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Modeling of Magnetic Field-Assisted Electron Manipulation in Nanogate-Donor System

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ABSTRACT: Numerical simulations of shallow donor states in external electric and magnetic fields near semiconductor surface are carried out. It is considered that the electric field is applied by a disc-shaped metallic gate and magnetic field is uniform and perpendicular to semiconductor interface. The stationary Schrödinger equation is solved using finite element method. The dependences of main characteristics of electron shuttling from the donor to the gate on the magnetic field are obtained for different gate diameters and donor positions.

Keywords: energy level; wave function; modeling; donor; magnetic field

1 INTRODUCTION

Single atoms of dopant impurities in semiconductors under control of electric and magnetic fields are among the most promising physical systems for implementing a quantum computer (Kane, 1998). This problem has stimulated much theoretical studies and numerical simulations on the quantum states of donors localized near a semiconductor surface in a magnetic field (Li et al., 2013, Bruno-Alfonso et al., 2010, Calderon et al., 2007). In some applications, such as a Si-based quantum computer, electronic states are to be controled by small gates with nanometer sizes. However, in previous works the system has been considered without external electric field (Li et al., 2013, Bruno-Alfonso et al., 2010) or under uniform electric field (Calderon et al., 2007). So, in this work, we assume a disc-shaped gate as a source of the external electric filed, and study characteristics of electron shuttling from the donor to the gate in the presence of uniform magnetic field.

2 FORMULATION OF THE PROBLEM

We consider a donor, positioned at the distance z_0 from semiconductor surface where the disc-shaped gate with diameter d is situated. The gate is separated from the semiconductor by an infinitely thin and infinitely high dielectric barrier. A uniform magnetic field B is applied perpendicular to the semiconductor surface. Then, the stationary Schrödinger equation for the electron wave function Ψ and energy E in cylindrical coordinates is given by

$$\hat{H}\Psi = E\Psi \qquad (1)$$

with the Hamiltonian operator

$$\hat{H} = \hat{T} - i\mu\frac{\partial}{\partial\varphi} + \frac{\mu^2\rho^2}{4} + \hat{V}_D + \hat{V}_G, \qquad (2)$$

$$\hat{T} = -\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) - \frac{\partial^2}{\partial z^2} - \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}, \qquad (3)$$

where $\mu = (a^*)^2/\lambda_B^2$ with $\lambda_B = \sqrt{\hbar/eB}$ the magnetic length and a^* effective Bohr radius, $\hat{V}_D$ is the potential electron energy in the field of the donor centre, $\hat{V}_G = \Phi_0 f(\rho, z)$ describes the potential landscape due to the gate, Φ_0 is the gate potential. Two kinds of boundary conditions for the field applied by the gate are used. Firstly, we consider that the gate is surrounded by a dielectric material (BC-A). Secondly, we assume that the gate is surrounded by a metal, at which the potential equals zero (BC-B).

Energy in equation (1) is expressed in the units of effective Rydberg (Ry^*). Magnetic field μ is expressed in $\mu_0 = \hbar/(a^*)^2 e$.

3 NUMERICAL RESULTS

The problem for the equation (1) has been solved using finite element method (FEM).

Firstly, we consider the effect of the magnetic field on the structure of electron energy spectrum of near-gate states, i.e. when the donor is infinitely distant from the gate. The system in this case can be considered as a quantum dot induced by external electric field. Energies of ground and several lowest excited states are presented in Figure 1 (numerical data for states localized at near-donor region are taken from Makado and McGill, (1986)).

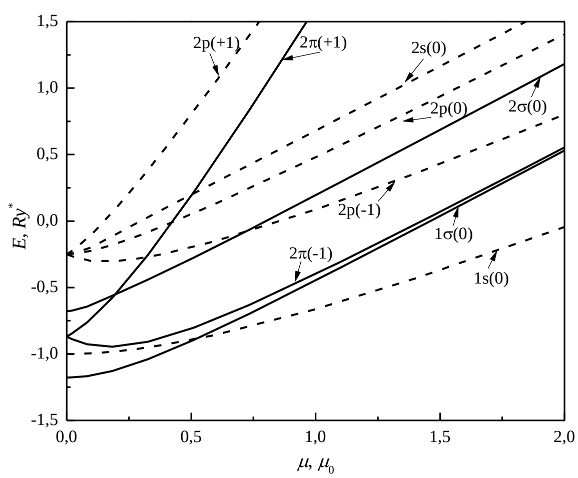

Figure 1: Energies of near-donor (dashed lines) and near-gate states (solid lines) as a function of magnetic field. The gate is surrounded with dielectric (BC-A) ($d = 7a^*$, $\Phi_0 = 3.9Ry^*/e$)

Two main characteristics of electron shuttling from the donor to the gate have been studied: critical gate potential at which the shuttling takes place and minimum energy gap ($g_{\min}$) between the ground and first excited σ-states, which can be used to estimate the tunnelling probability between these two states.

As one can see from Figure 1, energies of all σ-states become higher for larger magnetic fields if $d > a^*$. Energy level for 2π(–1) asymptotically approaches 1σ(0)-level for magnetic fields $\mu > 1$, which does not happen for near-donor states 1s(0) and 2p(–1). The effect of the magnetic field on ground state energy is stronger for near-gate 1σ(0)-state than for near-donor 1s(0)-state. This means that magnetic field increases the critical potential and can be used to tune this characteristic.

Figure 2 demonstrates difference of the effect of the magnetic field for different gate diameters and boundary conditions. The effect of the magnetic field is stronger for the larger gate diameters and for the BC-A boundary conditions as in these cases wave function is less localized in ρ direction. Using variational method, it has been shown that the presence of the magnetic field can be described by multiplying trial wave function of near-gate state ground by the factor $\exp(-\gamma\rho^2)$, where γ is variational parameter.

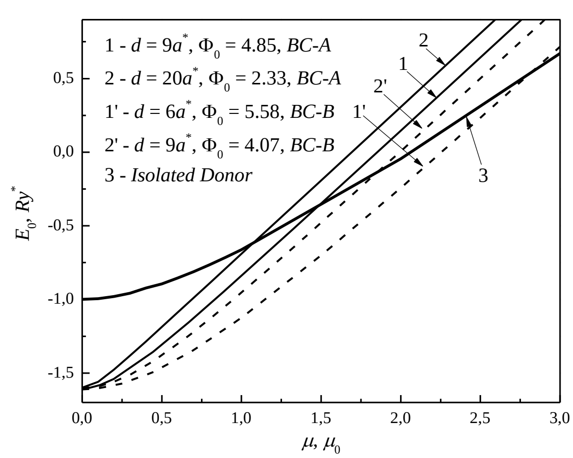

Figure 2: Ground state energy as a function of magnetic field for the electron in the field of isolated donor and in the field of the gate for different gate diameters and boundary conditions

We also consider a uniform external electric field, which is a limiting case of infinitely large gate diameter. The dependence of the critical potential on μ for both finite and infinite d can be approximated by a linear function: $a + b\mu$. It has been found that the value of b remains almost the same for different d and z_0.

The dependence of $g_{\min}$ in uniform external field on μ has been found to reveal nonmonotonic behaviour: the value of $g_{\min}$ increases on ~20% for $\mu < 0.2$ and decreases for larger magnetic fields (Figure 3).

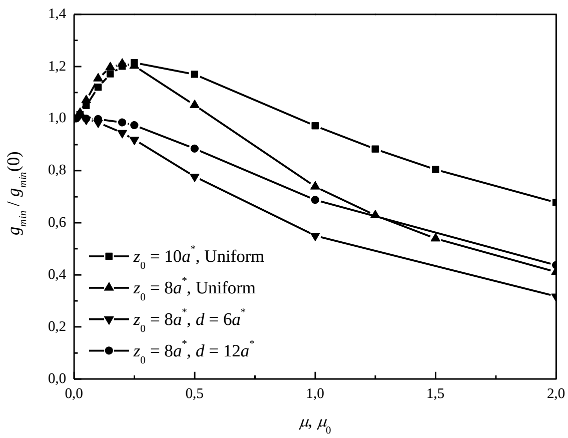

Figure 3: The dependence of the minimum gap on magnetic field for uniform external field and finite gate diameter. The value of the gap is normalized on the value of the gap on $\mu = 0$. Calculations are carried out for BC-A boundary conditions

At the same time, the minimum gap decreases for all values of the magnetic field when the gate diameter is finite. This fact can be explained as the result of less wave function overlapping for higher magnetic fields.

4 CONCLUSION

We have studied the effect of the magnetic field on donor electron energy spectrum in external electric field using the results of finite element calculations. It has been found that the effect of the magnetic field on the gate-induced electronic states is different as compared to electronic states hydrogenic donor.

It has been determined that the use of an external magnetic field leads to increasing of the critical potential. The effect of the magnetic field on the minimum gap between ground and first excited states depends on the gate size. If the gate diameter is finite, the minimum gap gradually gets smaller for larger magnetic fields. If the gate diameter is large enough (i.e. the electric field can be considered as uniform), the dependence of the minimum gap on magnetic field is nonmonotonic.

The results of the calculations can be used for the optimization of nanodevices that are based on the manipulation of shallow donor states by external fields.

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