \|V\|^{2} \|Z\|^{2} \left(2 + 8ka + \frac{k}{\alpha^{2}} 4\eta^{2} \frac{a^{2}}{\pi^{2}} (1+\varepsilon_{1}) / \|V\|^{2} \|Z\|^{2}\right) = \\ &= \frac{\alpha^{2}}{k} \|V\|^{2} \|Z\|^{2} (2+\varepsilon_{2}). \end{aligned}$$

This gives us the important alternative to the main lemma result that we can use in the subsequent proofs.  $\Box$ 

#### 5. Main result

**Theorem 4.** The Hamiltonian for the system of the three-dimensional waveguides coupled through small square window in transverse electric field has an eigenvalue below the lower bound of the continuous spectrum. The distance  $\delta$  between the eigenvalue and the threshold is estimated as follows:

$$\delta \geqslant \frac{3 \cdot 2^{17} a^6 \left(\frac{2m\lambda}{h^2} + \frac{E^2}{16\lambda^2}\right)^2}{\pi^{10} d^2 \left(3 + 2\varepsilon_1\right)^2 \|Z\|^4 \left(2 + \varepsilon_2\right)^2}$$

where d and 2l are correspondingly the thickness and the width of the waveguides, 2a is the window width, E is the electric field.

*Proof.* Let's consider the ratio  $\frac{M(\psi)}{\|\psi\|^2}$  using the expressions from lemma 2:

$$\frac{M(\psi)}{\|\psi\|^2} < \frac{\eta^2 \frac{\pi}{2} a(3+2\varepsilon_1) + \alpha^2 k \|V\|^2 \|Z\|^2}{\|\psi\|^2} + \frac{\left(\frac{\alpha^2}{k} + 2\alpha^2 a\right) \|V\|^2 \|Z'\|^2}{\|\psi\|^2} - \frac{64\eta \frac{a^2}{\pi^2} \alpha p^{-\frac{1}{12}} \left(\frac{\lambda}{E}\right)^{-\frac{5}{4}} \sqrt{C^2 + D^2} \sqrt{p(\frac{\lambda}{E})^3 + \frac{1}{16}\cos\gamma}}{\|\psi\|^2}.$$

It is easy to see that the first and the last terms of the numerator produce polynomial  $T(\eta)$ .

$$T(\eta) = = \eta^2 \frac{\pi}{2} a(3+2\varepsilon_1) - 64\eta \frac{a^2}{\pi^2} \alpha p^{-\frac{1}{12}} \left(\frac{\lambda}{E}\right)^{-\frac{5}{4}} \sqrt{C^2 + D^2} \sqrt{p\left(\frac{\lambda}{E}\right)^3 + \frac{1}{16}} \cos\gamma.$$

Let's find the value for the parameter  $\eta$  which minimizes the polynomial  $T(\eta)$ :

$$\mathbf{T}'(\eta) = = \eta \pi a (3 + 2\varepsilon_1) - 64 \frac{a^2}{\pi^2} \alpha p^{-\frac{1}{12}} \left(\frac{\lambda}{E}\right)^{-\frac{5}{4}} \sqrt{C^2 + D^2} \sqrt{p \left(\frac{\lambda}{E}\right)^3 + \frac{1}{16}} \cos \gamma = 0.$$

Let us take the following value of the parameter  $\eta$ :

$$\eta_0 = \frac{64a\alpha p^{-\frac{1}{12}} (\frac{\lambda}{E})^{-\frac{5}{4}} \sqrt{C^2 + D^2} \sqrt{p(\frac{\lambda}{E})^3 + \frac{1}{16}} \cos\gamma}{\pi^3 (3 + 2\varepsilon_1)}.$$

Variational estimations of the eigenvalues for 3D quantum waveguides

In this case one has:

$$T(\eta) = -\frac{2^{11}a^3\alpha^2 p^{-\frac{1}{6}} \left(\frac{\lambda}{E}\right)^{-\frac{5}{2}} (C^2 + D^2)}{\pi^5 (3 + 2\varepsilon_1)} \frac{\left(p\left(\frac{\lambda}{E}\right)^3 + \frac{1}{16}\right)\cos^2\gamma}{\pi^5 (3 + 2\varepsilon_1)}.$$

Hence, the considered ratio is estimated by the following expression:

$$\frac{M(\psi)}{\|\psi\|^2} < \frac{\alpha^2 k \|V\|^2 \|Z\|^2 + \left(\frac{\alpha^2}{k} + 2\alpha^2 a\right) \|V\|^2 \|Z'\|^2}{\|\psi\|^2} - \frac{2^{11} a^3 \alpha^2 p^{-\frac{1}{6}} \left(\frac{\lambda}{E}\right)^{-\frac{5}{2}} (C^2 + D^2) \left(p \left(\frac{\lambda}{E}\right)^3 + \frac{1}{16}\right) \cos^2 \gamma}{\pi^5 \left(3 + 2\varepsilon_1\right) \|\psi\|^2}.$$

Lemma 3 allows one to simplify the first ration in the expression:

$$\frac{\alpha^{2}k \left\|V\right\|^{2} \left\|Z\right\|^{2} + \left(\frac{\alpha^{2}}{k} + 2\alpha^{2}a\right) \left\|V\right\|^{2} \left\|Z'\right\|^{2}}{\left(\frac{\alpha^{2}}{k} + 2\alpha^{2}a\right) \left\|V\right\|^{2} \left\|Z\right\|^{2} (2 + \varepsilon_{2})} = \frac{\alpha^{2}k}{\left(\frac{\alpha^{2}}{k} + 2\alpha^{2}a\right) (2 + \varepsilon_{2})} + \frac{\left\|Z'\right\|^{2}}{\left\|Z\right\|^{2} (2 + \varepsilon_{2})}.$$

Throw off the positive  $2\alpha^2 a$  member from the first denominator because it will only increase the overall value and don't affect our upper estimate. So, we have:

$$\frac{\alpha^2 k}{\left(\frac{\alpha^2}{k} + 2\alpha^2 a\right)(2+\varepsilon_2)} + \frac{\|Z'\|^2}{\|Z\|^2(2+\varepsilon_2)} = \frac{k^2}{(2+\varepsilon_2)} + \frac{\|Z'\|^2}{\|Z\|^2(2+\varepsilon_2)}.$$

Let's make the conversion on the second ratio using the values for the norms:

$$\frac{\|Z'\|^2}{\|Z\|^2} = \frac{2\int_{-l}^{-a} \left\{ \frac{2(l+z)}{(l-a)^2} e^{k(z+a)} + k \frac{(l+z)^2}{(l-a)^2} e^{k(z+a)} \right\}^2 dz}{\int_{-l}^{l} \left\{ \min(1, \frac{(l-|z|)^2}{(l-a)^2} e^{-k(|z|-a)}) \right\}^2 dz} = \frac{k^2 I + 4k \int_{-l}^{-a} \frac{(l+z)^3}{(l-a)^4} e^{2k(z+a)} dz + 4 \int_{-l}^{-a} \frac{(l+z)^2}{(l-a)^4} e^{2k(z+a)} dz}{I+a}.$$

We can throw off also the negative members outside of integral after the integration by parts and also to skip the positive members from the denominator, the ratio will only increase.

$$\frac{\|Z'\|^2}{\|Z\|^2} \leqslant \frac{k^2 I + \frac{2}{3}k^2 I}{I+a} = \frac{5}{3}k^2.$$

The second part of the main expression can be simplified by using of the alternative result of lemma 2 in the denominator:

$$\frac{2^{11}a^{3}\alpha^{2}p^{-\frac{1}{6}}\left(\frac{\lambda}{E}\right)^{-\frac{5}{2}}(C^{2}+D^{2})\left(p\left(\frac{\lambda}{E}\right)^{3}+\frac{1}{16}\right)\cos^{2}\gamma}{\pi^{5}\left(3+2\varepsilon_{1}\right)\left\|\psi\right\|^{2}} = \frac{2^{11}a^{3}kp^{-\frac{1}{6}}\left(\frac{\lambda}{E}\right)^{-\frac{5}{2}}(C^{2}+D^{2})\left(p\left(\frac{\lambda}{E}\right)^{3}+\frac{1}{16}\right)\cos^{2}\gamma}{\pi^{5}\left(3+2\varepsilon_{1}\right)\left\|V\right\|^{2}\left\|Z\right\|^{2}\left(2+\varepsilon_{2}\right)}.$$

And we have for the ratio:

$$\frac{M(\psi)}{\|\psi\|^2} < \frac{8k^2}{3(2+\varepsilon_2)} - \frac{2^{11}a^3kp^{-\frac{1}{6}}\left(\frac{\lambda}{E}\right)^{-\frac{5}{2}}(C^2+D^2)\left(p\left(\frac{\lambda}{E}\right)^3+\frac{1}{16}\right)\cos^2\gamma}{\pi^5(3+2\varepsilon_1)\|V\|^2\|Z\|^2(2+\varepsilon_2)}.$$

Again, we received the polynomial but this time it depends on the parameter k, let's mark it as H(k) and search for the minimum value. It is for  $k = k_0$ :

$$k_{0} = \frac{3 \cdot 2^{11} a^{3} p^{-\frac{1}{6}} \left(\frac{\lambda}{E}\right)^{-\frac{5}{2}} (C^{2} + D^{2}) \left(p \left(\frac{\lambda}{E}\right)^{3} + \frac{1}{16}\right) \cos^{2} \gamma}{16 \pi^{5} \left(3 + 2\varepsilon_{1}\right) \|V\|^{2} \|Z\|^{2}}.$$

One has

$$H(k_0) = -\frac{3 \cdot 2^{17} a^6 p^{-\frac{1}{3}} \left(\frac{\lambda}{E}\right)^{-5} \left(C^2 + D^2\right)^2 \left(p \left(\frac{\lambda}{E}\right)^3 + \frac{1}{16}\right)^2 \cos^4 \gamma}{\pi^{10} \left(3 + 2\varepsilon_1\right)^2 \|V\|^4 \|Z\|^4 \left(2 + \varepsilon_2\right)}.$$

Consequently, the ratio is estimated as follows:

$$\frac{M(\psi)}{\|\psi\|^2} < -\frac{3 \cdot 2^{17} a^6 p^{-\frac{1}{3}} \left(\frac{\lambda}{E}\right)^{-5} \left(C^2 + D^2\right)^2 \left(p \left(\frac{\lambda}{E}\right)^3 + \frac{1}{16}\right)^2 \cos^4 \gamma}{\pi^{10} \left(3 + 2\varepsilon_1\right)^2 \|V\|^4 \|Z\|^4 \left(2 + \varepsilon_2\right)}$$

The received result already gives us the required proof of the gap existence, because the expression in the right hand side of the inequality is negative. Really, all the terms, except  $p^{-\frac{1}{3}}(\frac{\lambda}{E})^{-5}$ , contain even powers. The marked term can be considered as:

$$p^{-\frac{1}{3}} \left(\frac{\lambda}{E}\right)^{-5} = \left(\frac{\hbar^2}{2mE}\right)^{\frac{1}{3}} \left(\frac{E}{\lambda}\right)^5 = E^{\frac{14}{3}}\beta,$$

hence, it is also positive.

We, really, have a lack of dependencies of the gap size on the system parameters in the estimate. Let's simplify the received result taking into account that it is the upper estimation on the eigenvalue. We have for the weak field:

$$\int_{0}^{d} V^{2}(y) dy = \int_{0}^{d} \left(C^{2} + D^{2}\right) p^{-\frac{1}{6}} \left(y + \frac{\lambda}{E}\right)^{-\frac{1}{2}} \times \\ \times \cos^{2} \left(\frac{2}{3} \left(y + \frac{\lambda}{E}\right)^{\frac{3}{2}} p^{\frac{1}{2}} + \frac{\pi}{4} - \operatorname{arctg} \frac{D}{C}\right) dy_{E \to 0} = \\ = \int_{0}^{d} \left(C^{2} + D^{2}\right) p^{-\frac{1}{6}} \left(\frac{\lambda}{E}\right)^{-\frac{1}{2}} \cos^{2} \left(\frac{2}{3} \left(\frac{\lambda}{E} p^{\frac{1}{3}}\right)^{\frac{3}{2}} + \frac{\pi}{4} - \operatorname{arctg} \frac{D}{C}\right) dy.$$

Let's choose D = 0 (V becomes even). Don't forget that  $\gamma$  also depends on D:

$$\gamma = \frac{2}{3} \left(\frac{\lambda}{E}\right)^{\frac{3}{2}} p^{\frac{1}{2}} + \frac{\pi}{4} + \operatorname{arctg} \frac{\frac{1}{4}C(\frac{E}{\lambda})^{\frac{3}{2}} + Dp^{\frac{1}{2}}}{Cp^{\frac{1}{2}} - \frac{1}{4}D(\frac{E}{\lambda})^{\frac{3}{2}}} = \frac{2}{3} \left(\frac{\lambda}{E}\right)^{\frac{3}{2}} p^{\frac{1}{2}} + \frac{\pi}{4}.$$

So, for the ratio we have:

$$\begin{aligned} & \frac{M(\psi)}{\|\psi\|^2} < \\ & < -\frac{3 \cdot 2^{17} a^6 \left(\frac{\lambda}{E}\right)^{-4} (C^2 + D^2)^2 \left(p \left(\frac{\lambda}{E}\right)^3 + \frac{1}{16}\right)^2}{\pi^{10} \left(3 + 2\varepsilon_1\right)^2 d^2 \left(C^2 + D^2\right)^2} \frac{\cos^4 \left(\frac{2}{3} \left(\frac{\lambda}{E} p^{\frac{1}{3}}\right)^{\frac{3}{2}} + \frac{\pi}{4}\right)}{\cos^4 \left(\frac{2}{3} \left(\frac{\lambda}{E} p^{\frac{1}{3}}\right)^{\frac{3}{2}} + \frac{\pi}{4} - \operatorname{arctg} \frac{D}{C}\right) \|Z\|^4 \left(2 + \varepsilon_2\right)} = \\ & = -\frac{3 \cdot 2^{17} a^6 \left(\frac{2m\lambda}{h^2} + \frac{E^2}{16\lambda^2}\right)^2}{\pi^{10} d^2 \left(3 + 2\varepsilon_1\right)^2 \|Z\|^4 \left(2 + \varepsilon_2\right)}. \end{aligned}$$

Theorem is proved - the gap in the spectrum can be estimated as the norm of the expression in the right hand side.  $\hfill \Box$ 

## 6. Conclusion

The main result of the paper is received and is formulated in the theorem. Namely, the existence of the eigenvalue below the lower bound of the continuous spectrum of the Laplacian for the system of the coupled 3D waveguides in the transverse electric field is proved. The gap width between the eigenvalue and the threshold is estimated. More precisely, the gap's width depends on the window's width in the sixth degree (or a less because we have only the upper estimate for the eigenvalue position and the corresponding lower estimate for the gap's width). Also it inversely depends on the waveguides thickness in the second degree (and even sixth after simplifying the numerator's brackets). Dependency on the waveguides width was broken by the exponential character of the trial function term, and we have not obtained here the power estimate. Also we have not the evident power dependence in respect to the electric field. Nevertheless, one can see that the electric field allows one to manage the gap size for the fixed structure parameters that is very important for the nanoelectronic applications.

The work was supported by Federal Targeted Program "Scientific and Educational Human Resources for Innovation-Driven Russia" (contracts P689 NK-526P, 14.740.11.0879, and 16.740.11.0030), grant 11-08-00267 of Russian Foundation for Basic Researches and by Federal Targeted Program "Researches and Development in the Priority Directions Developments of a Scientific and Technological Complex of Russia 2007-2013" (state contract 07.514.11.4146).

## References

- Alferov Zh. I., Aseev A. L., Gaponov S. V., Kop'ev P. S., Suris R. A. // In: Nanomaterials and Nanotechnologies, Part 1, Analytics. – Moscow, 2008 [in Russian].
- [2] Ho J., Yerushalmi R., Jacobson Z. A., Fan Z., Alley R. L., Javey A. // Nature Mater. 2008. V. 7. P. 62.
- [3] Ferry D.K., Goodnick S.M. Transport in Nanostructures. Cambridge: Cambridge University Press, 1997.
- [4] Zutic I., Fabian J., Das S. SARMA Spintronics: Fundamental and Applications // Rev. Mod. Phys. 2004. V. 76. – P. 323–386.
- [5] Bader S.D. Colloquium: Opportunities in nanomagnetism // Rev. Mod. Phys. 2006. V. 78. P. 1-15.
- [6] Grunberg P. Layered magnetic structures: facts, figures, future // J. Phys.: Condens. Matter. 2001. V. 13. P. 7691–7706.
- [7] Exner P. Laterally coupled quantum waveguides // Cont. Math. 1998. V. 217. P. 69-82.
- [8] Matveev D. G., Popov I. Yu. Bound electron states in a system of coupled quantum waveguides in a transverse electric field // Tech. Phys. Lett. – 2009. – V. 35 (11). – P. 1007–1009.
- [9] Exner P., Vugalter S. Bound state asymptotic estimates for window-coupled Dirichlet strips and layers // J. Phys. A: Math. Gen. - 1997. - V. 30. - P. 7863-7878.

- [10] Melnichuk O.P., Popov I.Yu. Coupled dielectric waveguides: variational estimations // J. Math. Phys. 2005. V. 46, No. 7. – P. 073501/1-073591/17.
- [11] Popov I.Yu. Asymptotics of bound states and bands for laterally coupled waveguides and layers // J. Math. Phys. 2002. V. 43, No. 1. P. 215-234.
- [12] Popov I.Yu. Asymptotics of bound states and bands for laterally coupled three-dimensional waveguides // Rep. on Math. Phys. - 2001. - V. 48, No. 3.
- [13] Bagraev N., Martin G., Pavlov B. S., Yafyasov A. Landau–Zener effect for a quasi-2D periodic sandvich // Nanosystems: Phys., Chem., Math. – 2011. – V. 2 (4). – P. 32-50.