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Spin–spin and spin–orbit interaction effects of two-electron quantum dots

B. Vaseghi [a,*], G. Rezaei [a], S.F. Taghizadeh [a], Z. Shahedi [b]

[a] Department of Physics, College of Sciences, Yasouj University, Yasouj 75914-353, Iran
[b] Department of Physics, Payame Noor University, Shiraz, Iran

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ABSTRACT

Simultaneous effects of spin–spin and spin–orbit interactions on the energy spectrum of a two-electron spherical quantum dot with parabolic confinement and under the influence of external electric and magnetic fields are investigated. We have calculated energy eigenvalues and eigenvectors of the system for different spin states. Results show that effects of spin–spin interactions are negligible in comparison with those of the spin–orbit interactions. Spin–orbit interaction splits energy levels and removes degeneracy of different spin states. Moreover it is seen that energy eigenvalues and levels splitting strongly depend on the external magnetic field and the dot dimensions.

1. Introduction

Spintronics has attracted great interest in the scientific community recently [1,2]. This growing field refers to the study of the role played by electron's spin in the solid state physics, and possible devices that specifically exploit spin properties instead of or in addition to charge degrees of freedom. For example, spin relaxation and spin transport in metals and semiconductors are of fundamental research interest not only for being basic solid state physics issues, but also for the already demonstrated potential that these phenomena have in electronic technology [3–5].

In addition, the ability to create and manipulate charge and spin populations in low-dimensional quantum systems by tailoring the structural and electronic environment of localized electrons generates a wide class of applications such as spin-field effect transistor that uses the spin–orbit interaction (SOI) of electrons in a two-dimensional electron gas (2DEG) [6] spin interference devices [7,8], and a non-magnetic spin filter using a resonant tunneling structure [9].

For most experimental and theoretical realizations and studies, QDs can be described as an effective two-dimensional systems in a confining potential which is usually modeled as hard-wall or parabolic confinement [10–13]. Rashba SOI in these structures rises from the structure inversion asymmetry and is one of the most important phenomena realizing spin properties [14–16]. This phenomena has considerable effects on the electrical and optical properties of QDs and can be used as a mechanisms to control these properties via external gates and fields [17–22].

To our knowledge the most existing theoretical studies of SOI effects in such systems rely on the single electron schemes and without spin–spin (SS) interactions. In a more realistic model one may use a two-electron system in which the interactions between the spins can be considered either [23]. To this aim in the current work electronic structure of a two-electron parabolic QD under the influence of external magnetic field is studied. In comparison with the single electron systems, different states from the addition of spin angular momentums appear here and we have investigated combined effects of SS interaction, SOI, external magnetic field and confinement potential on the energy eigenvalues and functions of the system. It is shown that energies strongly depend on the SOI but, SS interaction effects are very weak and ignorable. Moreover, SOI removes the degeneracy of the states and shifts their energies proportional to the magnetic field and SOI strengths.

2. Model

Within the framework of effective mass approximation the Hamiltonian of a system consisting of two electrons, inside a spherical QD with parabolic confinement, can be written as

$$H = H_1 + H_{ss} + H_{so}, \tag{1}$$

in which H_{ss} and H_{so} are SS and SOI Hamiltonians, respectively, and H_1 is given as follows:

$$H_1 = H_0 + H_c + H_z, \tag{2}$$

* Corresponding author. Tel./fax: +98 741 222 3048.
E-mail address: vaseghi@mail.yu.ac.ir (B. Vaseghi).

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with

$$H_0 = \sum_{j=1,2} \frac{1}{2m^*}(\vec{P} + e\vec{A})_j^2 + \frac{1}{2}m^*\omega_0^2\rho_j^2 + \frac{1}{2}m^*\omega_z^2 z_j^2, \quad (3)$$

$$H_c = \frac{e^2}{4\pi\varepsilon|\vec{\rho}_1 - \vec{\rho}_2|}, \quad (4)$$

$$H_z = \sum_{j=1,2} g\mu_B \vec{B}.\vec{S}_j, \quad (5)$$

where P is the momentum operator, ρ_j and z_j are the electron positions in the cylindrical coordinate, $\vec{B} = B\hat{z}$ is the magnetic field, g is the gyroscopic ratio, μ_B is the bohr magneton, m^* is the effective mass, ε is the dielectric constant, and ω_0 and ω_z are the confinement frequencies in the $x-y$ plane and along the z-direction, respectively. Also, for this structure it is assumed that the confinement along the z-axis is much greater than that of in plane direction.

Energy eigenvalues and functions of the single-electron system are given by [24]

$$\varphi(\rho_j,\theta_j)\chi(\sigma_j) = C_{nm}\xi_j^{|m|}e^{-\xi_j^2/2}e^{im\theta_j}L_n^{|m|}(\xi_j^2)\chi(\sigma_j), \quad (6)$$

with $C_{nm} = \sqrt{n!/\pi L_B^2(n+|m|)!}$, $L_n^{|m|}$ is the Laguerre polynomial, $\xi_j = \rho_j/L_B$ is a scaled radius with $L_B = \sqrt{\hbar/(m^*\Omega)}$, $n(m)$ is the principal (azimuthal) quantum number, and $\chi(\sigma)$ is the electron spinor [24]. The corresponding eigenvalues of H_1 are

$$E = (2n+|m|+1)\hbar\Omega - \frac{m}{2}\hbar\omega_c + \frac{\sigma}{2}g\mu_B B, \quad (7)$$

where $\Omega = (\omega_0^2 + \omega_c^2/4)^{1/2}$, $\omega_c = eB/m^*$ is the cyclotron frequency and $\sigma = \pm 1$ denote spin up and down orientations, respectively.

In addition to the confinement effects and external factors that modify the electronic structure of QDs, in a more realistic model which consists of two electrons their spin interaction plays a crucial role on the electronic properties of these structures. In the current work since the system consists of two electrons, two interaction models which originate from the electron's spin are considered. The first type is the spin–spin interaction of the two electrons with the spin magnetic dipoles μ_1 and μ_2 and relative distance ρ in the form of [25]

$$H_{ss} = \frac{1}{\rho^3}\left[\mu_1\cdot\mu_2 - \frac{3(\mu_1\cdot\rho)(\mu_2\cdot\rho)}{\rho^2}\right], \quad (8)$$

and the other one is the Rashba SOI Hamiltonian [16,18]

$$H_{SO} = \frac{\alpha}{\hbar}\sum_{j=1,2}\left[\vec{\sigma}_j \times \left(\vec{P} + \frac{e}{c}\vec{A}\right)_j\right]\hat{n}, \quad (9)$$

where $\vec{P}$ is the momentum operator, α is the strength of spin–orbit interaction, $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ denotes the Pauli spin matrices, $\hat{n}$ is normal to the surface and $\vec{A} = (-By/2, Bx/2, 0)$, is the vector potential in the symmetry gauge. Expanding Eq. (9) in the cylindrical coordinate gives

$$H_{so} = \frac{\alpha}{\hbar}\sum_{j=1,2}\left[\frac{1}{\rho_j}\frac{\partial}{\partial\varphi_j} + \frac{eB}{2c}\rho_j\right]\sigma_{jz}, \quad (10)$$

where we have considered that $\hat{n} = \hat{\rho}$ and spins along the z-direction. Since this systems consists of two electrons, its wave function has to be antisymmetric. So either the spatial part is antisymmetric or the spin part is symmetric

$$\psi(\vec{r}_1, \vec{S}_1; \vec{r}_2, \vec{S}_2) = \frac{1}{\sqrt{2}}[\varphi_1(\rho_1,\theta_1)\varphi_2(\rho_2,\theta_2) - \varphi_1(\rho_2,\theta_2)\varphi_2(\rho_1,\theta_1)]\chi_{triplet}, \quad (11)$$

or the spatial part is symmetric and the spin part is antisymmetric

$$\psi(\vec{r}_1, \vec{S}_1; \vec{r}_2, \vec{S}_2) = \frac{1}{\sqrt{2}}[\varphi_1(\rho_1,\theta_1)\varphi_2(\rho_2,\theta_2) + \varphi_1(\rho_2,\theta_2) \times \varphi_2(\rho_1,\theta_1)]\chi_{Singlet}, \quad (12)$$

where $\chi_{triplet}$ and $\chi_{singlet}$ are two-electrons spin states. To find the energy eigenvalues and functions of the system, matrix representation of total Hamiltonian, H, is calculated and diagonalized numerically in the basis set that are presented in Eqs. (6), (11) and (12) with different values of n and m corresponding to different energy states of the unperturbed Hamiltonian, H_1.

3. Results and discussions

To investigate the effects of SS and SOI on the energy spectrum and its variations with external factors, we have calculated numerically energy eigenfunctions and eigenvalues of a two-electron spherical QD in this section. We do our calculations for a typical GaAs QD with $m^* = 0.067m_0$ (m_0 is the free electron mass), $\epsilon = 13.18\epsilon_0$ (ϵ_0 is the susceptibility of vacuum) and $\mu = (eB/m^*)\vec{S}$. In all figures the states represented by $\uparrow\uparrow, \downarrow\downarrow$ and one of the $\uparrow\downarrow$ are related to the triplet states and the other $\uparrow\downarrow$ arrows shows the singlet state.

To study the effects of SS interaction on the energy spectrum of the system in Fig. 1 energy is plotted as a function of ω_0, for different spin states. Since the parabolic confinement frequency, ω_0, plays the same role as the inverse of length, it is seen that energy increases with increasing ω_0. Effects of SS interactions are negligible, whereas different spin states remain degenerate and SS interaction cannot lift the degeneracy of the states. Due to the small effects of SS interaction on the energy eigenvalues and functions of the system in the remaining part we have focused on the SOI and related phenomena only.

In Figs. 2 and 3 energies of the ground and the first excited states are plotted as a function of SOI interaction parameter, α, which is tunable via external gates or fields [16]. In the figures the middle lines are corresponding to the energies of different spin states without considering the SOI, and very small energy difference originates from the Zeeman effect. It is seen that SOI splits and shifts the energies of different spin sates whereas, energies of spin-up states , $\uparrow\uparrow$, increase and spin-down states, $\downarrow\downarrow$, decrease as α increases. Also SOI splits the states with different spin orientations,

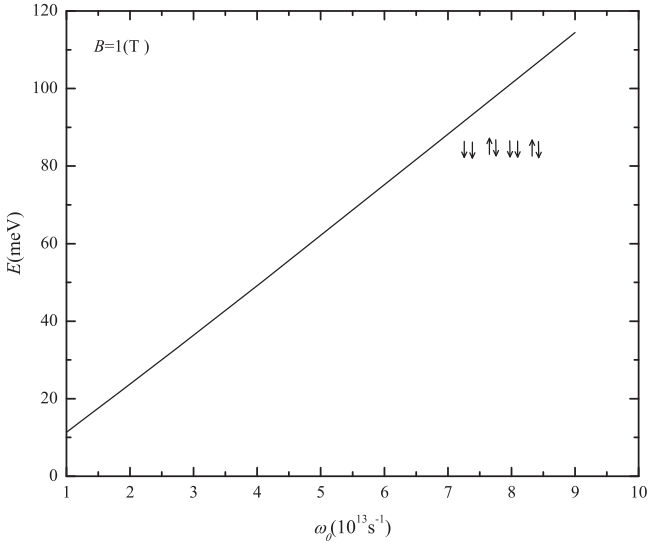

Fig. 1. Ground state energies of different spin-states as a function of ω_0 with considering the SS interaction.