Rashba effect in an asymmetric quantum dot in a magnetic field

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Abstract

We derive an expression for the total spin splitting energy in an asymmetric quantum dot with ferromagnetic contacts, subjected to a transverse electric field. Such a structure has been shown by one of us to act as a spintronic quantum gate with in-built qubit readers and writers [Phys. Rev. B, 61, 13813 (2000)]. The ferromagnetic contacts result in a magnetic field that causes a Zeeman splitting of the electronic states in the quantum dot. We show that this Zeeman splitting can be finely tuned with a transverse electric field as a result of non-vanishing Rashba spin-orbit coupling in an asymmetric quantum dot. This feature is critical for implementing a quantum gate.

1 Introduction

Consider the system shown in Fig. 1(a) consisting of a penta-layered quantum dot. The outer layers (contacts) are ferromagnetic and the thin insulating layers (tunnel barriers) facilitate spin coherent injection from the ferromagnetic layers into the semiconductor layer and vice versa [1]. The ferromagnets are spin polarizers and analyzers. They are used to inject and detect single electron spins. The insulating layers not only aid spin injection and detection, but they also provide a potential well to confine an electron in the semiconductor layer. The semiconductor layer has a graded composition (or doping) so that there is an in-built electric field between the contacts. This makes the quantum dot "asymmetric". The resulting conduction band diagram is shown in Fig. 1(b). This structure is a slightly modified version of a structure proposed by one of us more than two years ago to implement a universal quantum gate [2]. Note that the degeneracy between spins aligned parallel and anti-parallel to the magnetization of the contacts is lifted because of the Zeeman effect brought about by the magnetic field due to the contacts. We will call the spin parallel to the magnetization of the contacts the "upspin" state, while the spin anti-parallel to the magnetization will be called the "downspin" state.

In our quantum gate, a qubit is encoded by the *spin* of a single electron confined in the quantum dot [3]. The first step is to ensure that one, and only one, electron occupies the quantum dot. This is ensured by applying a positive bias to the gates *A, B, C...* (in Fig. 1(c)) simultaneously to lower the conduction band edge in the semiconductor layer with respect to the Fermi level in the metallic ferromagnetic contacts such that the Fermi level is above the upspin state, but below the downspin spin state in the semiconductor. This procedure ensures that a *single* electron occupies the quantum dot and its spin orientation is known (the spin is polarized along the direction of magnetization of the ferromagnetic contacts since the electron must occupy the lowest energy state). The conduction band diagram under single electron occupancy conditions are shown by the broken lines in Fig. 1(b). It is not difficult to ensure single electron occupancy in quantum dots; this experimental feat has been demonstrated many times in the past in large arrays of quantum dots [4].

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We now briefly show how this system acts as a universal quantum gate; that is, how one can execute the two features of a universal quantum gate, namely arbitrary single qubit rotation and the square-root-of-swap operation.

1.1 Single qubit rotation

In order to execute a single qubit rotation in a selected quantum dot, we must be able to tune the spin splitting energy in that dot so that it resonates with the frequency of an external global ac magnetic field. Below, we show that this can be realized by varying the spin splitting energy in any dot with a transverse electric field to induce a Rashba spin-orbit coupling effect between the upspin and downspin states [5]. This electric field is applied by imposing a *differential* potential between contacts *A* and *B*. By holding the dot in resonance with a small ac magnetic field for a time duration t, we can then rotate its host spin by an angle θ given by

$$\theta = \frac{\mu_B B_{ac} t}{\hbar} \tag{1}$$

where μ_B is the effective Bohr magneton for the electron and B_{ac} is the amplitude of the ac magnetic field flux density. Thus, by selecting the time duration of the ac signal, we can execute arbitrary qubit rotations.

1.2 Two qubit square-root-of-swap operation

In order to execute the two qubit square-root-of-swap operation, we need to couple two adjacent penta-layered quantum dots. Each dot hosts a spin or a qubit. The potential barrier between these two dots is gated as shown in Fig. 1(d). We can apply a slight positive voltage to the gate without pulling the higher spin state below the Fermi level (i.e. without upsetting the single electron occupancy). This positive voltage lowers the barrier between the two neighboring dots and makes the wavefunctions of electrons in the two dots overlap so that an exchange interaction develops between the two electrons (see Fig. 1(d)). The square-root-of-swap operation is executed by gating the barrier for a duration $h/4J$ where J is the exchange energy (essentially the energy difference between the triplet and singlet states of the two electron system) [6].

Recently, it has been shown that by executing a sequence of single qubit rotations and square-root-of-swap operations, one can realize the dynamics of a universal quantum gate [6]. Therefore, the two operations described here are sufficient to realize a universal quantum gate.

2 Controlling the spin splitting energy in a dot

We now calculate the total spin splitting energy in a quantum dot. It has has a contribution due to the Zeeman effect and another due to the Rashba effect.

The complete Hamiltonian for an electron in the semiconductor layer is

$$\begin{aligned} H &= \frac{(\vec{p}+e\vec{A})^2}{2m^*} + V_x(x) + V_y(y) + V_z(z) - e\mathcal{E}_y y + (g/2)\mu_B B_x \sigma_x + H_R \\ &= H_0 + H_R \end{aligned} \tag{2}$$

where $V_x(x)$, $V_y(y)$ and $V_z(z)$ are the confining potentials along the x-, y- and z-directions, g is the Landé g-factor, e is the magnitude of the electronic charge, μ_B is the Bohr magneton, σ_x is the x-component of the Pauli spin matrix, and H_R is the Rashba interaction given by

$$H_R = \frac{e\hbar}{2m^{*2}c^2}\vec{\mathcal{E}}_y \cdot \vec{\sigma} \times (\vec{p} + e\vec{A}) \tag{3}$$

where $\vec{\sigma}$ is the Pauli spin matrix, $\vec{p}$ is the momentum operator, and $\vec{\mathcal{E}}$ is the electric field inducing the Rashba effect.

We choose the Landau gauge $\vec{A}$ = (0, -Bz, 0). Since we have a y-directed electric field inducing the Rashba effect,

$$H_R = \frac{e\hbar}{2m^{*2}c^2}\mathcal{E}_y\left[\sigma_z p_x - \sigma_x p_z\right]. \tag{4}$$

The Zeeman term $(g/2)\mu_B B_x \sigma_x$ introduces an Zeeman splitting between the +x-polarized spin (upspin $|\uparrow>$) and the -x-polarized spin (downspin $|\downarrow>$). Since the potential confining the electron in the semiconductor quantum dot

(along the x-direction) is finite and there is an in-built electric field along the x-direction, therefore the spatial parts of the "upspin" (+x-polarized) and "downspin" (-x-polarized) states are slightly different since these two states have different eigenenergies *by virtue of the Zeeman splitting*. In stating this, we have assumed that the Zeeman splitting in the insulators is negligible (or has the opposite sign compared to the Zeeman splitting in the semiconductor). The wave function of the higher energy state will therefore be spread out a little bit more. This is shown in Fig. 1(e). If we assume that the the downspin state is at a higher energy (i.e., the g-factor in the semiconductor is negative), then the spatial parts of the wave functions of the two spin states in the lowest spin-split subband of the quantum dot can be written as

$$\phi\uparrow = \left(\frac{\sqrt{2}}{\sqrt{W_x}}\right) sin\left(\frac{\pi x}{W_x}\right)\phi_y(y)\phi_z(z)$$
$$\phi\downarrow = \left(\frac{\sqrt{2}}{\sqrt{W_x'}}\right) sin\left(\frac{\pi x}{W_x'}\right)\phi_y(y)\phi_z(z) \quad (5)$$

where $W_x' > W_x$. We have assumed that the confinement in the y-z plane is stronger than the confinement along the x-axis, so that the difference between the upspin and downspin wavefunctions is mostly in their x-component.

In the above equation, $\phi_y(y)$ and $\phi_z(z)$ are the y- and z-components of the wavefunctions. We will assume that the confinement along the y- and z-direction is parabolic. This is not only an appropriate assumption for realistic structures, but will also allow us to easily absorb the effect of the x-directed magnetic field by simply renormalizing the transverse confining potential according to

$$V_y(y) + V_z(z) = (1/2)m^*\omega^2\left(x^2+y^2\right) \rightarrow (1/2)m^*\left(\omega^2+\omega_c^2\right)\left(x^2+y^2\right)$$

where ω_c is the cyclotron frequency ($\omega_c = eB/m^*$) and B is the x-directed magnetic flux density. The wavefunction $\phi_z(z)$ is a "simple harmonic oscillator" wavefunction and $\phi_y(y)$ is a shifted simple harmonic oscillator wavefunction (shifted because of the electric field $\mathcal{E}_y$). In other words, $\phi_y(y)$ is not centered at the center of the well, but is displaced from the center by an amount proportional to the electric field $\mathcal{E}_y$. At this point, we should mention that the simple harmonic confining potentials give rise to additional electric fields that are equal to $-\nabla V_y(y)/e$ ($= m^*\omega^2 y$) and $-\nabla V_z(z)/e$ ($=m^*\omega^2 z$) along the y- and z-directions. Moreover, the in-built electric field along the x-direction also needs to be considered. These electric fields will give rise to additional Rashba interaction, but we will assume these internal fields are much weaker than the *externally applied* electric field $\mathcal{E}_y$. Therefore, we will only consider the Rashba contribution due to the external electric field $\mathcal{E}_y$.

The time-independent Schrödinger equation describing the ground state of the system is

$$(H_0 + H_R)\psi = E\psi \quad (6)$$

We expand ψ in the basis functions of the two lowest spin-resolved eigenstates of the Hamiltonian H_0. We can neglect the higher subband states as long as the Rashba spin splitting Δ_R and Zeeman spitting energy are much smaller than the energy separation between the lowest two subbands in the quantum dot in the absence of magnetic field. This is a reasonable assumption, since the spatial dimensions of the dots are just a few nanometers in all directions.

Accordingly,

$$\psi = a_\uparrow\phi\uparrow + a_\downarrow\phi\downarrow \quad (7)$$

Substituting this result in Eq.(6), we get

$$\begin{bmatrix} <H_1> + <H_R>_{11} & <H_R>_{12} \\ <H_R>_{21} & <H_2> + <H_R>_{22} \end{bmatrix}\begin{pmatrix} a_\uparrow \\ a_\downarrow \end{pmatrix} = E\begin{pmatrix} a_\uparrow \\ a_\downarrow \end{pmatrix}, \quad (8)$$

where $<H_1> = <\phi\uparrow|H_0|\phi\uparrow>$, $<H_2> = <\phi\downarrow|H_0|\phi\downarrow>$, $<H_R>_{11} = <\phi\uparrow|H_R|\phi\uparrow>$, $<H_R>_{22} = <\phi\downarrow|H_R|\phi\downarrow>$, $<H_R>_{12} = <\phi\uparrow|H_R|\phi\downarrow>$, and $<H_R>_{21} = <\phi\downarrow|H_R|\phi\uparrow>$.

Diagonalizing the above Hamiltonian, we get that the total energy splitting between the two orthogonal spin states is

$$E_\downarrow - E_\uparrow = 2\sqrt{\left(\frac{<H_1> - <H_2> + <H_R>_{11} - <H_R>_{22}}{2}\right)^2 + <H_R>_{12}<H_R>_{21}}$$

$$= 2\sqrt{\left(\frac{g\mu_B B}{2} - \frac{e\hbar}{2m^{*2}c^2}\mathcal{E}_y < p_z >\right)^2 + \left[\frac{e\hbar}{2m^{*2}c^2}\mathcal{E}_y\right]^2 < p_x >< p_x' >} \quad (9)$$

where $< p_z > = < \phi\uparrow | -i\hbar(\partial/\partial z|\phi\uparrow > = < \phi\downarrow | -i\hbar(\partial/\partial z|\phi\downarrow > = 0$, $< p_x > = < \phi\uparrow | -i\hbar(\partial/\partial x|\phi\downarrow >$ and $< p_x' >$ $= < \phi\downarrow | -i\hbar(\partial/\partial x|\phi\uparrow >$. We should point out that because of the Rashba coupling, the actual eigenspinors are no longer pure "upspin" and "downspin" states in the sense that they are not pure +x-polarized and -x-polarized spins. However the Rashba coupling is very weak in this quantum dot (there are ways to make it much stronger, which will be discussed in a forthcoming publication), so that we can still approximately label the eigenspinors as up- and down-spin states.

Using the wavefunctions in Equation 5, it is easy to show that

$$\begin{aligned} < p_x > &= -\frac{8i\hbar}{\sqrt{W_x W_x'}} cos^2\left(\frac{\pi}{2}\frac{W_x'}{W_x}\right)\frac{W_x/W_x'}{(W_x/W_x')^2 - 1}, \\ < p_x' > &= -\frac{8i\hbar}{\sqrt{W_x W_x'}} cos^2\left(\frac{\pi}{2}\frac{W_x}{W_x'}\right)\frac{W_x'/W_x}{(W_x'/W_x)^2 - 1}. \end{aligned} \quad (10)$$

Therefore the total splitting is

$$\Delta = E_\downarrow - E_\uparrow = 2\sqrt{\left(\frac{g\mu_B B}{2}\right)^2 + \mathcal{E}_y^2 \frac{16e^2\hbar^4}{m^{*4}c^4 W_x W_x'} f(W_x, W_x')} \quad (11)$$

where the function $f(W_x, W_x')$ is given by

$$f(W_x, W_x') = cos^2\left(\frac{\pi W_x}{2W_x'}\right) cos^2\left(\frac{\pi W_x'}{2W_x}\right)\frac{1}{((W_x'/W_x)^2 - 1)^2((W_x/W_x')^2 - 1)^2}. \quad (12)$$

The last term under the radical in Eq.(11) is the Rashba effect which can be varied by the electric field $\mathcal{E}_y$. Note that this term would vanish if $W_x = W_x'$, that is, if the spatial parts of the upspin and downspin wave functions were identical. Here, we have made the spatial parts different by using a finite potential barrier, an in-built electric field, and (the fortuitously present) magnetic field due to the ferromagnetic contacts. All three of these ingredients are necessary to have a non-vanishing Rashba effect in this type of quantum dot.

2.1 Total spin splitting energy as a function of the external electric field

We have calculated the total spin splitting energy Δ as a function of the external electric field $\mathcal{E}_y$ using Equation 11. Estimates of the quantities W_x and W_x' were found by solving the transcendental equations to find the wavefunctions in a finite square potential well [7]. We have used the parameters corresponding to a GaAs quantum well of width 100$\AA$ sandwiched between two $Ga_{0.7}Al_{0.3}As$ barriers. The effective mass was assumed to be constant throughout and equal to $m^* = 0.067\ m_o$, where m_o is the free electron mass. Furthermore, we used a total Zeeman splitting energy $g\mu_B B =$ 2 meV. To illustrate the influence of the Rashba interaction on the overall spin splitting energy, we plot in Fig.2 the following quantity

$$R(\mathcal{E}_y) = \frac{\Delta(\mathcal{E}_y) - \Delta 0)}{\Delta 0} \quad (13)$$

which is a measure of how the Zeeman splitting can be modulated by the Rashba effect.

Figure 2 indicates that the Rashba effect has a very small influence on the overall spin splitting energy. However, this small influence allows us to fine tune the spin splitting energy of a particular dot to bring it in resonance with the external frequency of the small external ac magnetic field. In large arrays of quantum dots, this fine tuning would need to be performed on a large sample of dots until a large number of specific qubits are found which can be used for quantum computation, i.e. which can be brought into resonance with a global ac magnetic field selectively. Much stronger Rashba modulation of the Zeeman splitting is possible by employing bandgap engineering in a quantum dot. This is the subject of a forthcoming publication.

3 Reading and writing of the qubit

We have, in effect, already described the writing (initialization) of the qubit in every quantum dot. Since the ground state in each dot is spin polarized because of the spin splitting, the lowest energy state corresponds to spin orientation along the magnetization vector in the ferromagnetic contacts. Thus, if the ferromagnets are magnetized along the +x-direction, then the initial state of every qubit is +x-polarized spin described by the eigenspinor $[11]^{\dagger}$. Therefore, all qubits are "written" as +x-polarized spins initially. To attain any other desired state, the qubit merely has to be rotated to the desired state following the prescription in Section 1.1.

Reading a qubit is actually much more difficult than writing, since reading a single spin in a solid has never been achieved before. State of the art magnetic resonance force microscopy can read about 100 polarized spins [8] which is still a far cry from reading a single spin.

A few proposals have appeared in the literature that can discriminate between the singlet and triplet states of two electrons [9, 10]. Recently, such a discrimination has been demonstrated experimentally in a coupled quantum dot [10]. However, all this can only tell us whether two spins are parallel or antiparallel. It does not tell which electron has which spin and therefore does not serve the purpose of "reading" qubits. More recently, there has been a proposal to read spin resonance signal from a single electron trap [11], but it too does not constitute a single spin measurement.

We have now proposed a scheme that truly can detect a single spin and tell whether it is "up" or "down". The details are omitted here but can be found in ref. [12]. This scheme is fully compatible with the universal gate described here and does not require any additional device.

4 Conclusion

We have shown how to finely tune the Zeeman spin-splitting energy of a specific asymmetric quantum dot in a large self-assembled array of dots based on the control of the Rashba coupling between the lowest up- and down-spin eigenstates in the dot using an external electric field. This fine tuning is critical to independently execute a single qubit rotation in a large array of dots.

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References

[1] E. I. Rashba, Phys. Rev. B, **62**, R16267 (2000).

[2] S. Bandyopadhyay, Phys. Rev. B, **61**, 13813 (2000).

[3] S. Bandyopadhyay and V. P. Roychowdhury, Superlat. and Microstruct., **22**, 411 (1997).

[4] B. Muerer, D. Heitman and K. Ploog, Phys. Rev. Lett., **68**, 1371 (1988).

[5] E. I. Rashba, Sov. Phys. Semicond., **2**, 1109-1122 (1960); Y. A. Bychkov and E. I. Rashba, J. Phys. C, **17**, 6039-6045 (1984).

[6] G. Burkard, D. Loss and D. P. DiVincenzo, Phys. Rev. B, **59**, 2070 (1999).

[7] L. I. Schiff, *Quantum Mechanics*, 3rd. edition (McGraw Hill, New York, 1968).

[8] D. Rugar, et. al., Science, **264**, 1560 (1994); Z. Zhang, P. C. Hammel and P. E. Wigen, Appl. Phys. Lett., **68**, 2005 (1996).

[9] B. E. Kane, et. al., *Phys. Rev B*, **61**, 2961 (2000).

[10] K. Ono, D. G. Austing, Y. Tokura and S. Tarucha, *Science*, **297**, 1313 (2002).

[11] I. Martin, D. Mozyrsky and H. W. Jiang, LANL e-print arXiv cond-mat/0208438.

[12] S. Bandyopadhyay, LANL e-print arXiv cond-mat/0210280.

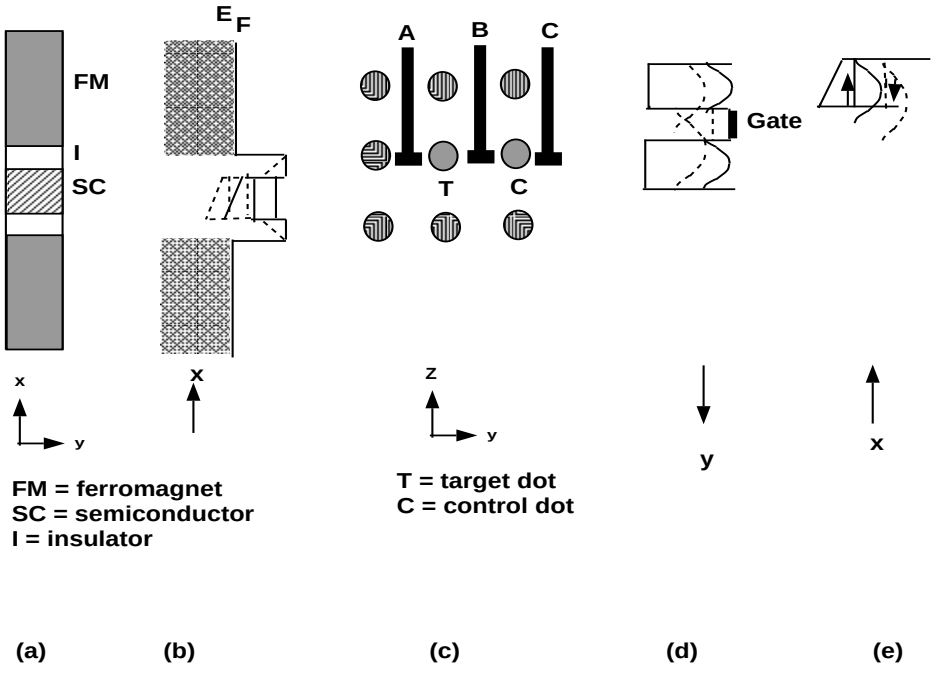

Figure 1: (a) Side view of a penta-layered quantum dot. (b) Conduction band diagram along the axis of the penta-layered dot. The solid line shows the diagram when the dot is completely depleted of all electrons, and the broken line shows the diagram when the conduction band edge is pulled down by external gates to inject a single (spin-polarized) electron into the semiconductor layer. (c) Top view showing the gates *A*, *B*, *C*... etc. used to inject a single electron into the dot and execute the 1- and 2-qubit operations. (d) Energy band diagram and wavefunctions in two adjacent dots (shown shaded in Fig. 1(c)) separated by an insulating barrier. To carry out the square-root-of-swap operation, the potential of gate *B* (which is a Schottky gate sitting on the barrier) is made slightly more positive. This lowers the barrier so that the wavefunctions of the electrons in adjacent dots leak out into barrier region, overlap and cause an exchange interaction between two neighboring electrons. The lowered barrier and the leaky wavefunctions are shown by broken lines while the raised barrier and the confined wavefunction is shown by solid lines. (e) the x-component of the wavefunctions $\phi\uparrow$ and $\phi\uparrow$. The wavefunction of the higher lying state is spread out a little bit more.

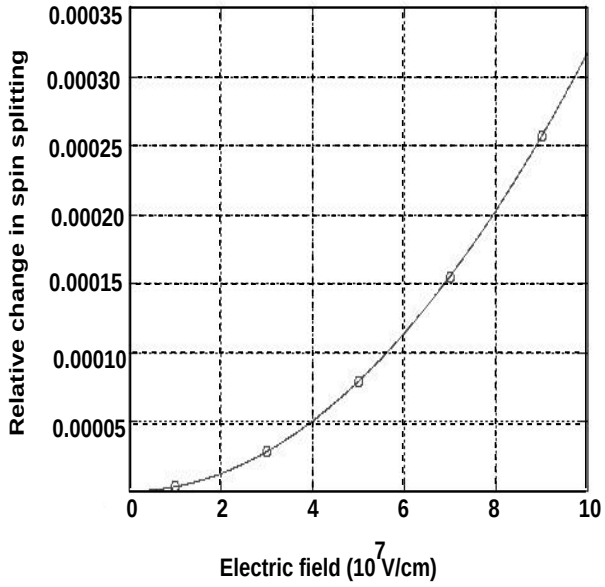

Figure 2: Dependence of the relative variation in the spin splitting energy as a function of the electric field inducing Rashba effect. The results are plotted for a quantum dot of dimension 10 nm in the x-direction. The potential barrier at the dot boundary (along the x-direction) is assumed to be 100 meV. The potential profiles along the y- and z-directions are parabolic with a curvature given by $\hbar\omega$ = 70 meV to simulate the hardwall boundary confinement in the y and z directions. For zero transverse electric field, the Zeeman splitting energy is assumed to be 2 meV.