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The discrete spectrum of the multiparticle Hamiltonian in the framework of the Hartree-Fock approximation

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Abstract. The paper deals with the problem of quantum particles storage in nanolayered structures. The system of a few interacting electrons placed into deformed waveguide is studied. Different interaction models — δ-type and Coulomb type — and different 2D geometries of the waveguide are under investigation. The ability to store or localize particles (“bound state”) corresponds to the existence of the discrete spectrum of the system Hamiltonian. The dimension of the problem growth with the number of particles. To avoid these difficulties we use Hartree-Fock method which gives the system of one particle equations. The equations are solved with the help of FEM. As the result we have the dependence of the minimal deformation coefficient which keeps bound states on the number of particles and its total spin. Comparison of the storage efficiencies is made.

1. Introduction
The problem of the existence of the system’s bound state is very important in many physical questions. One of its illustration is quantum particle storage problem. For example, it may be applied in a hydrogen accumulator based on nanolayered structure. One layer of such structure can be considered as a waveguide. In the terms of math, the ability to store a particle means the existence of the discrete spectrum of the corresponding Hamiltonian. It is known that single particle placed into straight waveguide has no bound states, so it can’t be stored or localized. Introducing a small deformation of the waveguide causes the eigenvalues appearance [1]-[7]. For many practical applications it’s necessary to store more than one particle. That leads to the multi-particle system [8], [9]. Straightforward solving of Schrödinger equation for such system is heavy task even for numerical methods. We use Hartree-Fock approximation to simplify the equations and solve it by FEM.

2. Governing equations
Consider a number of interacting electrons placed into a nanolayer or a waveguide. If we ignore the spin-orbit interaction then the Hamiltonian of the multi-particle system is written as follows

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

(1)
where \( m \) is particle’s mass, \( U_k \) is the external field potential, \( V_{jk} \) is the potential of the particles interaction. The multi-particle Schrödinger equation for (1) needs to be simplified. An approach based on the Hartree method is described in [10]. The drawback of this method is symmetry of the system’s wavefunction with respect to the interchange of particles spatial coordinates. Thus, it is not fully correct model for fermions.

In this article we offer an approach based on the Hartree-Fock method which allows one to avoid the described drawback. The idea of the method is to look for the system’s wavefunction in the form of Slater determinant:

\[
\psi(x_1, x_2, \ldots, x_n) = \frac{1}{\sqrt{n!}} \begin{vmatrix}
\psi_1(x_1) & \psi_2(x_1) & \cdots & \psi_n(x_1) \\
\psi_1(x_2) & \psi_2(x_2) & \cdots & \psi_n(x_2) \\
\vdots & \vdots & \ddots & \vdots \\
\psi_1(x_n) & \psi_2(x_n) & \cdots & \psi_n(x_n)
\end{vmatrix},
\]

where \( \psi_i \) is the single particle function, \( n \) is the number of particles, \( x_i \) represents the set of four (or three) spatial ones and a spin one.

Substituting (2) into (1) and using the variational principle, after simplification one can obtain the Hartree-Fock equations:

\[
\hat{F}^+ \psi_k^\uparrow = \left[ \hat{H}_k + \sum_{j=1}^{n^\uparrow} \left( \hat{J}_j^\uparrow - \hat{K}_j^\uparrow \right) + \sum_{j=1}^{n^\downarrow} \hat{J}_j^\downarrow \right] \psi_k^\uparrow = E_k^\uparrow \psi_k^\uparrow, \quad k = 1, n^\uparrow
\]

\[
\hat{F}^+ \psi_k^\downarrow = \left[ \hat{H}_k + \sum_{j=1}^{n^\uparrow} \hat{J}_j^\uparrow + \sum_{j=1}^{n^\downarrow} \left( \hat{J}_j^\downarrow - \hat{K}_j^\downarrow \right) \right] \psi_k^\downarrow = E_k^\downarrow \psi_k^\downarrow, \quad k = 1, n^\downarrow
\]

\[
\hat{J}_j^\uparrow \psi_k(r_k) = \left[ \int \psi_j^\uparrow(r_j) V_{jk} \psi_j^\uparrow(r_j) \, dr_j \right] \psi_k(r_k), \quad \hat{K}_j^\downarrow \psi_k(r_k) = \left[ \int \psi_j^\downarrow(r_j) V_{jk} \psi_j^\downarrow(r_j) \, dr_j \right] \psi_j^\downarrow(r_k),
\]

where the superscripts \( \uparrow \) and \( \downarrow \) denote to particles with different spins, \( \psi_i \) is a single particle function, \( r_i \) is the spatial coordinate of a particle. Now the \( n^\uparrow \) and \( n^\downarrow \) lowest eigenfunctions of the operators \( \hat{F}^\uparrow \) and \( \hat{F}^\downarrow \), respectively, are to be found. Equations (3)–(4) are solved numerically in the way similar to the one described in [10].

If all eigenvalues \( E_1^\uparrow, \ldots, E_{n^\uparrow}^\uparrow \) are less than the threshold, the bottom of the continuum spectrum of single particle, then the bound state exists. The threshold can be found by \( E_{thr} = \pi^2 \hbar^2 / (2mL^2) \), where \( L \) is the waveguide width at infinity.

### 3. Results

We studied two types of particles interaction, \( \delta \)-type and Coulomb, which are described by the following potentials:

\[
V_{ij}^\uparrow = U_\delta \delta(r_i - r_j), \quad V_{ij}^\downarrow = \frac{U_c}{|r_i - r_j|},
\]

where \( U_\delta \) and \( U_c \) are interaction intensity constants. Physically, they can be changed by the effective mass and charge of the particles.

All the problems are solved in 2D. In the case of \( \delta \)-interaction three geometries were studied: i) waveguide with locally deformed boundary (Fig. 1), ii) two waveguides coupled through a window (Fig. 2), iii) bent waveguide (Fig. 3). For all these cases the existence of single particle bound states has been proved [1] – [7]. The Coulomb interaction was studied for the coupled waveguides.

Comparing three types of the system geometry in the case of \( \delta \)-interaction we can conclude that the bent waveguide is the less efficient one. It can store only two particles with opposite
spins. Placing more particles or changing one particle’s spin leads to destroying of the bound state.

The window coupled layers appear the most efficient in the sense of particle storage. Increasing of the interaction intensity leads to destroying of the bound state. From the other hand, increasing of the window width leads to the rise of the discrete spectrum threshold. The correlation between the intensity and the deformation in the case of two particles in a window-coupled layers is shown on Fig. 4. To compare two types of potentials the relationship between the constants $U_{\delta}$ and $U_c$ must be established:

$$U_{\delta} = \alpha U_c, \quad \alpha = \frac{\iint \delta(|r_1 - r_2|) \, dr_1 \, dr_2}{\iint \frac{1}{|r_1 - r_2|} \, dr_1 \, dr_2}.$$ 

The domains below the curves corresponds to the existence of the bound states. One can see that for particles with collinear spins there is a threshold deformation which allows bound states. The system of two particles with collinear spins for $\delta$-interaction represents two single particles and doesn’t depend on the interaction intensity.

Figure 1. Deformed waveguide.  
Figure 2. Window-coupled waveguides.  
Figure 3. Bent waveguide.  
Figure 4. Domain on the dimensionless parameters plane $(a/L, U_c/E_0)$ corresponding to the existence of eigenvalues of two-particle Hamiltonian for coupled layers (below the curve), $E_0 = \hbar^2/(2mL^2)$.

- Coulomb interaction, zero total spin,  
- $\delta$-interaction, zero total spin,  
- Coulomb interaction, unit total spin.
Increasing of particles number or total system’s spin leads to larger deformation required to store the system. It is interesting to find what (minimal) deformation is sufficient for storage of a given system. On Fig. 5 the minimal window width keeping bound states is shown. The result on the plot is computed for $U_c = 0.01$ and corresponding $U_δ = 0.066$. The lower points corresponds to the lower total spin. One can see that for small interaction intensity the $δ$-type and Coulomb potentials gives one similar results. It can be seen that the required deformation depends on the number of the particles with the same spin. Thus, it is more efficient to store even number of particles with zero total spin than one particle less.

Fig. 6 shows the distribution of the electron density for the system of two particles with opposite spins in the layers with the window width $a/L = 1/2$.

The results of this work can be used to estimate the optimal parameters of a storage nanosystem.

![Figure 5](image1.png)  ![Figure 6](image2.png)

**Figure 5.** Minimal window width which keeps bound states for the case of layers coupled through a window, lower points correspond to smaller total spin. ○ Coulomb interaction, × $δ$-interaction.

**Figure 6.** Electron density distribution of the two-particle state for layers coupled through a window.

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