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HARTREE-FOCK APPROXIMATION FOR THE PROBLEM OF PARTICLE STORAGE IN DEFORMED NANOLAYER

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The paper deals with the problem of quantum particle storage in a nanolayered structures. The system of a few electrons interacting via a δ-potential is considered. The particles are placed into a two-dimensional deformed waveguide. From a mathematical point of view, the bound state of the system means that the corresponding Hamiltonian will have eigenvalues. To treat a multi-particle problem, the Hartree-Fock approach and the finite element method are used. Three different types of the perturbation are considered: deformation of the layer boundary, a small window in a wall between two layers and a bent layer. The systems of 2–10 particles with various total spins are studied. The dependence of the minimal deformation parameter, which keeps bound state on the number of particles, is given. Comparison of the storage efficiencies in those cases is made.

Keywords: discrete spectrum, multi-particle problem, waveguide.

1. Introduction

The problem of the existence of the bound states of quantum particles is very important in physics. Its usefulness is demonstrated by the particle storage problem. It is known that a particle can be stored in curved nanolayers. In the terms of math it means the existence of the discrete spectrum of the corresponding Hamiltonian. The single particle system in an undeformed nanolayer has an empty discrete spectrum. But deformation of the layer causes the appearance of an eigenvalue (see, e.g., [1–7]). Increasing the curvature leads to increasing eigenvalue numbers. In many applications it's necessary to store more than one particle and, consequently, to deal with the multi-particle problem [8, 9]. As an example of such an application, the storage of hydrogen in nanolayed structures can be given. This can be used to produce an effective and safe fuel container. In this work, the equations for multi-particle problem are simplified by the Hartree-Fock approach and the eigenvalue problem is solved numerically by the finite element method.

2. Theory background

Consider a number of interacting electrons placed into a nanolayer or a waveguide. Neglecting the spin-orbit interaction, one gets the following form for the Hamiltonian of the multi-particle system:

$$\hat{H} = \sum_k \left(-\frac{\hbar^2}{2m}\nabla_k^2 + U_k \right) + \frac{1}{2}\sum_{\substack{j,k \\ j\neq k}} V_{jk} = \sum_k \hat{H}_k + \frac{1}{2}\sum_{\substack{j,k \\ j\neq k}} \hat{H}_{jk}, \qquad (1)$$

where m is particle's mass, U_k is the external field potential, V_{jk} is potential of the particles' interaction. Solving the multi-particle problem is a Herculean task, so one needs to simplify the equation (1). Application of the *Hartree method* for two particle problem was described in [10]. In this case, the wavefunction of the system is sought in the form

$$\psi(x_1, x_2, \ldots, x_n) = \psi_1(x_1)\psi_2(x_2)\ldots\psi_n(x_n), \tag{2}$$

where ψ_i is the single particle function, x_i represents the set of four coordinates: three spatial ones and a spin one. Substituting (2) into (1) and using the variational principle, one can obtain *Hartree equations* (see [11]):

$$\left[\hat{H}_k + \sum_{\substack{j \\ j\neq k}} \int \psi_j^*(x_j)\hat{H}_{jk}\psi_j(x_j)\,dx_j\right]\psi_k(x_k) = E_k\psi_k(x_k) \qquad (k = \overline{1,n}). \tag{3}$$

The *Hartree method* is easy to implement but this approach has one significant disadvantage; the electronic wavefunction must satisfy the antisymmetry principle, i.e. it must be antisymmetric with respect to the interchange of all (space and spin) coordinates of one fermion with those of another. That is,

$$\psi(x_1, x_2, \ldots, x_i, \ldots, x_j, \ldots, x_n) = -\psi(x_1, x_2, \ldots, x_j, \ldots, x_i, \ldots, x_n). \tag{4}$$

This drawback was avoided by Fock. The idea of the *Hartree-Fock method* is to replace the wavefunction representation (2) by the *Slater determinant*:

$$\psi(x_1, x_2, \ldots, x_n) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_1(x_1) & \psi_2(x_1) & \ldots & \psi_n(x_1) \\ \psi_1(x_2) & \psi_2(x_2) & \ldots & \psi_n(x_2) \\ \ldots & \ldots & \ldots & \ldots \\ \psi_1(x_n) & \psi_2(x_n) & \ldots & \psi_n(x_n) \end{vmatrix}. \tag{5}$$

Again, engaging the variational principle, one can obtain (see [11]) the *Hartree-Fock equations*:

$$\left[\hat{H}_k + \sum_{\substack{j \\ j\neq k}} \int \psi_j^*(x_j)\hat{H}_{jk}\psi_j(x_j)\,dx_j\right]\psi_k(x_k) - \sum_{\substack{j \\ j\neq k}}\left[\int \psi_j^*(x_j)\hat{H}_{jk}\psi_k(x_j)\,dx_j\right]\psi_j(x_k) = \\ = E_k\psi_k(x_k) \qquad (k = \overline{1,n}). \tag{6}$$

To find the discrete spectrum, of the system one has to remember that all eigenvalues $E_1, \ldots, E_n$ must be less than the threshold (the bottom of the continuous spectrum, $E_{bot} = \pi^2\hbar^2/(2mL^2)$, where L is the waveguide width at infinity).

3. Numerical model

For the numerical model, we assume zero external field potential U_k and δ-potential of particles interaction:

$$V_{jk} = U_0\delta(r_j - r_k), \tag{7}$$

where U_0 is a constant which describes the intensity of the interaction, r_j and r_k are spatial coordinates of the particles. We assume every electron has predefined spin $s = 1/2$ or

$s = -1/2$. Applying those assumptions, one rewrites the *Hartree-Fock equations* (6) in simpler form:

$$\left[-\frac{\hbar^2}{2m}\nabla_k^2 + \sum_{\substack{j \\ j\neq k}} U_0 \left|\psi_j(r_k)\right|^2\right] \psi_k(r_k) - \sum_{\substack{j \\ j\neq k}} U_0 \delta_{s_j,s_k} \left|\psi_j(r_k)\right|^2 \psi_k(r_k) = E_k \psi_k(r_k) \qquad (k = \overline{1,n})$$

or

$$\left[-\frac{\hbar^2}{2m}\nabla_k^2 + \sum_{\substack{j \\ j\neq k}} U_0 (1 - \delta_{s_j,s_k}) \left|\psi_j(r_k)\right|^2\right] \psi_k(r_k) = E_k \psi_k(r_k) \qquad (k = \overline{1,n}), \tag{8}$$

where s_j, s_k are spin values of the corresponding electrons. All problems are solved in 2D. Three types of geometries are studied: i) a waveguide with deformed boundary (fig. 1); ii) two layers coupled through window (fig. 2); iii) a bent waveguide (fig. 3). Dirichlet conditions are valid at the waveguide boundaries and Neumann conditions are assumed at the ends of the waveguide. For the first configuration, the deformation is described by an analytical function. Its parameter is H/L (deformation width b is constant). The parameter of the second configuration is a/L. And for the last one is L/R (the length of the curved arc is constant). In all cases, larger geometry parameter values correspond to larger deformations of the waveguide. To find the numerical solution of (8), the FEM is

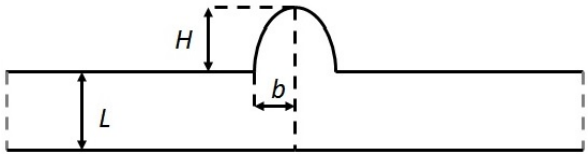

FIG. 1. Deformed waveguide

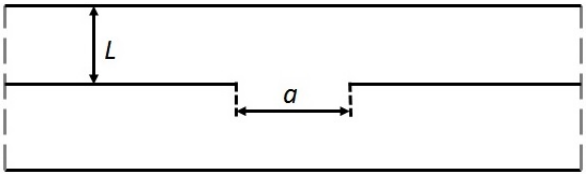

FIG. 2. Window-coupled waveguides

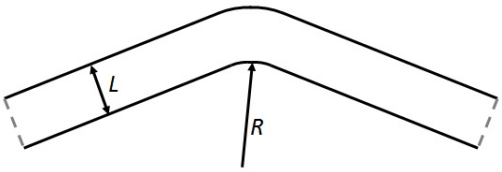

FIG. 3. Bent waveguide

used. The package FreeFEM++ is engaged. The algorithm of the solution is the same as in [10]. First, assume all functions ψ_k to be zero as the first approximation. Then solve the first equation for ψ_1. After that, insert it into the second equation and solve it with respect to ψ_2. The procedure is repeated until the difference between two last approximations becomes small enough.

4. Results

A number of computations for systems with different number of particles and various total spin values were made. While the interaction intensity was constant, the critical value of the geometry parameter was sought. The critical value is the minimal value of the parameter which maintains the bound state of the system. The results are shown at

the figures below. As expected, more particles and bigger total spins lead to increasing deformation which is needed to store the particles. This means that it is more difficult to store these particles. But, one sees an interesting effect which is valid for all geometries. It was shown that to store an even number of particles with zero total spin, the deformation may be the same or even less than that for a system of one less particle. Comparison of the dependencies slopes in figures 4–6 shows the efficiency of the window-coupled type deformation. In contrast, the bent waveguide is the least efficient.

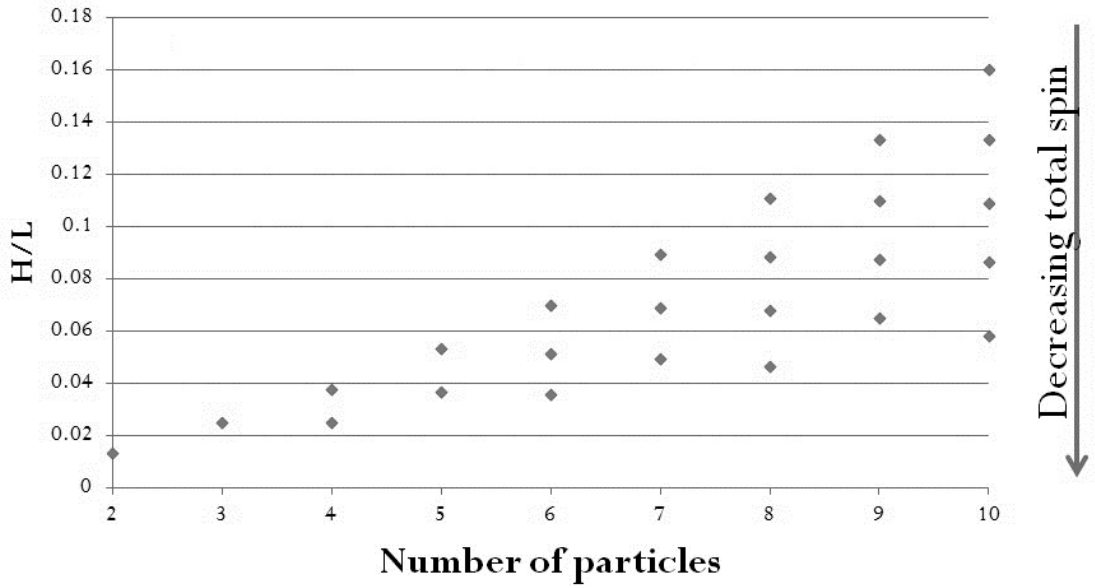

FIG. 4. Deformed waveguide: critical value of the geometry parameter

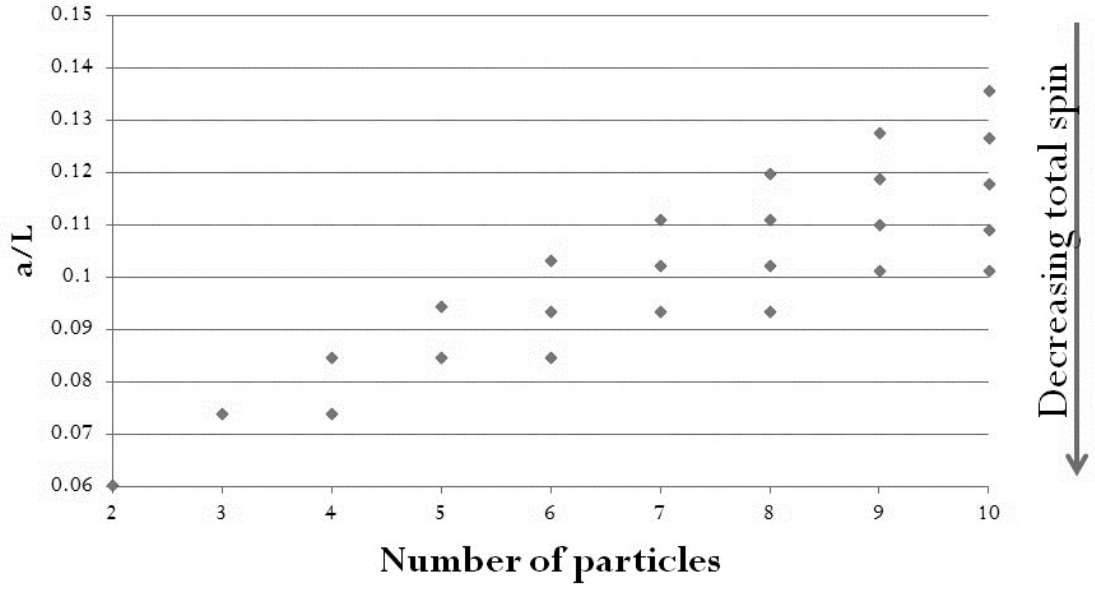

FIG. 5. Window-coupled waveguides: critical value of the geometry parameter

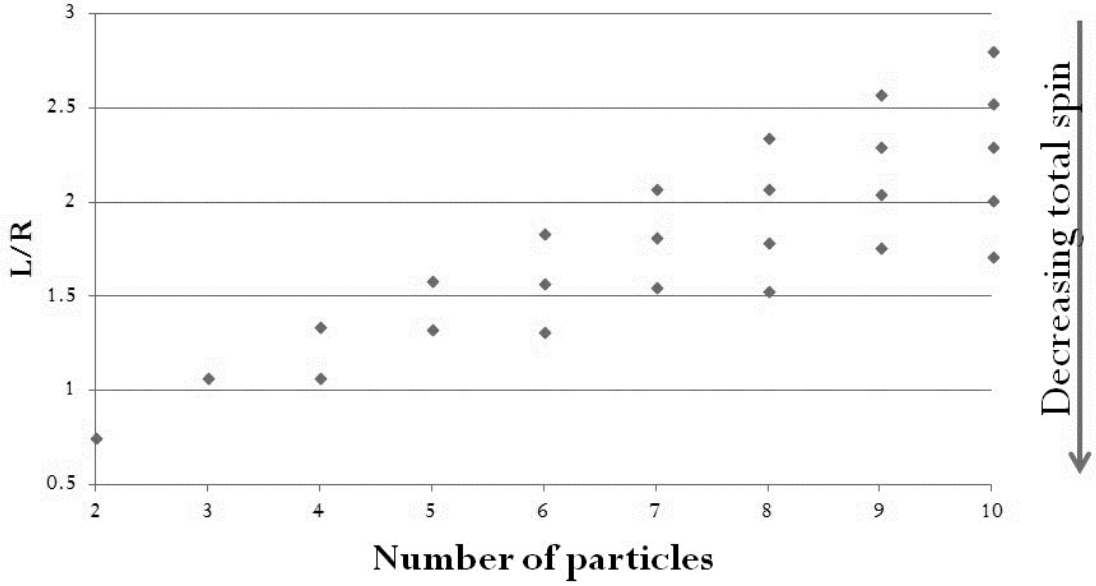

FIG. 6. Bent waveguide: critical value of the geometry parameter

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