Particles storage in locally deformed nanolayers

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INTRODUCTION

It is known that curved quantum layers can store particles. From mathematical point of view it is related with the existence of eigenvalues of the corresponding Hamiltonian. The increase of curvature leads to increasing of the eigenvalues number. This question is important in various physical problems. For example, to do two-qubit operation in 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 with the storage of hydrogen (or protons) in nanolayered structures. It can give effective and safe fuel container for hydrogen engine. One can note that layers with curved boundaries are more effective for particles storage because the increasing of the curvature (or boundary perturbation amplitude) leads to increasing of the discrete spectrum cardinality. Hence, the amount of the hydrogen stored in the layered structure will be greater. Note that the Hamiltonian for the corresponding plane layered structure has empty discrete spectrum.

TWO-PARTICLES PROBLEM

We seek a solution of multi-particle Schrodinger equation in Hartree approximation. Namely, we consider a waveguide with local perturbations: locally deformed boundary, two 2D waveguides coupled through small window, curved waveguide. For each system we consider a question whether there is two-particle bound state. The wavefunction is saught in the form

$$\psi(r_1,r_2)=\psi_1(r_1)\psi_2(r_2),$$

where ψ_1 and ψ_2 are one-particle wave functions. We use the model of point-like interaction between the particles. In this case one obtains the following system:

$$\begin{cases} -\dfrac{\hbar^2}{2m}\Delta\psi_1(r_1)+U_0\left|\psi_2(r_1)\right|^2\psi_1(r_1)=E_1\psi_1(r_1) \\ -\dfrac{\hbar^2}{2m}\Delta\psi_2(r_2)+U_0\left|\psi_1(r_2)\right|^2\psi_2(r_2)=E_2\psi_2(r_2) \end{cases}$$

To find the numerical solution we use FreeFem++ with the library ARPACK for searching of the matrix eigenvalues. For fixed geometry the convergence deteriorates when the interaction intensity U_0 increases. We find values of U_0, which guarantee the existence of the bound state. Increasing of U_0 leads to the destroying of the two-particles eigenstate. From other side, increasing of the boundary deformation d leads to increasing of the "eigenvalue-threshold" distance (the only reason for the eigenvalue existence is this deformation, plane waveguides haven't eigenvalues). It is interesting to find the correlation between the intensity and deformation, for which there exists two-particle bound state. It corresponds to the domain on the parameter plane. The boundary of this domain (in dimensionless form) is found (see Fig. 2). 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 proper parameters (proper deformation should correlates with the intensity of the particles interaction).

The analogous consideration is made for coupled layers and curved waveguides. We compare the results. It occurs that it is more effective to store two particles in the system of two layers coupled through small window. Fig. 3

shows that the result is natural due to specific distribution of particles wave functions density.

REFERENCES

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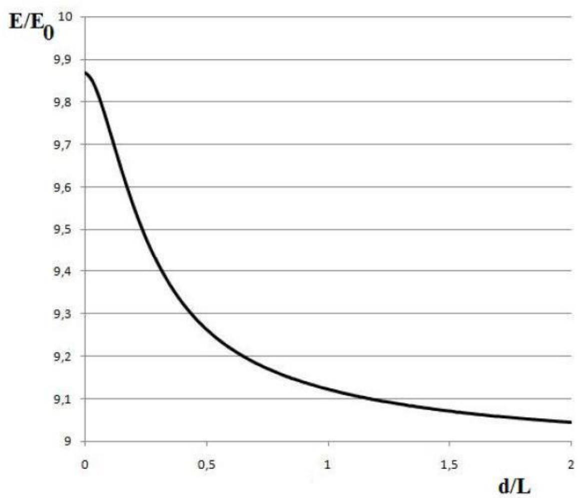

Fig. 1. Dependence of the eigenvalue on the deformation of the boundary.

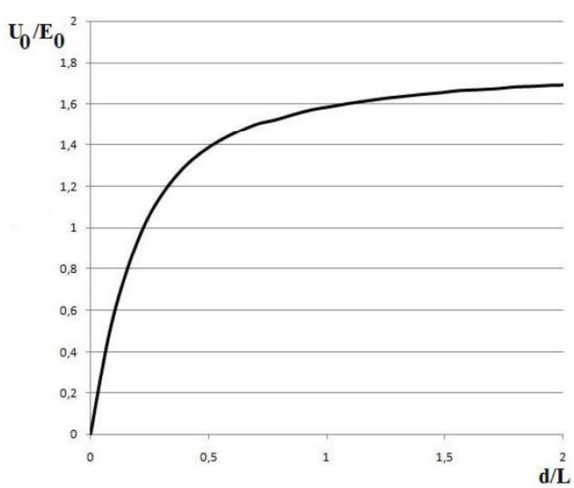

Fig. 22. Domain corresponding to the existence of two-particle bound state (below the line)..

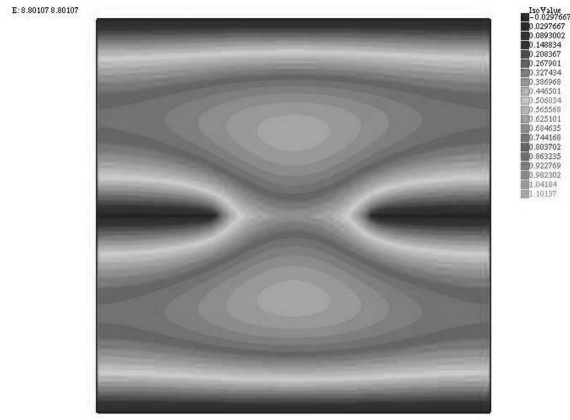

Fig. 3. Electron dansity distribution for coupled layers