MODELING OF LOCALIZED ELECTRONIC STATES IN NANOGATE-DONOR SYSTEM

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Recently there has been an enhanced interest to study the manipulation of donor electron wave functions near an interface of two materials by applying external electric field. This problem was investigated earlier in several works using variational methods. However, this approach does not allow to estimate errors for obtained energies and quality of trial functions. In this work main characteristics of such a system with electric field applied by a disc-shaped gate are studied using both the finite element method (FEM) and the variational method. The structure under study can be considered as a basic model for the development of quantum informatics devices.

The aim of this work is to understand effects of different system parameters on electron shuttling between the donor and gate. A joint problem for Laplace and stationary Schroedinger equation has been solved using FEM.

An external parameters controlling the electron state is electric field potential of the gate. The effect of gate potential depends on internal parameters of the problem. These are the gate diameter, the donor position, the thickness of an insulator layer and characteristics of semiconductor and insulator (band gaps, electron effective masses etc.). The last group of parameters on boundary and conjugation conditions for Laplace and Schroedinger equations.

One of the most important characteristics describing the given system is critical potential – the gate potential which corresponds to the electron transferring from the donor to the gate. Another considered characteristic is the minimum gap between ground and first excited state electron energies which allows to estimate the tunneling time.

We calculated ground and first excited state electron energy using FEM and the variational method with trial functions of a simple form, which consisted of two terms: the first one describes the influence of the gate potential, the second one represents electron wave function in the donor field. The results obtained using FEM were compared with the results obtained using the variational method. The variational method allows to determine energies for the gate field near the critical potential with errors less than 1 %. At the same time, the variational method provides convenient way for evaluating the characteristics of the system.

The dependence of ground state energy on the gate potential was defined using FEM. This dependence can be used for evaluating the critical potential in the system and empirical expression for it was obtained, which determines the effect of the gate size on the critical potential.

Similar approximations were obtained for the minimum gap, which appeared to be strongly dependent on the donor position and much less dependent on the gate configuration. Because of this different degree of influence, it is possible to manipulate both critical potential and minimum gap by modifying the donor position and the gate size.

Another way to manipulate the characteristics of the structure is choosing semiconductor material with appropriate electron effective mass. Relevant formulae were derived from the dependences of the critical potential and minimum gap on geometrical parameters. It was also found that the case of materials with anisotrope effective mass can be reduced to isotrope case with certain value of effective mass.

The first numerical computations of wave functions has been performed in 3D axisymmetric geometries. Computational process for a fully 3D setting with finite elements is under development.