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Computational Models for the Berry Phase in Semiconductor Quantum Dots

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Abstract. By developing a new model and its finite element implementation, we analyze the Berry phase low-dimensional semiconductor nanostructures, focusing on quantum dots (QDs). In particular, 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. Based on this study, we reveal that the Berry phase is highly sensitive to the Rashba and Dresselhaus spin-orbit lengths.

Keywords: Spin-Orbit Coupling, Semiconductor Quantum Dots, Finite Element Method, Berry Phase, spin-orbit coupling, Quantum Mechanical Transport
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INTRODUCTION

The geometric phase, known also as the Berry phase, is induced on the wavefunctions of quantum states during the adiabatic movement of a physical system. It plays an important role in many applications, including quantum computing and quantum information processing. The nature of this phase can be explained as follows. 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 such a geometric phase factor in addition to the conventional dynamic phase [1]. Furthermore, if the cyclic change of the system is adiabatic, then after one complete rotation of the physical system it acquires an additional phase factor, the Berry phase.

It is also known 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. This research has been carried our in both theoretical and practical dimensions. Indeed, there are proposals (e.g., [2]) to build a QD device in the absence of the magnetic field 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.

The above problems can be studied efficiently with the tools of mathematical medeling, once an adequate physical model is constructed. Here, based on the developed model, we demonstrate how the interplay between the Rashba and the Dresselhaus spin-orbit lengths on the scalar Berry phase [3] can be analyzed. It is assumed that 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. From a physics point of view, our model covers the situation where 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. This model is based on the time dependent Schrödinger equation and is not amenable to analytical solution. In order to investigate the evolution of spin dynamics in QDs, we solve it numerically, by using the finite element method. In the following sections we highlight the main details of our mathematical model, along with computational methodology, followed by a discussion of results and conclusions.

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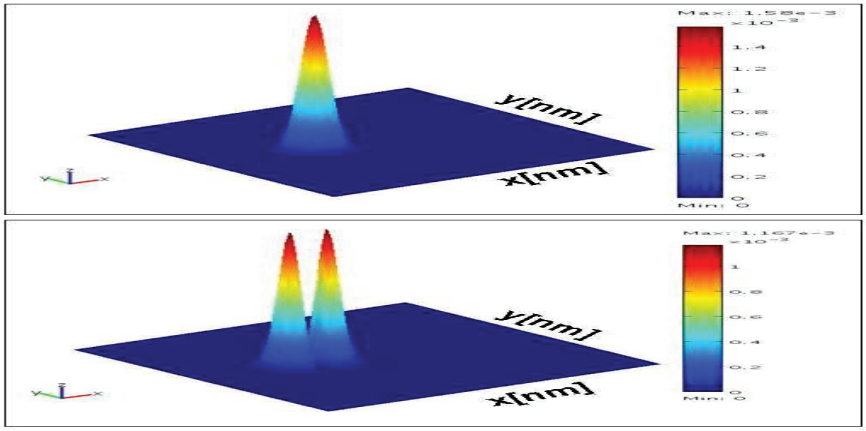

FIGURE 1. Modeling results of degenerate ground and first excited states wavefunction squared of GaAs quantum dots with no magnetic fields and no spin-orbit coupling. Here we chose $\theta = 0$ and $f_0 = 5 \times 10^3$ V/cm and $\ell_0 = 20$ nm and $m = 0.067$. Note that, by considering $\theta = 0$ and $f_0 = 5 \times 10^3$, the center of the QD shifts from $(x_0, y_0) = (0,0)$ to $(x_0, y_0) = (-70\text{ nm}, 0)$. As we vary $\theta = 0$ to 2π, the center of the QDs is transported along the circular trajectory.

THEORETICAL MODEL

The development of the mathematical model for the Berry phase analysis, we begin from the two band Kane Hamiltonian of an electron in a QD. Such a III-V semiconductor QD is located in the plane of a 2 Dimensional Electron Gas (2DEG) in the presence of external magnetic field B along the z-direction. In this case the Hamiltonia can be written as [4]

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

where the two parts of the Hamiltonian, H_R and H_D, are associated with the Rashba and the Dresselhaus spin-orbit couplings, respectively, and H_{xy} is the part of the Hamiltonian of the electron along the lateral direction in the plane of the 2DEG. We note that 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. Function $f(t) = eF_x(t) + eF_y(t)$ is the distortion potential, allowing the dot to move adiabatically in a closed loop in the 2D plane with no spin splitting energy difference disturbing, where $F_x = f_0 \cos(\omega t)$, $F_y = f_0 \sin(\omega t)$ with f_0 being the amplitude and $\omega t = \theta$ varying from 0 to 2π. 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. Other notations are standard. In particular, $-e < 0$ 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.

The Hamiltonians associated with the Rashba-Dresselhaus spin-orbit couplings can be written as [5, 6]

$$H_R = \frac{\alpha_R}{\hbar} (\sigma_x P_y - \sigma_y P_x), \tag{3}$$

$$H_D = \frac{\alpha_D}{\hbar} (-\sigma_x P_x + \sigma_y P_y). \tag{4}$$

Given the distortion potential, $f(t) = eF_x(t)x + eF_y(t)y$, as a time dependent function, the model is reduced to the two corresponding coupled Schrödinger equations which we solve by the finite element methodology.

Regarding the calculation of the Berry phase, we note that the state acquires phases after a period of the cycle T as

$$|\Psi_n(T)\rangle = \exp\left\{-\frac{i}{\hbar}\int_0^T \varepsilon_n(t)\,dt\right\} \cdot \exp\{i\gamma_n(C)\}\,|\psi_n\rangle, \tag{5}$$

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

$$\gamma_n(C) = -Im \oint_C d\mathbf{s} \cdot \sum_{m \neq n} \frac{< n|\nabla_R \hat{H}(\mathbf{R})|m > \times < m|\nabla_R \hat{H}(\mathbf{R})|n >}{(\varepsilon_m(\mathbf{R}) - \varepsilon_n(\mathbf{R}))^2}. \quad (6)$$

Here $\mathbf{R} = (F_x(t), F_y(t))$ and $d\mathbf{s}$ is the total area enclosed by the dots in one complete adiabatic rotation in the 2D plane at the heterojunction.

COMPUTATIONAL METHOD

Our basic premises here are that a QD is formed in the plane of a two dimensional electron gas of 200×200 nm^2 square geometry. The in-plane oscillating fields $F_x(t)$ and $F_y(t)$ are varied in such a way that the QD is transported in a closed loop of circular trajectory. 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 by finding the eigenvalues and eigenfunctions of the two coupled eigenvalue partial differential equations. This is done by using the UMFPACK solver. Since the geometry is much larger compared to the actual lateral size of the QD (computations have also been done for 400×400 nm^2), we impose Dirichlet boundary conditions. Computations have been carried out on a sequence of embedded grids, ensuring convergence.

RESULTS AND DISCUSSIONS

As a representative example, we provide details on the ground and first excited states wavefunctions squared of GaAs quantum dots with no magnetic and no spin-orbit coupling. The distortion potential ($f(t)$) allows the dot to be moved adiabatically in a closed loop in the 2D plane, in a way analogous to that described in [7]. Among important characteristics, electron wavefunctions of the dot at different locations ($\theta = 0, \pi/2, \pi, 3\pi/2$) in the 2D plane have been calculated. The actual values used for the distortion potential and other details are given in the caption to Fig. 1.

Our analysis has revealed that the Berry phase for the pure Rashba and pure Dresselhaus cases are well separated at smaller values of spin-orbit lengths due to the presence of the Rashba case and the Dresselhaus case. At large values of spin-orbit lengths, 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.

CONCLUSIONS

We have shown that the Berry phase for the pure Rashba and pure Dresselhaus cases are well separated at smaller values of the spin-orbit lengths due to the presence of large Rashba-Dresselhaus spin-orbit coupling coefficients. This has been done on the basis of the developed mathematical model, amenable to the finite element analysis of wavefunctions of electrons in QDs during the adiabatic movement of the dots along the circular trajectory.

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