Gated combo nanodevice for sequential operations on single electron spin

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Abstract

We present an idea for a nanodevice in which an arbitrary sequence of three basic quantum single qubit gates—negation, Hadamard, and phase shift—can be performed on a single electron spin. The spin state is manipulated using the Dresselhaus spin–orbit coupling intrinsically present in zinc blende materials. The electron trajectory within the device is controlled by voltages applied to a multiple gate system which is deposited on top of a planar semiconductor heterostructure. We present the results of simulations based on iterative solutions of the time dependent Schrödinger equation with the electric field within the entire nanodevice calculated in each time step. We estimate the gate operation times and provide spatial dimensions of the gates allowing for the spin transformations.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

One of the proposals for the construction of logical gates for quantum computing employs spins of electrons confined in semiconductor nanostructures [1–4] to store quantum bits of information. The original idea for the quantum computation on confined electron spins [1] assumed that the exchange of the spin states is performed with a controllable Heisenberg interdot coupling. Moreover, single spin rotations were required [1] for construction of a universal quantum gate. A natural way to rotate a single spin is to put the electron in an external magnetic field and apply a microwave radiation with a resonant frequency inducing the Rabi oscillations of the spin orientation. It was soon realized that this particular idea is of limited use since, due to the large microwave length, it would be difficult to address a single spin selectively, i.e. without an unintentional perturbation of the other electron spins. A number of alternative solutions to the single spin rotation problem have been proposed. In particular it was shown that single spin rotations can be performed by Heisenberg coupling uniquely with the use of additional registers [5], by exploiting an inhomogeneous Zeeman splitting [6], or using the spin–orbit coupling [7].

A number of gated nanodevices have been studied experimentally for operations on the electron spin [8–12]. Site-selective spin rotations were experimentally demonstrated only relatively recently [11] in a device with an embedded local microwave source. A more recent and simpler device [12] rotates the spin in AC electric fields by employing spin–orbit coupling. Recently, we proposed [13] a different device which requires the application of DC voltages only. The idea [13] combines the electron-wavepacket self-focusing effect with the Rashba spin–orbit coupling in which spin rotations are induced by the spatial motion of electrons [14, 15]. The self-focusing effect was introduced in [16] for an electron interacting with an infinite metal plate. In [17] we showed that for gates of finite size this effect leads to the formation of induced quantum dots and quantum wires, along which the electron can be transferred with a 100% probability to any desired location in the nanodevice.

The proposal of [13] was limited to materials of the diamond structure (Si, Ge) in which Dresselhaus [18] spin–orbit coupling, due to the inversion asymmetry of the crystal lattice, is absent. Moreover, in [13] we described systems in which separate devices were proposed for each spin transformation. The aim of the present paper is to generalize the previous proposal to materials of the zinc blende structure (III–V and II–VI semiconductors). In the present paper we show that for Dresselhaus coupling the spatial motion of the electron is associated with the spin rotation along the axis determined by the electron path. Since in a device based on induced quantum wires [17] the electron packet follows any desired trajectory, an arbitrary spin rotation can be obtained by the trajectory design. Moreover, we propose a single device
in which three most popular quantum transformations can be performed: negation (NOT), Hadamard, and phase shift.

In the present paper we assume that the quantum well in which the electron moves is perfectly symmetric, so that the Rashba coupling [19] constant is zero. Accordingly, we will consider pure Dresselhaus coupling only. In the proposed device the operations on the electron spin are induced by voltages applied to the electrodes. The spin transformations will be performed for small voltages applied to the gates, of the order of a fraction of millivolt, for which the asymmetry of the potential within the quantum well remains negligible.

2. Theory

The systems discussed below are based on a planar semiconductor structure as drawn schematically in figure 1. It contains a 10 nm wide quantum well sandwiched between tunnel barriers each 10 nm thick. The structure is separated from the strongly doped substrate by a undoped buffer layer 50 nm thick. Metal electrodes are deposited on top of the upper tunnel barrier. The electron gas within the electrodes is a source of the response potential which keeps the electron in motion with a controlled trajectory by the application of voltages supplied in this paper are given with respect to the semi-metallic strongly doped substrate.

The simulations that we performed were based on the time dependent Schrödinger equation

$$\Psi(t + dt) = \Psi(t - dt) - \frac{2i}{\hbar} H(t) \Psi(t) dt.$$  (4)

For a moving electron wavepacket the electrostatic potential must be evaluated in each time step, which introduces the time dependence of the Hamiltonian (1) entering into equation (4). In each simulation, as the initial condition we take a stationary wavepacket.

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Similarly one obtains the operator of the spin rotation around the $z$ axis for the electron moving along the $z$ axis:

$$U_z(\phi) = \begin{pmatrix} 1 & 0 \\ 0 & \exp(i\phi) \end{pmatrix}. \quad (10)$$

One can also derive the operator of the spin rotation around the $y$ axis:

$$U_y(\phi) = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1 + \cos(\phi)} & \sin(\phi) \\ -\sin(\phi) & \sqrt{1 + \cos(\phi)} \end{pmatrix}. \quad (11)$$

In contrast to $U_z$ and $U_x$, the $U_y$ operator is not associated with the time evolution of the spin, since electron movement in the $y$ direction is excluded. Nevertheless, it is useful for the system of reference transformations performed below.

### 3. Nanodevice

The system of electrodes deposited on top of the planar semiconductor structure is presented in figure 2. The system contains 13 electrodes serving various purposes. A small electrode $e_1$ plotted with the darkest shade of gray localized in the center of the device generates a quantum dot underneath it. The spin of the electron confined in this quantum dot will store the quantum bit, on which the logical operations will be performed. Pairs of electrodes $(e_2, e_3), (e_4, e_9), \text{ and } (e_0, e_{12})$ or their parts which are marked in figure 2 with medium shade of gray are used to set the electron in motion along closed loops. During the electron motion its spin undergoes time evolution corresponding to the logical gates: Hadamard, NOT, and phase shift $\pi$ gates. The parts of electrodes $e_4$ and $e_9$ marked with a lighter shade of gray serve to deliver the electron from the quantum dot to the NOT gate or the $\pi$ gate. The electrodes plotted with the lightest shade of gray are auxiliary and serve only to symmetrize the induced potential in order to make the electron trajectory as straight as possible.

The vertically oriented rectangle in the left part of figure 2 composed of electrode $e_{10}$ and the darker part of electrode $e_4$ form the NOT gate. An electron going along the shorter rectangle side travels a distance of $-\lambda_{w}/4$. Its spin is rotated around the $x$ axis by $-\pi/2$, or in other words a $U_x(-\pi/2)$ operation is performed on the spin state. At the end of the segment parallel to the $x$ axis there is a cut electrode corner. The electron packet is reflected off the cut corner under a right angle and starts to move parallel to the $z$ axis on a distance of $\lambda_{w}/2$ with the $U_z(\pi)$ operator acting on the spin state. Then the electron moves along the $x$ and $-z$ directions with $U_z(\pi/2)$ and $U_z(-\pi)$ operators acting on the electron spin sequentially. Assembling all the spin rotations we obtain the NOT transform, \[ U = U_z(-\pi)U_z(\pi/2)U_y(\pi)U_z(-\pi/2) \]

\[ = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]

\[ = -i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = U^{NOT}. \quad (12)\]

The electron is delivered to the NOT gate from under electrode $e_1$ along the quantum wire induced under the part of electrode $e_{10}$ which is plotted with the lighter gray shade in figure 2. We find that for the NOT gate the length of electrode $e_4$ is quite arbitrary, since, as can be verified by a direct algebra,

\[ U_x(\phi)U^{NOT}U_x(-\phi) = U^{NOT}. \quad (15)\]

### 4. Results

We first employ our device to perform the NOT operation on the electron spin. The subsequent steps of the spin state negation can be followed in figure 3, in which one can observe the time dependence of the position of the center of the wavepacket and the average values of the Pauli matrix operators. The electron trajectory in the NOT gate is depicted in figure 2 by the black color. At the initial moment the same voltage of $-0.2 \text{ mV}$ is applied to all the electrodes. The electron is localized under electrode $e_1$ in the ground state with the spin nearly parallel to the $z$ axis ($s_z \approx +\hbar/2$). The NOT operation on the electron spin starts by application of zero voltage to electrodes $e_4, e_{10}$, and $e_{11}$. The electron is first attracted under electrode $e_4$; it starts to move parallel to the $x$ axis and initially increases its velocity until the entire packet is transferred under $e_4$, when the velocity becomes constant and the motion of the packet acquires a ballistic character. The electron goes to under electrode $e_{10}$ from below the lighter part of electrode $e_4$. At $t = 100$ ps, when the electron is found at the uppermost electrode $e_{10}$ part, we decrease the voltage on $e_{10}$ and $e_{11}$ to $-0.4 \text{ mV}$ to make the electron reflect off the cut corner and leave the gate, changing its velocity direction to parallel to the $x$ axis in order to complete the full loop. The
The phase shift operation is performed in an exactly analogous way for the electron completing the loop along the rectangle of electrodes placed at the bottom of the device. The entire operation on the electron spin is performed by assembling separate rotations:

\[ U = U_z(-\phi) U_z(\pi) U_z(\pi/2) U_z(-\pi) U_z(-\pi/2) U_z(\phi) \]

\[ = i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = U^\pi. \]  

The phase shift \( \pi \) operation is performed for voltages \( e_9, e_{12}, \) and \( e_{13} \) set to zero at \( t = 0 \). For \( t = 100 \) ps, the voltage on electrodes \( e_{12} \) is lowered to \(-0.4 \) mV to make the electron change its direction and to return to electrode \( e_1 \) below electrode \( e_9 \). Then for \( t = 175 \) ps the electron is stopped by the voltage on electrode \( e_1 \) raised to \( 0.1 \) mV. The details of the time evolution of the position and spin can be followed in figure 4. This time we deliver the electron to the gate along the \( z \) direction. This choice results from the fact that for the \( \pi \) gate the length of the segment parallel to the \( z \) direction can be arbitrary, since \( U_z(\phi) U^\pi U_z(-\phi) = U^\pi \), for any \( \phi \).

One of the rectangles formed by electrodes in figure 2 is rotated with respect to the NOT gate by \( \pi/4 \) around the \( y \) axis.
5. Discussion

The relative positions of the parts of the nanodrive (see figure 2) performing the discussed rotations are not arbitrary. As discussed above, the horizontal part of electrode \( e_4 \) and the vertical part of electrode \( e_0 \) may have an arbitrary length since this is irrelevant for the operation of \( U_{\text{NOT}} \) and \( U^\pi \) gates, respectively. However, in order to deliver an electron from the induced quantum dot to the Hadamard gate, one should produce an electrode segment of a length exactly equal to \( \lambda_{\text{SO}} \), which is definitely inconvenient. For that reason the quantum dot electrode \( e_1 \) lies within the loop performing the Hadamard gate, so no initial electron delivery is required.

We have applied here material constants of ZnTe material, of the II–VI group of semiconductors. The most popular III–V material, GaAs, has a smaller effective mass and a larger dielectric constant. Therefore, the self-focusing effect in GaAs is much weaker than in ZnTe, and operation of the proposed device would be more susceptible to external perturbations. The Dresselhaus coupling constant in the two materials is comparable, but due to the dependence of \( \lambda_{\text{SO}} \) on the effective mass one should expect that the length of the electrodes in the GaAs-based device would be larger. For the above reasons II–VI materials should be more useful than III–V materials for construction of the proposed device.

For pure Rashba coupling, the spin is rotated in the direction perpendicular to the direction of the electron motion [17]. For both Rashba and Dresselhaus couplings present, the spin rotations with respect to the \( x \) and the \( z \) axes will occur for an electron moving in non-perpendicular spatial directions within a plane of confinement \((x, z)\). The specific value of the angle formed by these two directions depends on the coupling constants. A practical implementation of a device working with both couplings present is possible, although its design is somewhat more challenging.

In previous literature, Rashba coupling was proposed for the manipulation of the electron spin in opened quantum rings [14, 15]. In [14] a system of quantum rings is proposed for spin transformations according to three basic quantum gates: NOT, phase shift, and Hadamard transform, in a spin dependent scattering experiment. In [15], a programmable array of rings was proposed to split the incoming electron wavefunction into two parts, each corresponding to an opposite spin orientation. In these papers [14, 15], the time independent scattering problem is solved, with the electron spread all over the space with position dependent spin orientation. In contrast to quantum ring devices [14, 15], in the device discussed here the electron returns to its initial position when the spin transformation is completed. Therefore, the standard unitary time evolution operators used in the quantum computation theory (see section 2) act exclusively on the electron spin and not on the spatial wavefunction.

6. Summary and conclusion

The self-focusing effect due to the interaction of the electron packet with the charge induced on the electrodes placed on the surface of the semiconductor nanostructure allows for the electron transfer along a designed trajectory between chosen points in the device in the form of a wavepacket of a stable shape. In a semiconducting material in which the spin–orbit coupling is present, the electron motion is accompanied by rotation of its spin by an angle which depends on the direction of motion and the distance traveled. For carefully chosen lengths of the segments one can assemble the rotation into basic single qubit operations. For electrodes forming closed loops with a common quantum dot at the beginning and the end of each electron loop, one can apply the quantum gates sequentially in an arbitrary order. The nanodevice proposed in the present paper is designed to perform any sequence of operation of the most popular single qubit gates: NOT, Hadamard, and phase shift. The choice of operation and its implementation requires the application of weak DC voltages. The computer simulations performed were obtained by iterative solution of the time dependent Schrödinger equation. The simulations indicate that the operations designed algebraically based on elementary quantum mechanics can indeed be performed. The proposed device has realistic dimensions and can be produced by present technology. We have provided details of the spin rotation phenomena, including estimates for the spin rotation length and gate operation times.

References

[1] Loss D and Dincenzo D P 1998 Phys. Rev. A 57 120
[2] Datta S and Das B 1990 Appl. Phys. Lett. 56 665
[3] Awshalom D, Loss D and Samarth N 2002 Semiconductor Spintronics and Quantum Computation (Berlin: Springer)
[4] Hanson R, Kouwenhoven L P, Petta J R, Tarucha S and Vandersypen L M K 2007 Rev. Mod. Phys. 79 1217
[5] DiVincenzo D P, Bacon D, Kempe J, Burkard G and Whaley K B 2000 Nature 408 339
[6] Levy J 2002 Phys. Rev. Lett. 89 147902
[7] Stepanenko D and Bonesteel N E 2004 Phys. Rev. Lett. 94 140501
[8] Elzerman J M, Hanson R, Willems van Beveren L H, Witkamp B, Vandersypen L M K and Kouwenhoven L P 2004 Nature 430 431
[9] Meunier T, Vink I T, Willems van Beveren L H, Koppens F H L, Tantiz H P, Wegscheider W, Kouwenhoven L P and Vandersypen L M K 2006 Phys. Rev. B 74 195303
[10] Petta J R, Johnson A C, Taylor J M, Laird E A, Yacoby A, Lukin M D, Marcus C M, Hanson M P and Gossard A C 2005 Science 309 2180
[11] Koppens F H L, Buizert C, Tielrooij K J, Vink I T, Nowack K C, Meunier T, Kouwenhoven L P and Vandersypen L M K 2006 Nature 442 766
[12] Nowack K C, Koppens F H L, Nazarov Yu V and Vandersypen L M K 2007 Science 318 1430
[13] Bednarek S and Szafran B 2008 Phys. Rev. Lett. 101 216805
[14] Földi P, Molnar B, Benedict M G and Peeters F M 2005 Phys. Rev. B 71 033309
[15] Földi P, Kalman O, Benedict M G and Peeters F M 2006 Phys. Rev. B 73 155325
[16] Bednarek S, Szafran B and Lis K 2005 Phys. Rev. B 72 075319
[17] Bednarek S, Szafran B, Dudek R J and Lis K 2008 Phys. Rev. Lett. 100 126805
[18] Dresselhaus G 1955 Phys. Rev. 100 580
[19] Rashba E I 1960 Sov. Phys.—Solid State 2 1109