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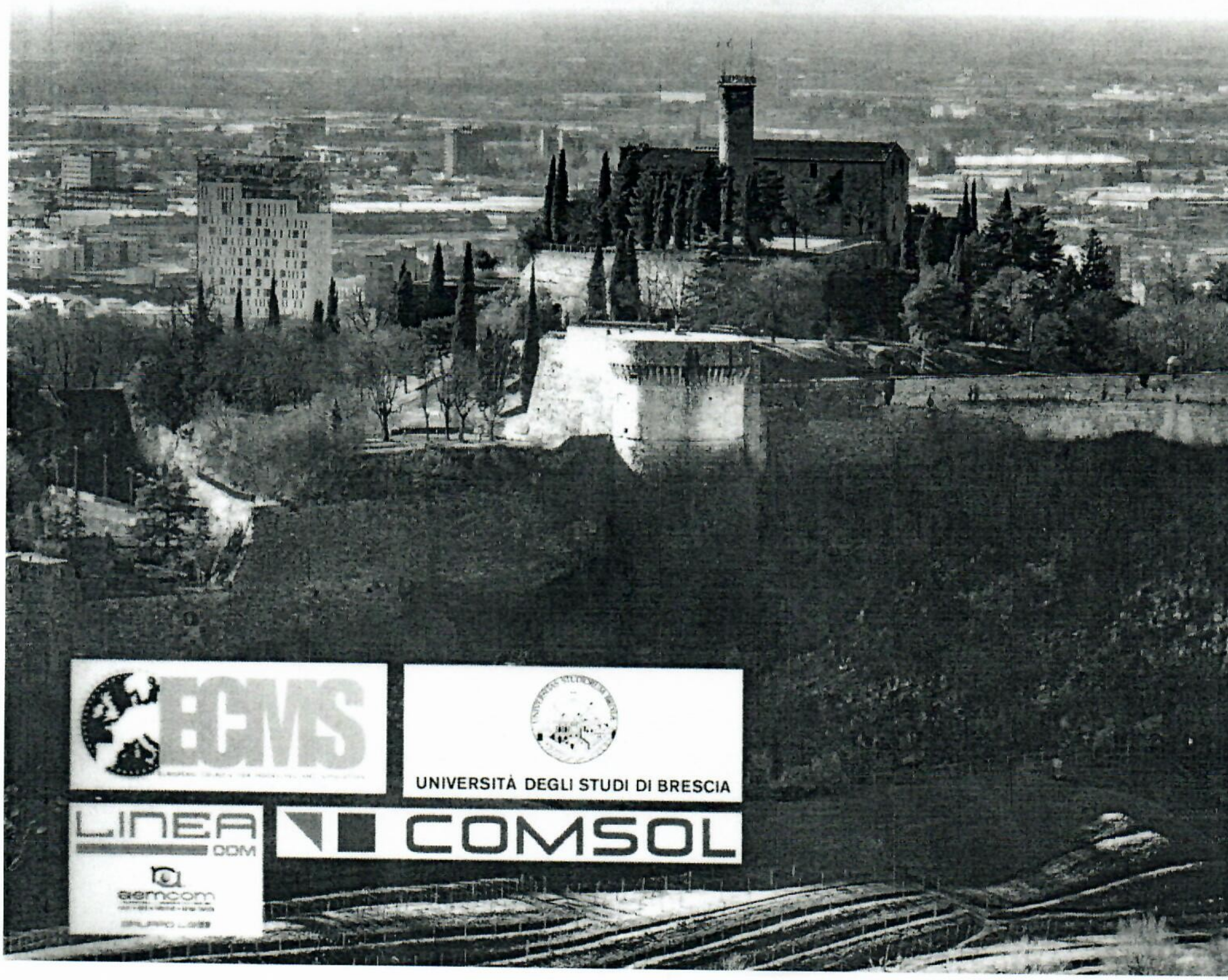

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Electrical and Electromechanical Engineering

MODELING AND CONTROL OF BERRY PHASE IN QUANTUM DOTS

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KEYWORDS

Semiconductor quantum dots, Finite Element Method (FEM), Berry phase, spin-orbit coupling, quantum mechanical transport.

ABSTRACT

We study numerically the Berry phase in semiconductor quantum dots (QDs) that is induced by letting the dots to move adiabatically in a closed loop in the 2D plane along the circular trajectory. We show that the Berry phase is highly sensitive to the Rashba and Dresselhaus spin-orbit lengths. Based on the Finite Element Method, we solve the Schrödinger equation and investigate the evolution of the spin dynamics during the adiabatic transport of the QDs in the 2D plane along circular trajectory. Results of numerical simulations are discussed in detail, indicating that this work might be used for the realization of solid state quantum information processing.

INTRODUCTION

Manipulating the single electron spins in QDs through the non-Abelean geometric phases has attracted considerable attention since the pioneering work of Berry (Aleiner & Fal'ko 2001, Wang & Zhu 2008, Yang & Hwang 2006, Eric Yang 2006, Yang 2007, Berry 1984). For a system of degenerate quantum states, Wilczek and Zee showed that the geometric phase factor is replaced by a non-Abelian time dependent unitary operator acting on the initial states within the subspace of degeneracy (Wilczek & Zee 1984, Prabhakar et al. 2010). Since then the geometric phase has been measured experimentally for a variety of systems such as quantum states driven by a microwave field (Pechal et al. 2012) and qubits with tilted magnetic fields (Berger et al. 2012, Leek et al. 2007). Manipulation of the spin qubits through the Berry phase implies that the injected data can be read out with different phase that can be topologically protected from the outside world (Das Sarma et al. 2005, Hu & Das Sarma 2000, Loss et al. 1990, Tserkovnyak & Loss 2011, San-Jose et al. 2008). Several recent reviews of the Berry phase have been presented in Refs. (Xiao et al. 2010, Nayak et al. 2008). One of the promising research proposals for building a solid state topological quantum computer is that the accumulated Berry phase in QD system can be manipulated with the interplay between the Rashba-Dresselhaus spin-orbit couplings (San-Jose et al. 2008, Aleiner & Fal'ko 2001). The Rashba spin-orbit coupling arises from the asymmetric triangular quantum well along the growth direction and the Dresselhaus spin-orbit coupling arises due to bulk inversion asymmetry in the crystal lattice (Bychkov & Rashba 1984, Dresselhaus 1955). A recent work by Bason et al. shows that the Berry phase can be measured for a two level quantum system in a superadiabatic basis comprising the Bose-Einstein condensates in optical lattices (Bason et al. 2012).

The geometric phase induced on the wavefunctions of quantum states during the adiabatic movement of the physical system plays an important role in numerous quantum computing and quantum information processing. When the state vector of a quantum system undergoes in a cyclic evolution and returns in its initial physical state then its wave function can acquire a geometric phase factor in addition to the familiar dynamic phase (Berry 1984, Prabhakar et al. 2010, Wang & Zhu 2008). If the cyclic change of the system is adiabatic then after one complete rotation of the physical system acquire an additional phase factor which is known as Berry phase (Berry 1984). Recently, it has also been shown that the geometric phase can be induced on the electron spin states in QDs by moving the dots adiabatically in a closed loop in the 2D plane with the application of gate controlled electric field (Prabhakar et al. 2010, San-Jose et al. 2008). Furthermore, the authors in Refs (Bednarek et al. 2012, 2008, Bednarek & Szafran 2008) have recently proposed to build a QD device in the absence of the magnetic fields that can perform the quantum gate operations (NOT gate, Hadamard gate and Phase gate) with the application of the externally applied gate potential modulated by a sinusoidal varying potential. All these problems can be studied efficiently with the tools of mathematical medeling, once an adequate physical model is constructed. In this paper, we focus on modeling of transport of the electron spin states in QDs in presence of the externally applied magnetic fields along z-direction in a closed loop in the 2D plane with the application of time dependent distortion potential. Based on our model, we investigate the interplay between the Rashba and the Dreeselhaus spin-orbit lengths on the scalar Berry phase (Yang & Hwang 2006, Wu et al. 2011). The transport of the dots is carried out very slowly so that the adiabatic theorem can be applied on the evolution of the spin dynamics. We show that the Berry phase in QDs can be engineered and can be manipulated with the application of the spin-orbit couplings through gate controlled electric fields. We solve the time dependent Schrödinger equation and investigate the evolution of spin dynamics in QDs. Details of the corresponding mathematical model and computational methodology are provided.

MATHEMATICAL MODEL

The model construction starts from the two band Kane Hamiltonian of an electron in QDs in the plane of a 2 Dimensional Electron Gas (2DEG) in the presence of an external

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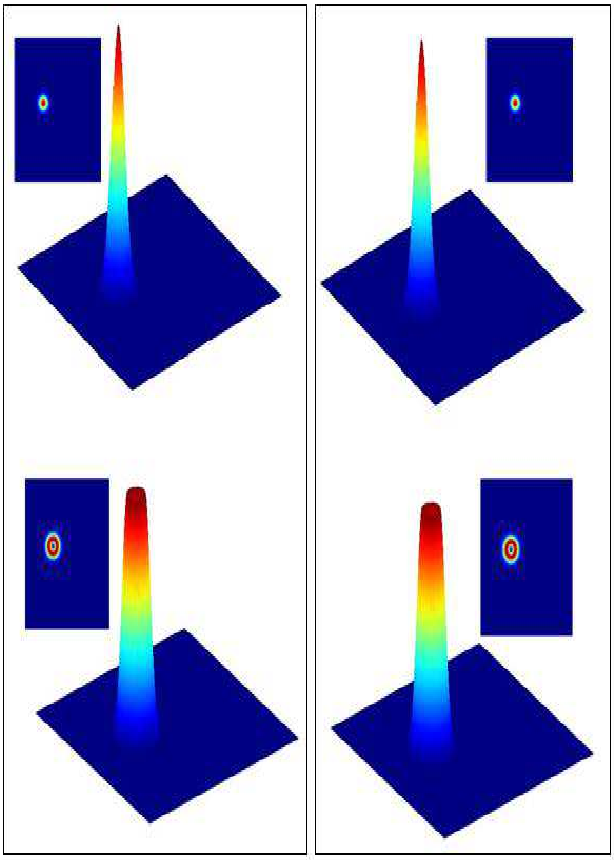

Fig. 1. Modeling results for four lowest states of the wavefunction squared in GaAs quantum dots. Here we chose $B = 1T$ and $E_0 = 5x10^3\ V/cm$. Note that the spin split wavefunctions shown in the left and right columns look identical. However, their energy eigenvalues are different which can be used for the design of quantum dots with different g-factors and Berry phases (see Figs. 2 and 5).

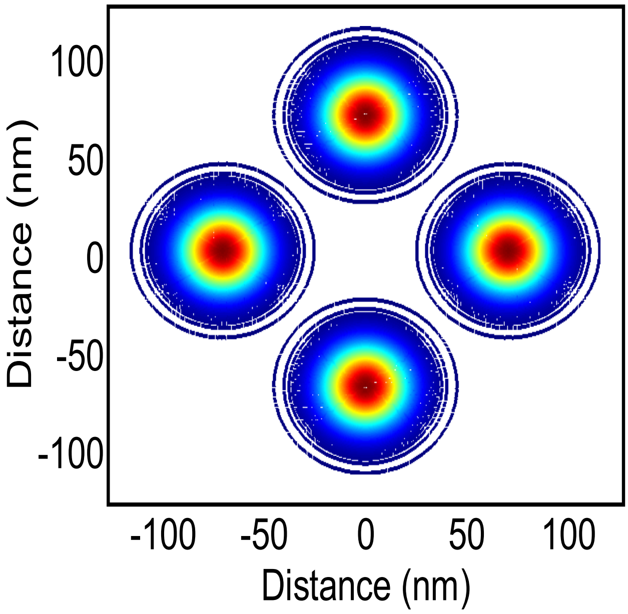

Fig. 3. Contour plots of the realistic electron wave function of GaAs QDs that are adiabatically transported along the circular trajectory under the influence of externally applied time dependent gate potential. We choose the amplitude $f_0 = 5\times10^3$ V/cm, electric field $E = 10^5$ V/cm, $B = 1$T and QD radius $\ell_0 = 20\ nm$.

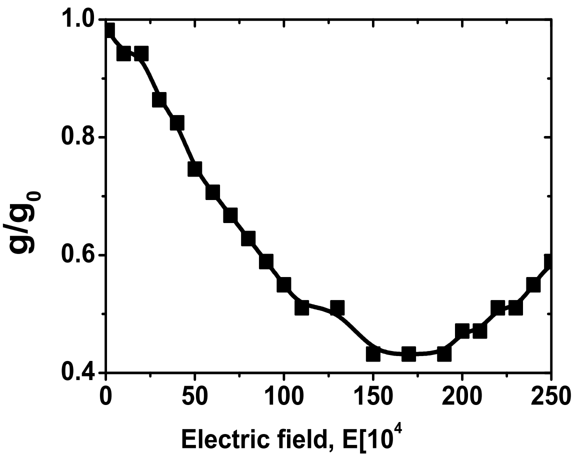

Fig. 2. g-factor (absolute value) vs applied electric fields with no time dependent distortion potential. We chose $g_0 = -0.44$, $m = 0.067$, $\gamma_R = -0.044$ nm^2 and $\gamma_D = -0.0026$ eV. nm^3.

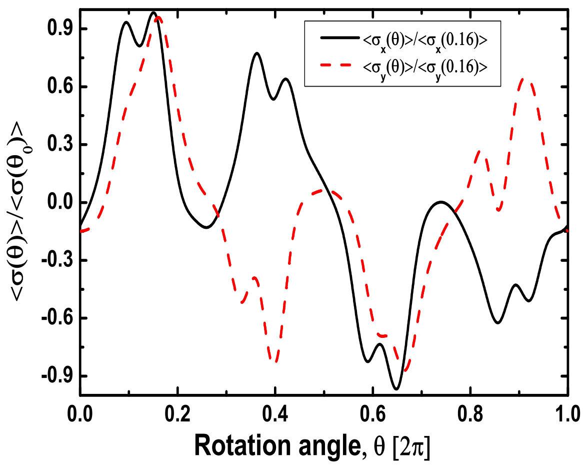

Fig. 4. Evolution of spin dynamics during the adiabatic transport of the GaAs quantum dots. We chose $E = 5\times10^5\ V/cm$ and the rest of the parameters are chosen the same as in Fig. 3.

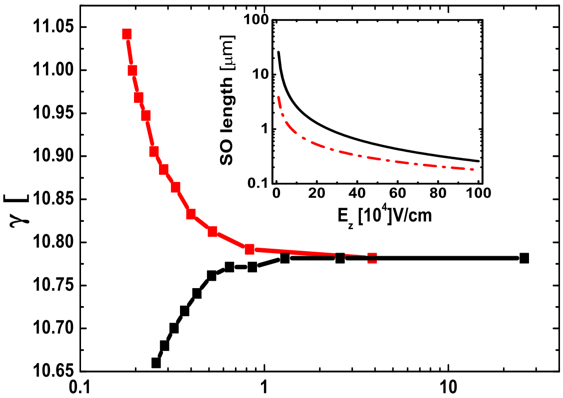

Fig. 5. Berry phase vs SO lengths on spin state $|0,0,+1\rangle$. Here we chose $\ell_0 = 20$ nm, $B = 1$ T and total enclosed adiabatic area is considered as $\pi d^2/4 = 7.85 \times 10^{-7}\text{eV}^2/\text{nm}^2$.

magnetic field B, along the z-direction in III-V semiconductor QDs can be written as (Prabhakar & Raynolds 2009, Prabhakar et al. 2011)

$$H = H_{xy} + H_R + H_D, \tag{1}$$

where the Hamiltonians H_R and H_D are associated with the Rashba and the Dresselhaus spin-orbit couplings and H_{xy} is the Hamiltonian of the electron along the lateral direction in the plane of the 2DEG. H_{xy} can be written as

$$H_{xy} = \frac{\vec{P}^2}{2m} + \frac{1}{2}m\omega_o^2(x^2+y^2) + f(t) + \frac{\hbar}{2}\omega_z\sigma_z, \tag{2}$$

where $\vec{P} = \vec{p} + e\vec{A}$ is the kinetic momentum operator, $\vec{p} = -i\hbar(\partial_x, \partial_y, 0)$ is the canonical momentum operator and $\vec{A}$ is the vector potential in the symmetric gauge, $\omega_z = g_0\mu_B B/\hbar$ is the Zeeman frequency and g_0 is the bulk g-factor. Here, $-e < 0$ is the electronic charge, m is the effective mass of the electron in the conduction band, μ_B is the Bohr magneton, σ_z is the Pauli spin matrix along z-direction. Also, $\omega_0 = \frac{\hbar}{m\ell_0^2}$ is a parameter characterizing the strength of the confining potential and ℓ_0 is the radius of the QD. The time dependent function $f(t)$ is the distortion potential that can be used to let the dot to move adiabatically in a closed loop in the 2D plane without disturbing the spin splitting energy difference. We use the functional form of $f(t)$ in our theoretical model as (Yang & Hwang 2006)

$$f(t) = eF_x(t)x + eF_y(t)y, \tag{3}$$

where $F_x = f_0\cos(\omega t)$, $F_y = f_0\sin(\omega t)$, f_0 is the amplitude and ωt varies from 0 to 2π.

The Hamiltonians associated with the Rashba-Dresselhaus spin-orbit couplings can be written as (Bychkov & Rashba 1984, Dresselhaus 1955)

$$H_R = \frac{\alpha_R}{\hbar}\left(\sigma_x P_y - \sigma_y P_x\right), \tag{4}$$

$$H_D = \frac{\alpha_D}{\hbar}\left(-\sigma_x P_x + \sigma_y P_y\right). \tag{5}$$

The strength of the Rashba-Dresselhaus spin-orbit couplings is characterized by the parameters α_R and α_D which are given by

$$\alpha_R = \gamma_R eE, \qquad \alpha_D = 0.78\gamma_D\left(\frac{2me}{\hbar^2}\right)^{2/3} E^{2/3}. \tag{6}$$

Finally we write the two coupled Schrödinger equations as:

$$-i\hbar\partial_t\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} h_{11}+\frac{\Delta}{2} & h_{12} \\ h_{21} & h_{22}-\frac{\Delta}{2} \end{pmatrix}\begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, \tag{7}$$

where $\Delta = g_0\mu_B B/2$ and

$$\begin{aligned} h_{11} &= -\frac{\hbar^2}{2m}\left(\partial_x^2+\partial_y^2\right) + \frac{1}{2}m\Omega^2\left(x^2+y^2\right) + f(t) \\ &\quad -\frac{i\hbar\omega_c}{2}\left(y\partial_x - x\partial_y\right), \end{aligned} \tag{8}$$

$$h_{12} = \hbar\alpha_R\left(\partial_x - i\partial_y\right) + \hbar\alpha_D\left(i\partial_x - \partial_y\right). \tag{9}$$

Also, $h_{11} = h_{22}$ and $h_{21} =$ hermitian conjugate of (h_{12}). Finally we define the g-factor of electron in quantum dots by the expression

$$g = \frac{\varepsilon_1 - \varepsilon_2}{\mu_B B}, \tag{10}$$

where ε_1 and ε_2 are the ground and first excited states eigenvalues of the corresponding two coupled Schrödinger equations (7). In principle, one can design GaAs/AlGaAs quantum dots and vary the g-factor of the dots by letting the wavefunction of electrons to penetrate from one material (GaAs) into the other material (AlGaAs) (Prabhakar & Raynolds 2009).

We now turn to the calculation of the Berry phase in QDs. According to works of Berry, if parameters contained in the Hamiltonian of a quantal system are adiabatically carried around a closed loop, an extra geometric phase (Berry phase) is induced in addition to the familiar dynamical phase (Berry 1984, Prabhakar et al. 2010). A slow variation of such parameters along a closed path C will return the system to its original energy eigenstate with an additional phase factor $\exp\{i\gamma_n(C)\}$. More specifically, the state acquires phases after a period of the cycle T as

$$|\Psi_n(T)\rangle = \exp\left\{-\frac{i}{\hbar}\int_0^T \varepsilon_n(t)\,dt\right\}\cdot\exp\left\{i\gamma_n(C)\right\}|\psi_n\rangle, \tag{11}$$

where the coefficients $\gamma_n(C)$ can be written as

$$\begin{aligned} \gamma_n(C) &= -Im\oint_C d\mathbf{s}\cdot\sum_{m\neq n} \\ &\quad \frac{<n|\nabla_R\hat{H}(\mathbf{R})|m> \times <m|\nabla_R\hat{H}(\mathbf{R})|n>}{\left(\varepsilon_m(\mathbf{R}) - \varepsilon_n(\mathbf{R})\right)^2}, \end{aligned} \tag{12}$$

where $\mathbf{R} = (F_x(t), F_y(t))$ and $d\mathbf{s}$ is the total area enclosed by the dots in one complete adiabatic rotation in the 2D plane at the heterojunction. Here ε_m and ε_n correspond to the eigenvalues of (7) associated to the quantum states $|m\rangle$ and $|n\rangle$.

COMPUTATIONAL METHOD

We suppose that a QD is formed in the plane of a two dimensional electron gas of 400×400 nm^2 geometry. The in-plane oscillating fields $F_x(t)$ and $F_y(t)$ is varied in such a way that the QD is transported in a closed loop of circular trajectory (see Fig. 3). To find the Berry phase by an explicit numerical method, we diagonalize the total Hamiltonian $H(t)$ at any fixed time using the Finite Element Method. In particular, We utilize the UMFPACK solver in the COMSOL multiphysics package (n.d.) to find the eigenvalues and eigenfunctions of the two coupled eigenvalue partial differential equation (7). The geometry contains 24910 elements. Since the geometry is much larger compared to the actual lateral size of the QD, we impose Dirichlet boundary conditions. Error vs iteration number shows the convergence of simulations is good.

RESULTS AND DISCUSSIONS

In Fig. 1, we have plotted the modeling results of ground and first excited states wavefunctions squared of GaAs quantum dots with no magnetic and no time dependent distortion potential. In Fig. 3, we use the distortion potential ($f(t)$) as a time dependent function and allow the dot to move adiabatically in a closed loop in the 2D plane. Realistic electron wavefunctions of the dots at different locations ($\theta = 0, \pi/2, \pi, 3\pi/2$) in the 2D plane are shown.

Based on FEM (n.d.), we solved the two coupled time dependent Schrödinger equations (7) with the initial condition $H(x,y,0)\psi(x,y,0) = \varepsilon\psi(x,y,0)$ in the fixed time interval $\theta = [0 : 0.1 : 2\pi]$. The adiabatic theorem guarantees that $\psi_\theta^{'}(x,y,\theta) = 0$. We plotted the evolution of the spin dynamics during the adiabatic movement of the QDs in the 2D plane in Fig. 4. Even in the presence of Zeeman energy, where the magnetic field is applied along z-direction, the spin components in the ground state of the QDs are not well defined due to the presence of spin-orbit couplings (Bednarek et al. 2008, Bednarek & Szafran 2008). It means, $<\sigma_z>$ is either 1 or -1 depending on the g-factor of electron in QDs and the components of $\sigma_i (i = x,y)$ varies during the adiabatic movement of the QDs in the 2D plane. Fluctuations in $<\sigma_z>$ can be made at degenerate sublevels where g-factor exactly vanishes. In this case, rather than finding a scalar Berry phase, one needs to find the matrix Berry phase acting on the initial states within the subspace of degeneracy. (Prabhakar et al. 2010) Since the motivation of the paper is to investigate the influence of electric field on the scalar Berry phase, we choose the parameters in Fig. 4 in such a way that the g-factor is negative and $<\sigma_z>= +1$ (Prabhakar & Raynolds 2009). For g-factor control in quantum dots, see Refs. (Prabhakar & Raynolds 2009, Prabhakar et al. 2011). If one choses $\ell_0 = 40$ nm, it can be found that the g-factor is positive and $<\sigma_z>= -1$. Depending on the choice of the parameters, one can construct the quantum gates (Hadmard, OR, Controlled NOT gates) with the application of the gate controlled electric fields (Bednarek et al. 2012). For example, when all the spin components are equal to unity, one can have Hadmard gates. Since spin components decay with different phase (see Fig. 4) but they all vanishes at certain degree of orientation in the Bloch sphere, one can find the controlled NOT gates. (Bednarek et al. 2008, Bednarek & Szafran 2008) Also, the transport of the QDs are carried out adiabatically, one can find the similar type of evolution of the spin dynamics (Fig. 4) in each cycle of rotation which is another efficient way to construct the quantum gates from QDs. Since the periodicity of the propagating waves is different for the pure Rashba and for the pure Dresselhaus case, we see the superposition effect in the x- and y-components of the electron spin in QDs (see Fig. 4).

We now turn to the results associated to the Berry phase that is accumulated during the adiabatic transport of the dots in the 2D plane.

In Fig. 5, we plot the characteristics of the Berry phase vs spin-orbit coupling length. As can be seen, the Berry phase for the pure Rashba and pure Dresselhaus cases are well separated at smaller values of the SO lengths due to the presence of the Rashba case and the Dresselhaus spin-orbit coupling case. At large values of spin-orbit lengths $\lambda_R = \lambda > 1.8\mu m$, the Berry phases for the pure Rashba and for the pure Dresselhaus spin-orbit coupling cases meet each other because extremely weak spin-orbit coupling coefficients are unable to break the in-plane rotational symmetry. Note that the spin-orbit length is characterized by the applied electric field along the z-dicrection (see inset plot in Fig. 5) (Prabhakar et al. 2013).

CONCLUSIONS

To conclude, based on the developed mathematical model, we have analyzed the wavefunctions of electrons in QDs during the adiabatic movement of the dots along the circular trajectory. By using the Finite Element Method, we have calculated the evolution of the spin dynamics and shown that the superposition effect can be observed during the adiabatic movement of the QDs in the 2D plane. We have shown that the Berry phase for the pure Rashba and pure Dresselhaus cases are well separated at smaller values of the SO lengths due to the presence of large Rashba-Dresselhaus spin-orbit coupling coefficients.

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