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NUMERICAL MODELING OF GEOMETRICAL EFFECTS ON MANIPULATION OF EXCHANGE INTERACTION FOR TWO-ELECTRON STATES IN NANOGATES-DONORS SYSTEM

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Numerical simulation results of exchange coupling in the system of near-surface donor and quantum dot pairs are presented. Exchange energy under the effect of external external electric field has been calculated using Hartree-Fock method. Fourier transform and finite element methods have been used to solve the problem for the Poisson equation. The dependences of exchange energy on external electric field have been obtained. Limits of applicability of electric field for the system control are discussed. The effect of donors position has been investigated.

Key words: qubit; two-electron system; nanogate; quantum dot; modeling.

INTRODUCTION

The potential realization of solid-state elements of quantum information has attracted a lot of attention due to long coherence times [1], promise to scalability and compatibility with existing semiconductor technologies. Recent progress in fabrication semiconductor nanodevices has stimulated a large variety of theoretical studies dedicated to modeling of quantum information structures for quantum computing, quantum communication, quantum sensing, etc. [2–3]. In particular, there are several proposals of quantum computer implementations: based on donor electron or nuclear spins in silicon [4–5], superconducting nanocircuits [6], single electron spins in quantum dots and quantum wires of different configurations [7–8].

One of the necessary elements for controlling spin-qubit operations for several quantum computing proposals is manipulating spin and exchange interaction between electrons by combining gate electrodes and magnetic field. Exchange splitting can be used for both two-qubit [4, 7] and single-qubit operations [1]. For example, according to Kane's proposal [4], quantum calculations are realized using the nuclear spins of phosphorus donors in silicon. The bound electron of single donor is affected by the electric field of main control gate (A-gate), which provides the electron density relocation to semiconductor surface. Two-qubit operations are implemented using the exchange interaction of two neighbouring electrons, regulated by the electric field of additional (exchange) gate (J-gate), located between A-gates. Exchange interaction is extremely sensitive to external fluctuations, which imposes restrictions both on the parameters of the J-gate and on geometric parameters of the whole system [9].

When modeling the effect of electric on a donor or a quantum dot pair [10–17], simplified structures are usually studied. External electric field (J-gate field) is often considered homogeneous [12] or parabolic [15], as well as quantum dot confining potential [10, 11]. Such potential configurations have significant differences from the real potential of finite-size gate. Another common simplification is considering bulk donors and quantum dots instead of near-surface structures.

In this paper, we study the effect of the electric field of the disk-shaped additional J-gate on the value of exchange interaction for different geometrical parameters of the two-qubit system.

FORMULATION OF THE PROBLEM

The stationary electronic states of the system under study are described by the Schrodinger equation

$$\left(\hat{H}^{(1)}\left(\vec{r}_1\right)+\hat{H}^{(1)}\left(\vec{r}_2\right)+\frac{2}{\left|\vec{r}_1-\vec{r}_2\right|}\right)\Psi\left(\vec{r}_1,\vec{r}_2\right)=E\Psi\left(\vec{r}_1,\vec{r}_2\right), \quad (1)$$

$$\hat{H}^{(1)}\left(\vec{r}\right)=-\nabla^2+\hat{V}_{A_1}\left(\vec{r}\right)+\hat{V}_{A_1}\left(\vec{r}\right)+\hat{V}_{D_1}\left(\vec{r}\right)+\hat{V}_{D_1}\left(\vec{r}\right)+\hat{V}_J\left(\vec{r}\right), \quad (2)$$

where $\hat{V}_{A_i}$, $\hat{V}_{D_i}$ are donor and A-gate potentials, $\hat{V}_J$ is J-gate potential. Distances are expressed in effective Bohr radius a^*, effective Rydberg Ry^* is used as energy unit. For silicon, averaged units are $a^* = 2$ nm and $Ry^* = 31.27$ meV. Disk-shaped gates potentials are defined by analytical expression [18].

For bound states, wave function vanishes at infinity:

$$\Psi(\vec{r}_1,\vec{r}_2)\xrightarrow[|\vec{r}_1|\to\infty]{}0,\quad \Psi(\vec{r}_1,\vec{r}_2)\xrightarrow[|\vec{r}_2|\to\infty]{}0,\quad z_1>0,\quad z_2>0. \tag{3}$$

As we consider half-space problem, additional boundary conditions on the plane $z = 0$ should be applied:

$$\Psi(\vec{r}_1,\vec{r}_2)\big|_{z_1=0}=0,\quad z_2>0,\quad \Psi(\vec{r}_1,\vec{r}_2)\big|_{z_2=0}=0,\quad z_1>0. \tag{4}$$

NUMERICAL METHOD

To solve the problem (1)–(4), Hartree-Fock method based on variational approach has been used. Trial functions have been chosen in the form [19]:

$$\varphi_{ij}^{(1)}=\exp\left(-\alpha_i\left(x\pm R/2\right)^2-\alpha_i y^2-\alpha_j\left(z-z_0\right)^2\right), \tag{5}$$

$$\varphi_{ij}^{(2)}=z\exp\left(-\beta_i\left(x\pm R/2\right)^2-\beta_i y^2-\beta_j z^2\right), \tag{6}$$

$$\varphi_{ij}^{(3)}=z\exp\left(-\beta_i x^2-\beta_i y^2-\beta_j z^2\right),\quad i,j=1..M, \tag{7}$$

where R is the distance between donors (QDs' centers), z_0 is the distance between donors and semiconductor surface. Parameters α_i have been chosen so that a linear combination of functions $\exp\left(-\alpha_i r^2\right)$ deliver minimum value for ground state energy of the electron in the field of isolated donor, and $\beta_i=\left(d/2\right)^{-1/2}\alpha_i$ to scale on gate diameter. Trial functions (5)–(7) demonstrate good results for modeling of corresponding one-qubit problem.

Calculation of exchange integrals has the greatest computational cost. To prevent such calculations on each iteration, we calculate integrals of the form

$$\iint \chi_i(\vec{r}_2)\chi_j(\vec{r}_2)\chi_k(\vec{r}_1)\chi_l(\vec{r}_1)\frac{2}{\left|\vec{r}_1-\vec{r}_2\right|}d\vec{r}_2 d\vec{r}_1 \tag{8}$$

preliminary and use it for all calculations with this basis. The inner integral (u_{ij}) is replaced by the problem for the Poisson equation. To approximate boundary conditions at infinity, asymptotic conditions have been used. This conditions are constructed under the assumption that gate potential at large distances is close to the potential of effective point charge. Thus, the function u_{ij} at the boundary has been approximated with the function

$$v\left(x,y,z\right)=\frac{q}{\sqrt{\left(x-X\right)^2+y^2+\left(z-Z\right)^2}}, \tag{10}$$

where (X, 0, Z) are approximate coordinates of average position of effective charge (for all basis functions this position is placed on y-axis), q is overall charge.

The problem for the Poisson equation has been reduced to two-dimensional problem using cosine Fourier transform on y direction. The resulting problem has been solved using the finite element method with linear triangular elements.

APPROXIMATION OF THE GATE POTENTIAL

To reduce calculation efforts, the integrals of donor potential are calculated analytically on y variable, and numerically on x and z variables. The integrals which include the gates potential can not be calculated analytically. Thus, to approximate the potential created by the thin disk-shaped gate, expressions of the form

$$\hat{V}_G=-c\exp\left(-a\rho^2-bz\right) \tag{11}$$

has been used. Potential of the form (11) is more preferable at large distances than usually used parabolic potential [15], as it vanishes at infinity and demonstrates good approximation for one-electron axis-symmetric systems. However, it distorts electric field with the distance from the gate center.

Parameters a and b in Eq. (11) have been chosen in two ways. According to the first on, parameters have been chosen so that, the value of the critical potential (the potential at which the maximum electron density of the ground state passes from the donor to the gate) remains unchanged compared to the exact value of the potential. This condition is satisfied by infinite number of values. We chose such values of parameters a and b that the dependence of ground state energy on gate potential Φ_0 have been close to the dependence in the field created by a real disk-shaped metal gate and suppose $c = \Phi_0$. Then due to the fact that the whole system can be scaled on gate diameter and critical potential practically does not depend on the distance from the donors to the interface, a disk-shaped gate of diameter d corresponds to parameter values $a \approx 1.098/d^2$, $b \approx 1.268/d$.

The second way to define parameters a and b is to minimize the difference between potential values and electric field components for exact and approximate expressions at certain points. We have used gates centers and donors positions as such points. The drawback of this way to choose parameters is the necessity to find new parameters for different gate diameters and donor-interface distances. For $z_0 = 6a^*$, $d = 2a^*$, we get $a \approx 0.154$, $b \approx 0.61$, $c \approx \Phi_0$.

The results of using these two kinds of potential approximation for two-donor system is presented in Fig. 1. The difference between two types of approximation potentials is considerable, and the result can differ by two times. To find more accurate results, we have also used another function

$$\hat{V}_G = -c_1 \exp\left(-a_1\rho^2 - b_1 z\right) - c_2 \exp\left(-a_2\rho^2 - b_2 z\right), \tag{12}$$

with fitting parameters on the potential and field values at donors and gates centers. With approximation (12), we have gotten error in exchange energy of about 10%, although singlet and triplet energies separately are less accurate.

Expressions (11)–(12) can be considered not only as approximations of the potential of disk-shaped gate, but also as the potential of electrodes with another configuration. In such way, different gate configurations can be regarded as additional control parameter of the system.

To verify the calculation procedure, we have used asymptotic expression for the dependence of exchange energy on inter-donor distance for two bulk donors:

$$K \approx 1.64 \frac{e^2}{\varepsilon\varepsilon_0 a^*} \left(\frac{R}{a^*}\right)^{5/2} \exp\left(-\frac{2R}{a^*}\right). \tag{13}$$

We have compared exchange energy (13) with the values for two-donor system positioned at the distance $z_0 = 6a^*$ from semiconductor interface. The surface effects at such distances can be neglected. For inter-donor distances from $6a^*$ to $10a^*$, calculations get results which are in good agreement with Eq. (13).

CALCULATION RESULTS AND DISCUSSION

Calculations shows that J-gate potential does not have great effect on exchange interaction in two-donor systems, in contrast to uniform electric field. For example, in Ref. [15] exchange energy changes by several order of magnitude without electron density reloca-

tion, whereas J-gate potential of diameter $d = 2a^*$ only doubles it. This difference arises due to the rapid decrease in electric field in the case of a finite size gate. For larger d, exchange energy varies over a wider range, but the gate diameter can not be used for improving the system efficiently, as its value is limited with the distance between neighbouring qubits.

Exchange energy becomes more sensitive to change of the J-gate potential with decreasing z_0, which means that switching spin exchange coupling between neighbouring qubits can be performed more efficiently for smaller z_0.

A-gate potential has also slight effect on exchange interaction, as its range is limited by electron density relocation as well as J-gate potential. It can be used for increasing exchange energy by several times due to electron wave function deformation.

In the case of a quantum dot pair, the dependence of exchange energy on J-gate potential is more prominent, than in two-donor state. Such a difference can be explained by the less distance between the gates, than between donors and J-gate. At the same time, exchange energy is more sensitive to the A-gate potential, than to the J-gate potential (Fig. 2). This means that A-gate potential can also be used more tuning exchange interaction for two-QD system.

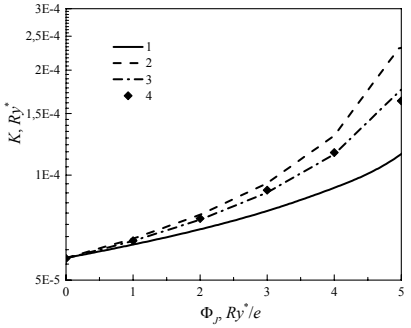

Figure 1. – The dependence of exchange energy on J-gate potential for two-donor system, J-gate diameter $d = 2a^*$, distance between donors $R = 8a^*$. Curves *1* and *2* corresponds to J-gate potential approximated with Eq. (11) using fitting on critical potential and field values at several points, respectively. Curve 3 corresponds to approximation (12). Values with exact potential are denoted as 4

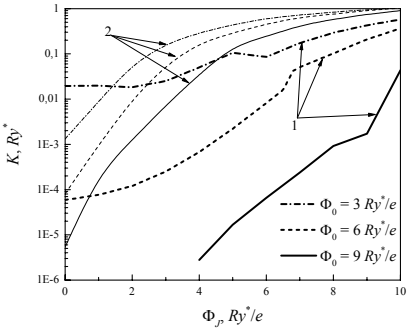

Figure 2. – The dependence of exchange energy on J-gate potential for two-QD system; curves *1* correspond to gates diameter $d = 2a^*$, curves *2* – $d = 4a^*$, distance between gate centers $R = 8a^*$

CONCLUSIONS

In conclusion, the system of near-surface donors and quantum dots induced by electric field of nanosized gate has significant differences with the bulk case. For near-surface donors, the use of electric field for exchange coupling control is limited with electron density relocation, which takes place for large enough gate potentials. On the other hand, positioning donors closer to semiconductor surface can widen the range of the gate potentials that can be used for exchange coupling manipulation. For in two quantum dot system manipulation of exchange splitting can be implemented more effectively using the gates, which in-

duce quantum dots, rather than the external exchange gate. Based on the calculation results, optimal system configurations can be proposed for more efficient exchange energy control.

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LINEAR MAGNETORESISTANCE IN GRAPHENE FORMED ON SILICON CARBIDE: TWO DIMENSIONAL MAGNETOTRANSPORT

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In this study we have tested the magnetoresistance (MR) and Hall-effect in graphene formed on semi-insulating 4H-SiC substrate by thermal decomposition of its silicon face (0001) in Ar ambient at a high temperature of 1800–2000 °C over the large areas of SiC without any passivation for checking a possibility for sensor applications. Testing was done in a relatively low magnetic fields (up to 3 T) in the temperature range from 300 to 4.2 K. A large (up to 10%) and linear magnetoresistance was observed at 300 K, which is distinctively different from the other carbon nanomaterials. Furthermore, negative magnetoresistance behavior at a low field regime for low temperatures is recognized as a weak localization in graphene. This study suggests the potential of utilizing graphene formed on semi-insulating 4H-SiC for room temperature magneto-electronic device applications and for the sensors of first order phase transitions ice–water.