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Single Electron Spin Operations Employed for Logical Gates of Quantum Computer

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Electron localized in a quantum dot in the vicinity of conductor surface, causes an induced potential to appear. This potential enables self-focusing of electron wave function. Because of this feature, in a planar nanostructure consisting of a quantum well covered with a layer of an insulator, on top of which metal electrodes are deposited, formation of induced dots and quantum wires is possible. By applying appropriate voltages to the electrodes, it is feasible to transport an electron in a fully controllable way in a form of a stable wave packet between two specific locations in a nanodevice. While transporting an electron along properly shaped closed loops, spin–orbit coupling intrinsically present in a semiconductor nanostructure can be employed to perform operations on an electron spin.

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1. Introduction

The hopes based on the tremendous calculation capabilities of a quantum computer caused many people to look for its physical implementation. One of the research areas is to construct a quantum computer employing semiconductor nanostructures. A huge advantage of such solutions is the possibility to join it with the classical computer structures. The most promising realization of a quantum bit (qubit) in semiconductor nanostructures are spin states of a single electron confined in a quantum dot [1–3]. At present in such nanodevices it is possible to rotate electron spin [4-8] as well as perform a read/write operations [9–11]. In most cases in order to rotate the spin an electron is inserted in a magnetic field which splits energy states with a spin parallel and antiparallel to the magnetic field. By applying a microwave radiation with energy equal to the energy shift between two split spin states, transitions between these states are obtained (the Rabi oscillations). However even in the presence of a strong magnetic field the spin splitting energy is low, hence microwave wavelength used for spin rotation is of an order of millimeters (for 10 T – 6 mm). Due to this fact it is very hard to apply this mechanism while building multi-qubit registers. If the distance between qubits forming a register is of the order of micrometers and a microwave used for rotation purpose has wavelength of the order of millimeters, the microwave would interact with many qubits simultaneously (it would be impossible to rotate only one spin). The latest solution is to force spin rotation using AC voltage applied to electrodes in an electrostatic quantum dot. This approach does not suffer from the disadvantage described above. In such device the spin rotation is obtained due to joined magnetic field interaction and spin–orbit coupling [8].

In this paper we review our previous works [12–16], where we proposed totally new construction of a nanodevice, which allows performing a single electron spin operations corresponding to the most important one-qubit quantum gates.

2. Self-focusing mechanism of an electron wave function — inducton efect

Classical charge localized in the vicinity of a grounded conductor is a source of an electric field, which leads to a redistribution of charge on a conductor and effectively causes an induced charge to appear on a conductor surface. The induced charge is then a source of a potential attracting the original charge. Similar effect can as well be observed in a quantum case [12, 13].

Let us consider a planar nanostructure formed by parallel layers: conductor, insulator or semiconductor blocking barrier (AlGaAs), semiconductor quantum well (GaAs) and a second barrier (AlGaAs). Exemplary structure is presented in Fig. 1.

If we form an electron wave packet of a finite size in a quantum well, an induced charge will appear on the conductor surface and will be a source of a potential attracting the original charge.

Wave packet moving parallel to the structure surface with a small velocity causes the induced charge to move with it. Packet velocity is marked in Fig. 1 as a black arrow directed to the right. Assuming that we have an ideal conductor, charge redistribution occurs immediately without any energy loss. We have to bare in



Fig. 1. Schematics of the considered structure, the wave packet and the induced charge. Solid vector shows the packet velocity, and the dashed vectors — the forces acting on the electron in the front and the tail of the wave packet.

mind that a force acting on a front of the packet consists of a component acting in the opposite direction to the packet's velocity (retarding), on the other hand force acting on a back of the packet has a component acting in the same direction as packet's velocity (accelerating). Forces acting on a packet are illustrated in Fig. 1 as dotted arrows. It is a known mechanism leading to the process of forming and preserving a soliton shape.

3. Calculation method

In case of an infinite metal surface, an image charge method known from electrostatics, can be employed to compute an induced potential. However in a case of finite-size electrode, the self-focusing effect of an electron wave function appears as well, but the image method is no longer applicable. In order to calculate the induced potential we have to use calculation method basing on a Poisson equation solution [14]:

$$\nabla^{2} \Phi(\mathbf{r}) = -\frac{1}{\varepsilon \varepsilon_{0}} \rho(\mathbf{r}) \,. \tag{1}$$

We are solving a Poisson equation in a 3D cuboid includes the whole nanodevice. We choose such cuboid sizes in all three dimensions, that for the infinite metal electrode the Poisson-based solution corresponds to an image-method solution which can be used in this case. To solve the Poisson equation we use boundary conditions imposing the disappearance of an electric field component parallel to the cuboid surface. While defining boundary conditions we also take into consideration voltages applied to the electrodes.

The charge density localized under the metal electrode is a source of an electric field. We express it with an electron wave function $\psi(\mathbf{r})$ and its charge -e:

$$\rho(\mathbf{r}) = -e \left| \psi(\mathbf{r}) \right|^2.$$
(2)

Electrostatic potential $\Phi(\mathbf{r})$ obtained using this method is a total potential which, thanks to a superposition principle, can be broken in two components originating from two different sources

$$\Phi(\mathbf{r}) = \varphi_1(\mathbf{r}) + \varphi_2(\mathbf{r}).$$
(3)

First component $\varphi_1(\mathbf{r})$ originates directly from the charge density distribution and we can compute it as

$$\varphi_1(\mathbf{r}) = \frac{1}{4\pi\varepsilon\varepsilon_0} \int d^3 \mathbf{r}' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}.$$
(4)

Second component $\varphi_2(\mathbf{r})$ originates from a charge induced on the metal electrode. It is an induced potential, which we are looking for. To obtain the value of this component we subtract the potential (4) from the potential obtained by solving Poisson Eq. (1):

$$\varphi_{2}(\boldsymbol{r}) = \boldsymbol{\Phi}(\boldsymbol{r}) - \varphi_{1}(\boldsymbol{r}).$$
(5)

Potential computed in this way is then used in the Schrödinger equation for an electron confined in the induced potential. For a nanostructure proposed in Fig. 2 we can neglect an electron motion in a direction parallel to a growth direction. As a result of this simplification we are solving 2D Schrödinger equation with a following Hamiltonian:

$$H = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) - e \varphi_2(x, y, z_0), \qquad (6)$$

where z_0 is a center of a quantum well. In order to compute electron confinement energy and a wave function in a stationary state we solve a Hamiltonian (6) eigenequation

$$H\psi\left(\boldsymbol{r}\right) = E\psi\left(\boldsymbol{r}\right).\tag{7}$$

Because the electrostatic potential depends on an electron wave function $\psi(x)$ via the charge density, and the electron wave function depends on the potential φ_2 , we solve this problem using self-consistent iterations. To obtain a time evolution simulation we numerically solve a time-dependent Schrödinger equation using the following iterative form:

$$\psi(\mathbf{r}, t + \Delta t) = \psi(\mathbf{r}, t - \Delta t) - \frac{2i}{\hbar} H(\mathbf{r}, t) \psi(\mathbf{r}, t) \Delta t.(8)$$

In case of a motionless inducton trapped under the electrode, the Hamiltonian is time-independent. However, when the inducton is set in motion by the application of voltages to the electrodes, the electron distribution density introduces time dependence to the Hamiltonian

$$\rho(\mathbf{r},t) = -e \left| \psi(\mathbf{r},t) \right|^2.$$
(9)

In order to include time dependence in our calculations, within each time-step of an Eq. (8) we solve a Poisson equation.

4. Induced quantum dots and quantum wires

If a metal electrode is formed in a shape of any finite geometric figure (e.g. square or circle), an electron will be trapped directly beneath the electrode and will not be able to run away until it obtains a kinetic energy which is bigger than the binding energy. If the size of an electrode is comparable with the radius of a wave packet (inducton), lateral motion becomes impossible which results in a creation of an "induced" quantum dot [14] beneath the electrode. A density distribution $|\psi(x, y)|^2$ of an electron trapped under a square electrode (pictured with a blue square) of a side width b = 70 nm is presented in Fig. 2a. In our calculations we assumed material parameters characteristic of GaAs: the electron effective mass m = 0.067, dielectric constant $\varepsilon = 12.5$. In case of an electrode in the

rectangular shape, when one of the rectangle side is much bigger then the wave packet radius (like a straight current path), inducton remains with one spatial degree of freedom, to move along the path. "An induced" quantum wire is formed beneath the electrode [14]. The electrondensity distribution is presented in Fig. 2b.



Fig. 2. (a) Electron charge density in the quantum dot induced by square metal plate of width b = 70 nm. (b) Charge density of the wave packet confined under the metal bar of width b = 50 nm.

Let us consider a nanodevice with a cross-section presented in Fig. 1, and electrodes shape shown in Fig. 3b. There are three electrodes with gaps of a width of 10 nm between them. Beneath the first square electrode e_1 of size (70 nm, 70 nm) an induced quantum dot is formed, to which in an initial moment an electron is injected. Second electrode e_2 (current path) of size (50 nm, 500 nm) should effectively induce a quantum wire in a quantum well localized beneath. This quantum wire will be used to transport an electron to a quantum dot induced under the electrode e_3 of size (70 nm, 70 nm).



Fig. 3. (a) Electron charge density as a function of the x-variable and time calculated at the symmetry axis (y = 100 nm) of the electrode configuration presented with blue lines in (b). The contour plots in (b) display the charge density at subsequent moments in time.

We assume that an electron is confined in a quantum dot induced under the electrode e_1 time long enough to relax to the ground state. In order to obtain a minimum of a potential energy under electrode e_1 we apply following voltages (Schottky potential barrier is neglected): V1 = 0.0 mV, V2 = V3 = -0.1 mV. After the electron is put in the ground state we change applied volt-

ages: V1 = -0.1 mV, V2 = 0.0 mV, V3 = -0.1 mV and start to iterate time-dependent Schrödinger equation. The electron senses the potential differences, leaves the quantum dot induced under electrode e_1 and gains a kinetic energy. Going balistically along the quantum wire induced under the electrode e_2 it reaches the electrode e_3 . As soon as the electron reaches the electrode e_3 we change the voltage applied to the electrode e_2 and set it to V2 = -0.15 mV, so the electron is permanently trapped under electrode e_3 . The electron-density distribution wandering along the nanodevice is presented in a few successive time steps in Fig. 3b. In Fig. 3a $|\psi(x, y_0, t)|^2$ is presented, where $y_0 = 200$ nm is a coordinate of a geometric center for all three electrodes. In a t = 0 moment, which is the moment of applying a repulsive voltage to the electrode e_1 , the inducton is not moving, then it gains a velocity (accelerate) until there is non-zero electron-density within a gap between electrodes e_1 and e_2 . Further it goes with a constant velocity beneath the path e_2 . Finally the packet is caught under the electrode e_3 , and starts to oscillate, as not whole kinetic energy is lost while trapping inducton. It is extremely important to notice the fact that the electron has been transported (in 100%) between two induced quantum dots.

Let us consider a similar semiconductor nanostructure with different shape of electrodes deposited on its surface (width is the same). Let us assume a path e_2 with a 90° bend. We will force the trapped inducton to change its direction. The time-evolution result is presented in Fig. 4. There is one bend presented in Fig. 4a and two bends in Fig. 4b.



Fig. 4. Snapshots of the time evolution of the electron density following the path which is bended once (a) or twice (b). The arrows indicate the cut corners of the metal path. The electron leaves the quantum dot induced under the e_1 electrode and goes to the quantum dot under e_3 .

It occurs that we are able to lead the electron to any place in a nanostructure even along a bended path. Please draw your attention to the edge of the current path marked with arrows in Fig. 4. It ensures the change of the direction with conservation of a reflection law. If the path corner is not cut the electron reflects from the edge and comes back underneath the electrode e_1 .

5. Spin–orbit coupling

The ability to transport the electron along any curve allows using a spin-orbit coupling to perform electron spin operations. In order to take into account the spinorbit coupling during simulations, we add two terms to Hamiltonian (6):

$$H \to H + \beta \left(p_x \sigma_x - p_z \sigma_z \right) + \alpha \left(p_z \sigma_x - p_x \sigma_z \right).$$
(10)

First term describes a Dresselhaus coupling [17], which is intrinsically present in semiconductors with a crystal elementary cell without the inversion symmetry (semiconductor compounds), the other term describes a Rashba coupling [18], which originates from the asymmetry of a quantum well.

In both terms we can find Pauli matrices σ_i . In order to take spin into consideration, electron wave function is constructed in a form of a two-row column matrix

$$\Psi(x,z,t) = \begin{pmatrix} \psi_1(x,z,t) \\ \psi_2(x,z,t) \end{pmatrix}$$
(11)

and charge density used in a Poisson Eq. (1) is given with a following expression:

$$\rho(\mathbf{r},t) = -e\left(|\psi_1(x,z,y_0,t)|^2 + |\psi_2(x,z,y_0,t)|^2\right) \times \delta(y-y_0).$$
(12)

In further simulations we will use Hamiltonian (10).

Assuming that only the Rashba coupling is possible and Dresselhaus interaction is not taken into account, let us consider a system presented in Fig. 5a. It consists of two electrodes e_1 and e_2 placed along the x axis on the surface of the nanostructure presented in Fig. 1. In the starting moment on both electrodes we put a zero voltage with respect to the substrate $V_0 = 0.0$ mV. We form an electron wave function underneath the electrode e_1 (marked in darker grey) in an inducton ground state, simultaneously forcing such a spin state, that average values of all x, y, z spin coordinates are equal. Having a formed wave function in a staring moment we increase a voltage applied to the electrode e_2 by $V_2 = 0.2$ mV and start iterations according to the equation (8). Changed potential distribution causes an electron to be pulled under the electrode e_2 and starting to move along the z axis. It accelerates until whole wave function is localized beneath the electrode e_2 . Starting from this moment it moves with a constant velocity. Electron position as a function of time is presented in Fig. 5b as a black solid line.

The dotted lines show how the average values of spin coordinates change in time. We can see that while electron is moving towards the z axis, $\langle \sigma_x \rangle$ is not changing. $\langle \sigma_y \rangle$ and $\langle \sigma_z \rangle$ coordinations oscillate. We can observe a spin rotating around the x axis. In a similar way we can show that if electron is moving towards the x axis, the Rashba Hamiltonian is responsible for a spin rotation around the z axis, while the Dresselhaus Hamiltonian is responsible for a spin rotation around the axis, along which electron is moving.

Rotation angle depends on a spin-orbit coupling con-



Fig. 5. Inducton position as a function of time and time evolution of an average values of spin coordinates while electron moving along the z axis with Rashba coupling only. (a) Position of the electrodes e_1, e_2 (arrows) on top of the structure. (b) Electron packet z position vs. time (solid line, left axis). Average values (dashed lines) of the Pauli operators: $\langle \sigma_z \rangle$ [red (light gray) color], $\langle \sigma_x \rangle$ (black) and $\langle \sigma_y \rangle$ [blue (dark gray)] — referred to the right axis.

stant, electron effective mass and an electron travel distance. In a simulation presented in Fig. 5 we employed a coupling constant $\alpha = 0.0005$ in atomic units, which is the same as 7.2×10^{-13} eV m and corresponds to the range predicted for an asymmetric quantum well [19]. Quantum well width and a blocking barrier width were assumed 10 nm each, electron effective mass m = 0.19and dielectric constant $\varepsilon = 13$ correspond to material parameter for Si. Analyzing a spin oscillation graph presented in Fig. 5 we can see that to rotate the spin by 360° an electron has to cover distance of $\lambda_{\rm SO} = 1.6 \ \mu m$ (spin– orbit (SO) length).

6. Quantum gates

By choosing a suitable length of the path the electron has to traverse we can rotate the spin by any angle. Because movement in perpendicular directions results in the spin rotations around axes perpendicular to themselves, we can perform a specific electron spin rotation by forcing an electron to run under electrodes forming closed circuit [18]. A proposition for a device performing a logical NOT operation is presented in Fig. 6.

On a surface of a nanostructure consisting a quantum well (presented in Fig. 1), electrodes are deposited as it is shown in Fig. 6 in grey color. An induced quantum dot is created beneath the electrode e_1 . Spin of the confined electron is representing a quantum bit. Electrode e_2 will be used to transport the electron along a loop trajectory back underneath the electrode e_1 . Lengths of respective parts of the electrode e_2 : A, B, C, D are chosen in such a way, that while the electron is moving, its spin rotates by a defined angle.

Likewise in the simulation presented in Fig. 5, in a starting moment t = 0 we put equal voltages to all electrodes and form an electron wave function in an inducton ground state beneath the center of the electrode e_1 . Ad-



Fig. 6. An electrode arrangement performing a NOT operation on a single electron spin (assuming Rashba coupling). Electrodes are marked in grey color. A solid blue line shows electron wave packet trajectory. Spin directions are marked in red color.

ditionally we set an electron spin to an "up" direction at the beginning.

We increase a voltage applied to the e_2 and e_4 electrodes by 0.2 mV and start an iteration of the time depended Schrödinger Eq. (8) with the Hamiltonian (10). During each time step we solve Poisson Eq. (1) with an electron density derived from Eq. (12). The electron wave packet senses an electric field which was just created and accelerates in a direction of an x axis. During first stage it goes along a segment A, due to a cut electrode corner it reflects and changes its direction, goes along a part B and afterwards C and D. Just after the electron reaches the electrode e_1 we increase its voltage by 0.3 mV in order to trap the electron beneath it. Spin orientation is presented in Fig. 6 in red color. Initially electron had a spin directed parallel to z axis, while moving under A segment (along x axis) the electron spin remains parallel to the z axis. While in B segment (motion along the z axis) spin is rotated around the x axis by 90° and takes the "from the page" orientation. While going through C segment (along the x axis) spin is rotating by 180° around the z axis and takes the "to the page" orientation. While going under D segment spin rotates again around the xaxis by -90° and finally the trip is ended with the spin directed opposite to the initial direction. This is a NOT logical gate operation.

Other one-qubit logical gates can also be created. A nanodevice described in the work [16] is illustrated in Fig. 8. It allows performing any sequence of the three one qubit operations on a single electron spin: negation U^{NOT} , phase shift by $\pi - U^{\pi}$ and Hadamard operation — $U^{\rm H}$. The electron, whose spin will be used to perform an operation, is placed under the electrode e_1 . Afterwards we force it to move along appropriate trajectory by applying voltages to the electrodes. Average values of the electron localization computed during the simulation of an electron wave packet are presented in Fig. 7, NOT, phase shift and Hadamard trajectories are marked in black, red and blue colors respectively. ZnTe material constants were applied during these simulations. Since the Dresselhaus coupling is rather strong in this compound, for simplicity reasons we did not include Rashba coupling in our calculations. One should notice that because of different type of coupling, NOT gates presented in Fig. 6 and Fig. 7 have different spatial orientation.



Fig. 7. An electrodes system of a nanodevice performing negation U^{NOT} , Hadamard U^{H} and phase shift U^{π} operations on a single electron spin.

7. Summary

The inducton effect resulting in electron wave function self-focusing mechanism, caused by the interaction of the electron with the charge induced on the electrodes surface, allows to transport the electron in a form of a stable wave packet along a loop trajectories defined with the electrodes deposited on a nanostructure surface.

While electron is wandering through the semiconductor, due to a spin–orbit coupling, a spin precession round an axis depended on the coupling type and motion direction occurs. We are able to compose spin rotations, just by choosing appropriate lengths of respective segments, performing all one-qubit quantum gates operations. We have planned and simulated working devices performing a logical operations of a NOT, Hadamard and phase shift operations on a single electron spin. Transitions between spin quantum states are performed by applying small (fraction of a mV) DC voltages to the electrodes. This implementation allows us to change many qubits in an independent way.

Spin states time evolution were observed during the simulation of a working system, which was performed by an iterative solution of a time dependent Schrödinger equation. The quantum approach undoubtedly used in our simulation, shows without a question that because of the inducton effect the spatial part of an electron wave packet exhibits many features of a classical electron. Particularly it is able to transmit or reflect from the potential barrier with a 100% probability. These classical features of a wave packet allow performing a spin operation with a probability arbitrary close to 1.

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