NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2013, 4 (2), P. 173–181

MULTI PARTICLE STATES CALCULATIONS AND PARTICLES STORAGE IN PERTURBED NANOLAYERS

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PACS 02.30.Tb, 73.21.Ac, 03.65.Ge

The problem of particle storage in nanolayered structures will be considered. Local perturbations of nanolayers can lead to the appearanceof eigenvalues of the corresponding one-particle Hamiltonian. To study particle storage it is necessary to deal with the multi-particle problem. This problem faces essential computational difficulties due to the great increase of the spatial dimension. Using a composite of natural physical models, analytical methods and computational approaches allows one to simplify the problem and to obtain useful results for application. Particularly, the Hartree method and Finite Elements Method (FEM) are used. The discrete spectrum of the Hamiltonian for two interacting particles is considered. Two different types of perturbation are considered: deformation of the layer boundary and a small window in a wall between two layers. The relation between the system parameters (interaction intensity - waveguide deformation) ensuring the existence of a non-empty discrete spectrum is studied. A comparison of particle storage efficiencies is made for these two cases.

Keywords: discrete spectrum; few-particle problem; quantum waveguide.

1. Introduction

It is known that curved quantum layers can store particles. From a mathematical point of view, it is related with the existence of eigenvalues for the corresponding Hamiltonian. Increased curvature leads to larger eigenvalues figures. This question is important in various physical problems. For example, to do two-qubit operation in a quantum computer based on coupled quantum waveguides (see, e.g., [1], [2]), it is necessary to store two electrons in some bounded domain during the operation time. Another interesting application is related to the storage of hydrogen (or protons) in nanolayered structures. Storing hydrogen in this manner can give a safe and effective fuel container for a hydrogen engine. One can note that layers with curved boundaries are more effective for particle storage because increasing the curvature (or boundary perturbation amplitude) leads to an increase of the discrete spectrum cardinality. Hence, the amount of hydrogen stored in the layered structure will be greater. Note that the Hamiltonian for the corresponding plane layered structure has an empty discrete spectrum.

To solve the problem it is necessary to consider the multi-body system, which is the main source of difficulty. Many-particle problems appear in various situations. These problems have been studied by using a variety of different methods (see, e.g., [3], [4]). For the quantum waveguide multi-body problem, the majority of results concerns the use of one-dimensional wires. Many of these methods for dealing with this particular problem have been reported previously [5]. Interesting approaches are also based on scattering theory [6], operator extensions theory [7] and reducing the problem to a 2D diffraction [8].

In the discrete spectrum problem for curved or deformed 2D (3D) quantum waveguides, rigorous mathematical results are only available for the one-particle Hamiltonian (if we deal with non-interacting particles or interaction is taken into account as some mean field only, then we really deal with a one-particle problem). As for the many-particle problem for quantum waveguides, only approximated results have been obtained [9], [10], [11], [12]. For example, Exner estimates the number of neutral fermions which can be stored near the distortion of the layer as the dimension of the discrete spectrum subspace [10]. For charged (repulsing) particles, only rough variational estimation for the maximum number of stored particles can be obtained (the analogous rough variational results for attracting particles have been described [12]). Namely, consider 2D layer Σ – strip in $\mathbb{R}^2$ of width $2a$. Let Γ be the axis of Σ. The strip is determined by the semi-width a and the curvature $s \to \gamma(s)$, defined on Γ. Here s is the curve length. Assume that the following regularity conditions take place: a) Σ is non self-intersecting curve, b) $a\|\gamma\|_\infty < 1$, c) γ has bounded support and $\gamma \in C^2$, γ, γ' are bounded.

Let us first choose a system of units for which $\hbar = 2m = c = 1$, c is the speed of light, m is the particle mass. Using natural waveguide coordinates (s, u) in Σ, one reduces the one-particle Hamiltonian to the following operator:

$$H = -\partial_s(1 + u\gamma)^{-2}\partial_s - \partial_u{}^2 + V(s, u)$$

in $L^2(\mathbb{R} \times (-a, a))$ with the potential

$$V(s, u) = -\frac{\gamma(s)^2}{4(1 + u\gamma(s))^2} + \frac{u\gamma''(s)}{2(1 + u\gamma(s))^3} - \frac{5u\gamma''(s)^2}{4(1 + u\gamma(s))^4}.$$

The operator is defined and essentially self-adjoint on $D(H) = \{f : f \in C^\infty, f(s, \pm a) = 0, Hf \in L^2\}$. By means of the modes expansion, one reduces the problem to a one-dimensional case [13–15], for which we use the Birman-Shwinger estimations. The potential V is majorized by:

$$W = \frac{\gamma(s)^2}{4\delta_-^2} + \frac{a|\gamma''(s)|}{2\delta_-^3} + \frac{5a^2\gamma''(s)^2}{4\delta_-^4}, \quad \delta_\pm = 1 \pm a\|\gamma\|_\infty.$$

Let us introduce W_j, $j = 2, 3, \ldots$

$$W_j(s) = \begin{cases} 0, & \left(\frac{\pi}{2a}\right)^2 (j^2 - 1) > \|W\|_\infty, \\ W(s), & \left(\frac{\pi}{2a}\right)^2 (j^2 - 1) \leqslant \|W\|_\infty. \end{cases}$$

Then the number N of neutral fermions, with spins S, which can be bounded near the perturbation of the layer is estimated [10] as:

$$N \leqslant (2S + 1) \left(1 + \delta_+^2 \frac{\int\limits_{\mathbb{R}^2} W(s)\, |s - t|\, W(t) ds dt}{\int\limits_{\mathbb{R}} W(s) ds} + \sum_{j=2}^{\infty} \delta_+^2 \int\limits_{\mathbb{R}} W(s) ds \right).$$

Here we assume the Dirichlet condition. The Neumann and Robin conditions are analogous. As for the semi-transparent surface, it is possible to consider it as $\delta-$potential supported by curve [16], [17], [18].

In the case of charged particles (electrons, protons) it is necessary to consider their interaction. The simplest approximation was discussed previously [10], and some variational estimations were obtained. The discrete spectrum of a N-particle Hamiltonian can be empty. A sufficient condition for this is as follows:

$$T_\beta(N) + \frac{e^2 N(N - 1)}{2\beta\sqrt{7}} \geqslant \|W\|_\infty N + \left(\frac{\pi}{2a}\right)^2 N + \frac{e^2}{18\beta\sqrt{2}}$$

for some $\beta \geqslant \max\{2b, 596e^{-2}\}$, where $2b$ is the diameter of the support of function γ, e is the particle charge,

$$T_\beta(N) = \begin{cases} 2\sum\limits_{m=1}^{n} \lambda_m, & N = 2n, \\ 2\sum\limits_{m=1}^{n} \lambda_m + \lambda_m, & N = 2n+1, \end{cases}$$

λ_m are ordered eigenvalues of the Dirichlet Laplacian for the domain $\left[-\frac{3}{2}\beta\delta_+, \frac{3}{2}\beta\delta_+\right] \times [-a, a]$.

The computational problem for an $N-$particle state is rather difficult due to the essential increasing of the space dimension (N times). To simplify the problem, it is possible to use natural physical models and some preliminary analytical considerations. Particularly, the Hartree method permits the reduction of the problem to a sequence of one-particle problems. By using analytically obtained asymptotics, one can choose an initial approximation more effectively. Such a combination of analytical and computational methods seems to be the most promising approach to this problem.

2. One-particle problem for waveguide with deformed boundary

Variational estimates for the eigenvalues of the problem were obtained [19]. The domain is determined as follows:

$$\Omega = \{(x, y) \in R^2 :\ 0 < y < a(1 + \lambda f(x))\}, \text{supp} f = [-b, b], f \in C_0^\infty(R).$$

The trial function is sought in the form

$$\psi = \begin{cases} (1 + \lambda\eta f(x))\chi_1(y), & |x| \leqslant b, \\ e^{-h|x \mp b|}\chi_1(y), & |x| > b. \end{cases}$$

Let

$$z = \frac{\pi^2}{a^2}\frac{\|f\|^2}{\|f'\|^2},$$

The parameter η is chosen by the condition

$$\eta^2 - 2\eta z + 3z + K^2 < 0,\ \ K = \sqrt{\sum_{n=2}^{\infty}\left(\frac{2n}{n^2-1}\right)} = \sqrt{\frac{\pi^2}{3} + \frac{1}{4}},$$

which can be valid if $z^2 - 3z - K^2 > 0$, particularly, one can take $\eta = z$, that corresponds to the parabola minimum.

$$\chi_n = \sqrt{\frac{2}{a}}\sin\frac{\pi n y}{a}.$$

$$h = \frac{1}{2}\lambda^2 d_1\|f\|^2, d_1 = \frac{\pi^2}{a^2 z}(z^2 - 3z - K^2).$$

The eigenvalue distance from the bottom of the continuous spectrum is estimated as follows;

$$-\lambda^4 {d_0}^2\|f\|^4 + O(\lambda^5) \leqslant E - \frac{\pi^2}{a^2} \leqslant -\frac{1}{4}\lambda^4 {d_1}^2\|f\|^4 + O(\lambda^5),$$

$$d_0 = \left(\frac{4\pi b}{a^2}\right)^2 - 3\frac{\pi^2}{a^2}.$$

The eigenvalue problem is solved numerically by the Finite Elements Method (FEM). Namely, we consider the minimization problem for the functional (in natural system of units)

$$a(\psi, \phi) = \int_\Omega \left(\frac{\hbar^2}{2m}\left(\frac{\partial\psi}{\partial x}\frac{\partial\phi}{\partial x} + \frac{\partial\psi}{\partial y}\frac{\partial\phi}{\partial y}\right) + E\psi\phi\right) d\Omega \qquad (1)$$

in the waveguide domain of length $2k$, width $2a$ with sine-like deformation of height d and width $2b$, $b \ll k$: $f(x) = d \sin\left(\frac{(x-b)\pi}{2b}\right)$, $|x| \leqslant b$. In real physical systems the thickness (width L) of the layer is about the de Broglie wavelength (few nanometers for the electron) The Dirichlet condition are valid at the waveguide boundaries, while Neumann conditions are assumed at the waveguide ends ("formal" boundaries). One can use "non-reflecting" conditions at the ends, but this type of this condition doesn't influence the results. The reason is very simple — the corresponding eigenfunction decays exponentially outside of the perturbation region. To find the numerical solution, we used FreeFem++ with the library ARPACK to search for the matrix eigenvalues. Domain was Ω is divided into triangular subdomains with determined quadratic functions (see Fig. 1). The dependence of the eigenvalue (energy level) on the height of the deformation is shown on Fig. 2. Note that the eigenvalue is less than the threshold, i.e. the bottom of the continuous spectrum, $E/E_0 = \pi^2$. Our results are in good correlation with Exner's estimations.

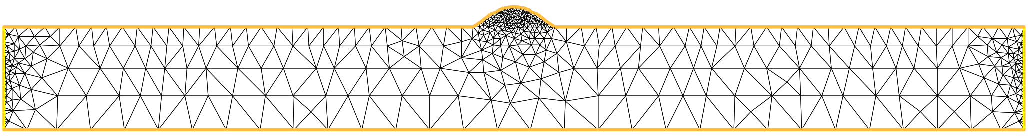

Fig. 1. Triangulation of the domain

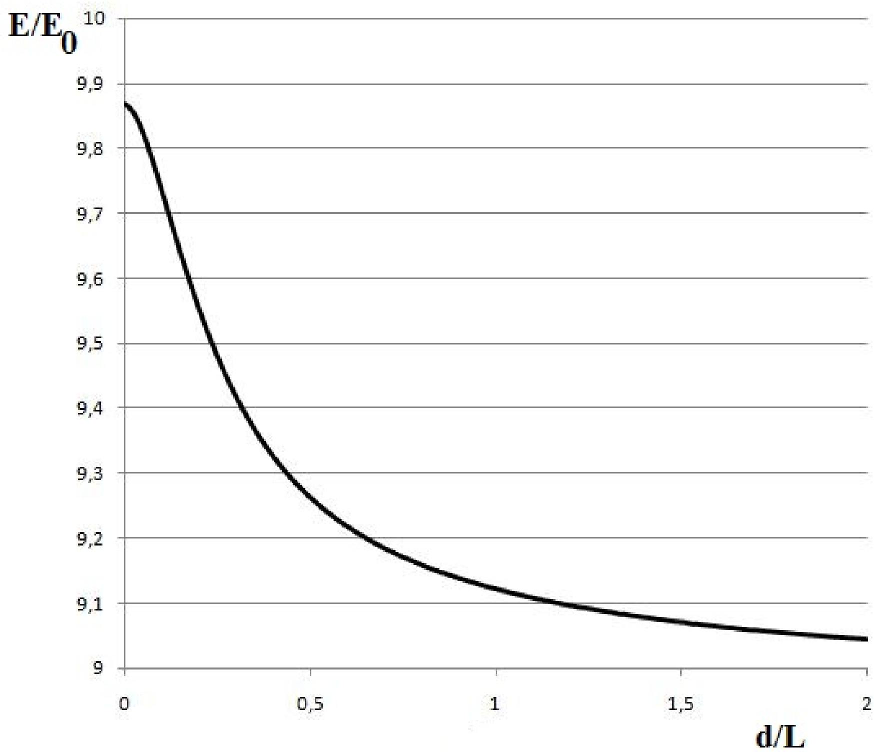

Fig. 2. Dependence of the eigenvalue (energy level) E/E_0 on the height d/L of the deformation (in dimensionless form); $L = 2a$, $E_0 = \frac{\hbar^2}{2mL^2}$, $b = 0.4L$

3. Two-particle problem for waveguide with deformed boundary

Consider two interacting particles in 2D waveguide with a perturbed boundary, i.e. we deal with the two-particle Schrödinger equation

$$-\frac{\hbar^2}{2m}\Delta\psi(r_1,r_2)+U(r_1,r_2)\psi(r_1,r_2)=E\psi(r_1,r_2).$$

The one-particle Hamiltonian for aquantum waveguide exhibits bound states if it is bent, protruded or allowing a leak to another duct [19], [20], [21], and the discrete spectrum depends substantially on the shape of the channel. The same is true for non-interacting particles. The most interesting question is whether the discrete spectrum's non-emptiness is preserved if we switch on the interaction between particles. A search was begun for system parameters that ensured this. Working with the Hartree approximation, the wavefunction is sought in the form

$$\psi(r_1,r_2)=\psi_1(r_1)\psi_2(r_2), \tag{2}$$

where ψ_1 and ψ_2 are one-particle functions and r_1 and r_2 are coordinate vectors of the corresponding particles. Using conventional methods, one obtains the following system for ψ_1 and ψ_2:

$$\begin{cases} -\frac{\hbar^2}{2m}\Delta\psi_1(r_1)+U_1(r_1)\psi_1(r_1)=E_1\psi_1(r_1),\\ -\frac{\hbar^2}{2m}\Delta\psi_2(r_2)+U_2(r_2)\psi_2(r_2)=E_2\psi_2(r_2),\end{cases} \tag{3}$$

where

$$U_n(r_n)=\int_\Omega |\psi_{3-n}(r_{3-n})|^2\,u(r_1,r_2)dr_{3-n}, \tag{4}$$

$u(r_1,r_2)$ is the interaction potential, e.g., for Coulomb repulsion it has the form $u(r_1,r_2)=\frac{e^2}{|r_1-r_2|}$. The simplest type of interaction is a $\delta-$potential (see, e.g., [22], [23], [24]). For this case, $U_n(r_n)$ takes the form:

$$U_n(r_n)=\int_\Omega |\psi_{3-n}(r_{3-n})|^2\,U_0\delta(r_1,r_2)dr_{3-n}=U_0\,|\psi_{3-n}(r_n)|^2\,,$$

where U_0 describes the intensity of the interaction. As a result, we get the following system:

$$\begin{cases} -\frac{\hbar^2}{2m}\Delta\psi_1(r_1)+U_0\,|\psi_2(r_1)|^2\,\psi_1(r_1)=E_1\psi_1(r_1),\\ -\frac{\hbar^2}{2m}\Delta\psi_2(r_2)+U_0\,|\psi_1(r_2)|^2\,\psi_2(r_2)=E_2\psi_2(r_2).\end{cases} \tag{5}$$

To find eigenvalues of the two-particle Hamiltonian, FEM is used. For this purpose, the problem needs reformulation in order to study the variational problem. At this stage, the system of differential equations (5) is replaced by integral relations:

$$\begin{aligned} &\int_\Omega\left(\frac{\hbar^2}{2m}\nabla\psi_1\cdot\nabla\phi_1+U_0\,|\psi_2|^2\,\psi_1\phi_1\right)dr_1-E_1\int_\Omega\psi_1\phi_1dr_1=0,\\ &\int_\Omega\left(\frac{\hbar^2}{2m}\nabla\psi_2\cdot\nabla\phi_2+U_0\,|\psi_1|^2\,\psi_2\phi_2\right)dr_2-E_2\int_\Omega\psi_2\phi_2dr_2=0.\end{aligned} \tag{6}$$

The algorithm for the solution begins by taking as the first approximation the following functions $\psi_1=\psi_2=0$leading naturally, to a one-particle problem. Once the one-particle problem is solved, that solution (approximation for the one-particle eigenfunction) is inserted into (5) (or (4) in the general case), then, problem (6) is solved with the obtained potential. The solution is inserted into (5), and the procedure is repeated. Due to spatial symmetry, the values of E_1 and E_2 should coincide, so, the algorithm is made up to the instant when coincidence with the chosen accuracy appears. Bound states corresponds to values less than the lower bound of the continuous spectrum (π^2). For fixed geometry, the convergence deteriorates when the interaction intensity U_0 increases. Values of U_0 are found which guarantee the existence of the bound state. Increasing U_0 leads to the destruction of the two-particles eigenstate. Conversely, increasing the boundary deformation d leads to an increase of the “eigenvalue-threshold” distance (the only reason for the eigenvalue’s existence is this deformation, as plane waveguides have no eigenvalues). It is interesting to find the correlation between the intensity and deformation, for which there exists a two-particle bound state. This corresponds to the domain on the parameter plane. The boundary of this domain (in dimensionless form) is found (see Fig. 3). The domain in question is below the curve on the Figure. One can use this curve to predict the possibility of particle storage, and consequently, to create systems with the proper parameters (proper deformation should correlates with the intensity of the particle’s interaction).

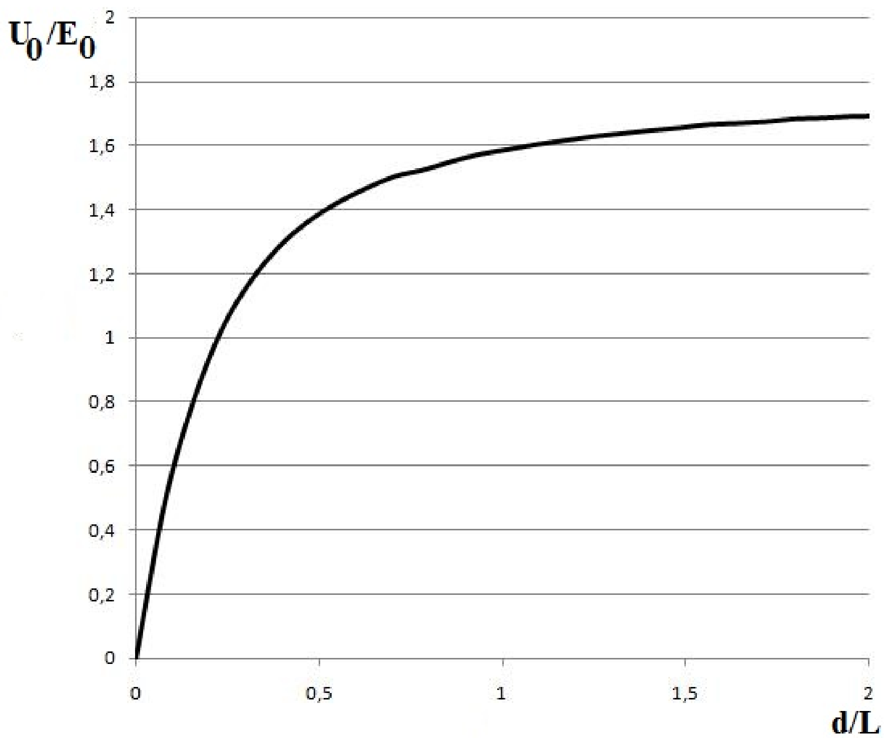

Fig. 3. Domain on the dimensionless parameters plane $(d/L, U_0/E_0)$ corresponding to the existence of eigenvalues of the two-particle Hamiltonian (below the curve); $2a = L$, $E_0 = \frac{\hbar^2}{2mL^2}$, $b = 0.4L$; the domain is below the curve

4. Layers coupled through window

Local perturbation of the layered structure boundary isn’t a unique one that leads to the appearance of bound states below the continuous spectrum. Consider two nanolayers coupled through a narrow slot. It can be considered as a two-dimensional system, i.e. two strips coupled through window. The Dirichlet Laplacian for such system is known to have an eigenvalue below the threshold. The eigenvalue tends to the lower bound of the continuous spectrum when the window width tends to zero. Let d and a be the widths of the strip and the window, correspondingly. Exner and Vugalter [25] obtained an estimation of the eigenvalue distance from the threshold for a small window. The asymptotics (in the width of coupling window) of the eigenvalue were obtained by matching the asymptotic expansions for solutions to the boundary value problem [26], [27]:

$$\lambda_a = \frac{\pi^2}{d^2} - \left(\frac{\pi^3}{2d^3}\right)^2 a^4 + o(a^4). \tag{7}$$

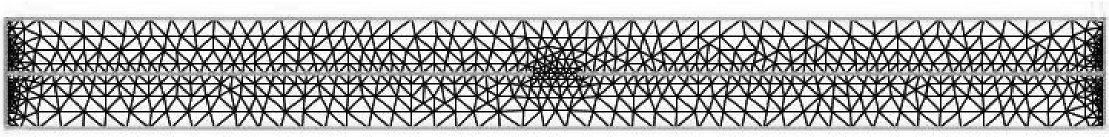

Fig. 4. Triangulation of coupled layers

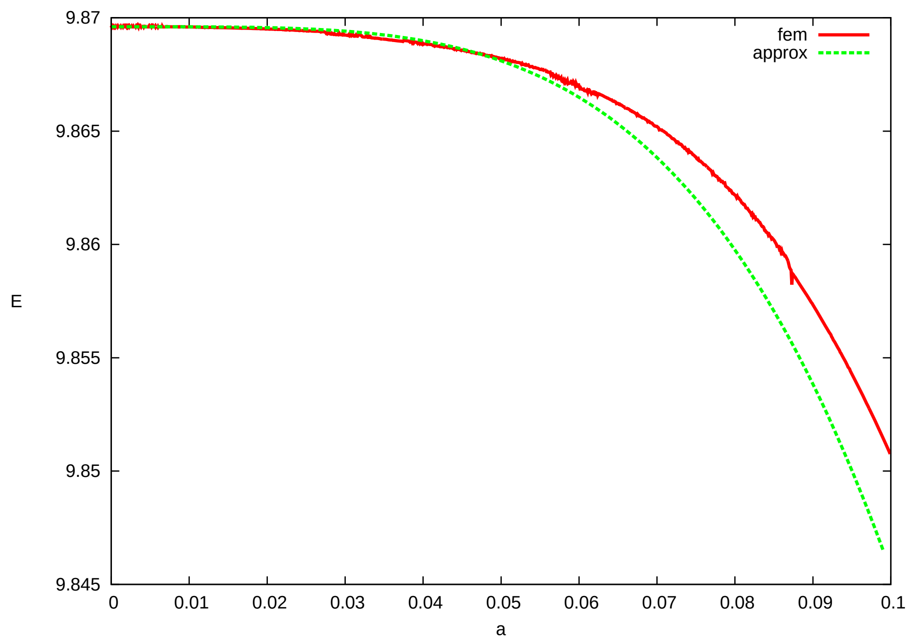

Fig. 5. Comparison of eigenvalue asymptotics ("approx") (7) and exact eigenvalue ("fem") for small coupling window

These results concern the one-particle Hamiltonian. As for the corresponding two-particle problem, there are no results. In the present paper, as a first step, we consider the one-particle problem for the system of arbitrary window size. Computations are made by FEM. Triangulation is made as shown on Fig. 4 One can see (Fig. 5) that for a small window, the results are in good correlation with the asymptotics. The main subject of this section is the two-particle problem for this system. We consider the delta-interaction between the particles. Delta-repulsion leads to the destruction of the one-particle bound state. We found the domain on the parameter's plane ("interaction intensity - window width"), which corresponds to the existence of the two-particle bound state. The results are shown on Fig.6. It is interesting to compare these results with the analogous one obtained for the deformed boundary layer. One can see that two layers with a coupling window is essentially more effective for the storage of two particles than the nanolayer with a deformed boundary (the destroying electrostatic repulsion intensity is many times greater). The result becomes clear if we look through the distributions of electron density (Fig. 7).

Acknowledgements

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, 16.740.11.0030), grant 11-08-00267 of Russian Foundation for Basic Researches.

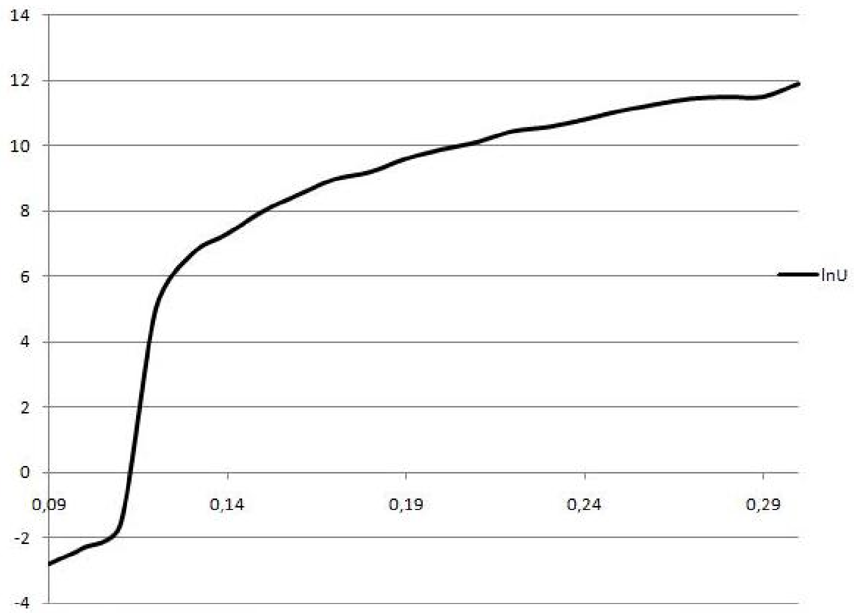

Fig. 6. Domain on the dimensionless parameters plane $(d/L, \log U_0/E_0)$ corresponding to the existence of eigenvalues of the two-particle Hamiltonian (below the curve)

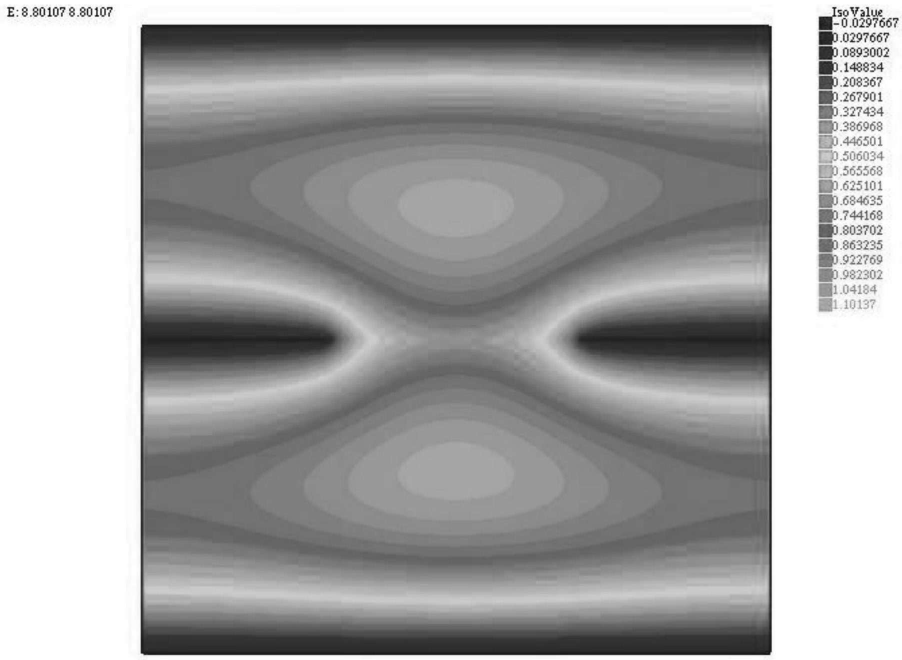

Fig. 7. electron density distribution of two-particle state for layers coupled through window

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