Spin-orbit effects on two-electron states in nanowhisker double quantum dots

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We investigate theoretically the combined effects of the electron-electron and the Rashba spin-orbit interactions on two electrons confined in quasi-one-dimensional AlInSb-based double quantum dots. We calculate the two-electron wave functions and explore the interplay between these two interactions on the energy levels and the spin of the states. The energy spectrum as a function of an applied magnetic field shows crossings and anticrossings between triplet and singlet states, associated with level mixing induced by the spin-orbit coupling. We find that the fields at which these crossings occur can be naturally controlled by the interdot barrier width, which controls the exchange integral in the structure.

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I. INTRODUCTION

Substantial efforts have been devoted to understanding and manipulating the electron spin aiming at potential applications in semiconductor spintronics. While the spin-orbit interaction in quantum dots has been extensively studied from the single-electron perspective, its combined effects with the Coulomb interaction in few-particle systems has only recently begun to be explored. Especially in nanowhiskers, Fasth et al. measured the strength of the spin-orbit interaction in two-electron InAs cylindrical dots (diameter ∼ 50 nm, length ∼ 120 nm), and Pfund et al. studied spin relaxation in a similar system. Here we examine two-electrons in a double quantum dot system with only one transverse quantum mode active. The one-electron spectrum of this thin nanowhisker semiconductor structure has been treated by us previously as well as the phonon-mediated spin-relaxation.

In this paper we calculate and analyze in detail the two-electron states in such a system, taking into account the Rashba spin-orbit coupling and the Coulomb interaction between the electrons. We pay special attention to the degree of admixture of different two-electron spin wave-functions, which will influence the spin-flip transitions in this system.

The paper is organized as follows. In Sec. II we introduce the effective quasi-one-dimensional Hamiltonian of two interacting electrons in the presence of the Rashba interaction and describe the method and approximations used in the calculations. In Sec. III we investigate the effects of the electron-electron interaction on the energy levels with and without Rashba interaction and their dependence on an applied magnetic field. We monitor the mean value of the spin projection as a function of the structural parameter that determines the strength of the Rashba spin-orbit coupling. In Sec. IV we provide some concluding remarks.

II. THEORETICAL DESCRIPTION

We investigate the problem of two interacting electrons in a quasi-one-dimensional double quantum dot structure in the presence of the structural or Rashba spin-orbit interaction. We study two identical 30 nm wide dots, separated by an interdot barrier, 3 nm or 5 nm wide. In our calculations we consider an Al0.1In0.9Sb-InSb structure which has a potential energy depth of 100 meV. In Fig. 1 we show the confining potential in the longitudinal direction, $V_z(z)$, and the eigen-functions $u_n(z)$ of the single-particle Hamiltonian $H_0 = \frac{p_z^2}{2m} + V_z(z)$, displaced vertically according to their corresponding energy levels, $E_n$.

The nanowisker where the double dot structure is defined is assumed to be so thin (∼ 2 nm) that only the lowest transverse mode is active. As such, the effective one-dimensional Hamiltonian of two interacting electrons with Rashba interaction, in the absence of a magnetic field, can be written as

$$H = H_0 + H_{1dR} + V_{int},$$

where $H_0 = \frac{p_z^2}{2m} + V_z(z)$, $m^*$ is the conduction-band effective mass, $z_1$ and $z_2$ are the $z$-coordinates of the two electrons, and $p_{z,1}$ and $p_{z,2}$ are the $z$-components of their linear momentum. $H_{1dR}$ and $V_{int}$ are the Rashba spin-orbit coupling and the electron-electron interaction potential, respectively. The Rashba spin-orbit coupling in the quasi-one-dimensional structure considered here is given by

$$H_{1dR} = \sum_{i=1}^2 \frac{\gamma_R}{\hbar} \langle \frac{\partial V_z}{\partial x} \rangle p_{z,i}(\sigma_{x,i} - \sigma_{y,i}),$$

where $\gamma_R = 500 \, \text{Å}^2$ is the Rashba field parameter, where the mean
value is taken over the ground state $\Phi$ of the laterally-confining potential $V_z = V'_z$ ($V_z$ is assumed to be the same as $V'_z$ for simplicity). The electron-electron interaction is given by

$$V_{\text{int}}(|z_2 - z_1|) = \int dx_1 dx_2 dy_1 dy_2 \frac{e^2 \Phi(x_1)^2 \Phi(x_2)^2 \Phi(y_1)^2 \Phi(y_2)^2}{\epsilon \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}},$$

(3)

where $r_i = (x_i, y_i, z_i)$, $i = 1, 2$, are the electron positions, and $\epsilon$ is the dielectric constant of the material (16.8 for InSb). In Eq. (3) we approximate $\Phi$ by the ground state (spatial extent $\sim 2$ nm) of a harmonic oscillator potential defined over the cross section of the whisker.

As a basis set for the two-electron Hilbert space we take

$$\varphi_1 = u_1(z_1)u_1(z_2) \ket{0, 0},$$

$$\varphi_2 = \frac{1}{\sqrt{2}} (u_1(z_1)u_2(z_2) + u_2(z_1)u_1(z_2)) \ket{0, 0},$$

$$\varphi_3 = u_2(z_1)u_2(z_2) \ket{0, 0},$$

$$\varphi_4 = \frac{1}{\sqrt{2}} (u_1(z_1)u_2(z_2) - u_2(z_1)u_1(z_2)) \ket{1, 1},$$

$$\varphi_5 = \frac{1}{\sqrt{2}} (u_1(z_1)u_2(z_2) - u_2(z_1)u_1(z_2)) \ket{1, -1},$$

$$\varphi_6 = \frac{1}{\sqrt{2}} (u_1(z_1)u_2(z_2) - u_2(z_1)u_1(z_2)) \ket{1, 0}. \quad (4)$$

The two-particle spin wave functions are the usual singlet $\ket{S} = \ket{S = 0, m_S = 0}$ and triplet states $\{\ket{T^+} = \ket{1, 1}, \ket{T^0} = \ket{1, 0}, \ket{T^-} = \ket{1, -1}\}$. This truncated basis set $\{\varphi_i, i = 1, 6\}$ takes into account only the two lowest eigenstates of $H^0$, $u_1(z)$ and $u_2(z)$ (see Fig. 1). This truncated basis simplifies the analysis and presentation without leaving out essential physics. We have checked that the truncation introduces only small quantitative differences, of the order of 1 percent, in the results.

In order to solve the eigenvalue problem of the full two-electron Hamiltonian given in Eq. (1), we expand the two-electron wave functions

$$\psi_i = \sum_{j=1}^{6} a_{ij} \varphi_j,$$

(5)

where $i = 1, \ldots, 6$, and determine the coefficients $a_{ij}$ by numerical diagonalization. It is clear that the Rashba coupling mixes states with different spin wave functions, although the mixing depends strongly in structure parameters and applied magnetic field, as we will see in the next section.

![FIG. 1: The Al$_3$In$_9$Sb-InSb double-well confining potential in the longitudinal direction of the quasi-one-dimensional nanowhisker quantum dots. The single-particle eigenfunctions and energies are also shown.](image1)

![FIG. 2: (color online) Probability density of two electrons in the double quantum dot with Coulomb interaction but without Rashba coupling. $\psi_1$: ground state (GS), $\psi_{i=2, \ldots, 6}$ excited states. Notice $\psi_5$ and $\psi_6$ describe states with both electrons in the same dot, while the others can be seen more as having one electron in each dot.](image2)

III. RESULTS

We solve the eigenvalue problem of the two-electron Hamiltonian $H$ given in Eq. (1) with the goal of understanding the interplay between the electron-electron Coulomb interaction and the single-particle Rashba coupling. In order to gain some initial insight into the nature of the two-electron states, in Fig. 2 we show the probability density of the six eigenstates for the two electrons in a double-dot structure with a 3 nm barrier without Rashba coupling. As expected, in the ground state the two electrons are essentially localized in different dots,
due to their mutual Coulomb repulsion, and on “bonding” single-particle states with a non-zero amplitude in the interdot barrier region. In contrast, states $\psi_2$ to $\psi_4$ have electrons localized in each dot too, but with an “antibonding” orbital with zero amplitude in the central barrier. Notice also that the two higher energy states, $\psi_5$ and $\psi_6$, correspond to singlet states with two electrons in each dot. Furthermore, in order to fully characterize the two-electron system in what could be realistic experimental situations we introduce a magnetic field along the $z$-direction. The field is chosen small enough (and the whisker so thin) that the $x$-$y$ orbital wave functions are not perturbed significantly by it. Thus, the field contributes only a Zeeman term to the Hamiltonian:

$$H_Z = \frac{g_0 \mu_B B}{\hbar} S_z,$$

where $\mu_B$ is the Bohr magneton, $g_0$ is the Landé factor ($g_0 = -51$ for InSb), and $S_z = S_{1,z} + S_{2,z}$ is the $z$-component of the total spin operator. In Fig. 3 we plot the energy and expectation value of $S_z$, for all the two-electron eigenstates vs. the applied magnetic field without Rashba interaction, in the double dot with a 3 nm barrier.

Let us point out some basic features of the results without Rashba coupling seen in Fig. 3. First notice that since the spatial wave functions do not depend on the magnetic field and only the Zeeman energy changes with $B$, this explains the linear field dependence of the energies. At zero magnetic field, the ground state $\psi_1$ is a singlet $(|0,0\rangle$, $S_z = 0)$, but around $B \approx 2.2$ T there is a level crossing and its spin part becomes $|1,1\rangle (S_z = 1)$. This change occurs due to the competition between the Zeeman energy, on one hand, and the Coulomb interaction and $E_2 - E_1$ on the other. At the crossing, the first excited state $\psi_2$ goes, naturally, from $S_z = 1$ to $S_z = 0$. $\psi_2$, $\psi_3$ and $\psi_4$ are degenerate at $B = 0$, but having $S_z = 1, 0, -1$, respectively, their degeneracy is broken for non-zero $B$. $E_4$ and $E_5$ have a level crossing at $B \approx 6$ T, and, finally, $E_5$ and $E_6$ cross at $B > 7$ T (not shown). There are no further crossings at higher magnetic fields.

![FIG. 3: (color online) (a) Energy levels and (b) mean value of $S_z = S_{1,z} + S_{2,z}$ versus applied magnetic field for the two-electron eigenstates including Coulomb and Rashba interactions. The strength of the Rashba coupling is given by $\langle \frac{\partial V}{\partial x} \rangle = 1$ meV/Å. Barrier width: 3 nm. $|S\rangle = $ singlet state, $|T^{\pm,0}\rangle = $ triplet state.](image1)

We next include the Rashba interaction with a coupling parameter $\langle \frac{\partial V}{\partial x} \rangle = 1$ meV/Å. The results for the energy levels and mean value of $S_z$ are shown in Fig. 4. The main differences with Fig. 3 are as follows:

(i) With Rashba interaction, at $B = 0$, $\psi_2$ and $\psi_4$ are not spin eigenstates anymore, as can be seen in Fig. 4(b). However, we still label the states as if they were pure spin states, as one spin state dominates the admixture (far from the avoided crossings discussed next).

(ii) Two of the level crossings in Fig. 3 ($E_1$ with $E_2$ at $B \approx 2.2$ T, and $E_5$ with $E_6$ at $B > 7$ T) become avoided crossings here, as the pair of states involved are coupled by the Rashba interaction. The other crossing, between $E_4$ and $E_5$ at $B \approx 6$ T, is shifted slightly upward due to the effect of the Rashba interaction on each individual level, but it does not become avoided because the levels are not coupled to each other through the Rashba interaction. This lack of mixing arises from the different spatial symmetry of the states and the strong Coulomb interac-

![FIG. 4: (color online) (a) Energy levels and (b) mean value of $S_z = S_{1,z} + S_{2,z}$ versus applied magnetic field for the two-electron eigenstates including Coulomb and Rashba interactions. The strength of the Rashba coupling is given by $\langle \frac{\partial V}{\partial x} \rangle = 1$ meV/Å. Barrier width: 3 nm. $|S\rangle = $ singlet state, $|T^{\pm,0}\rangle = $ triplet state.](image2)
The symmetry under space reversal (odd vs. even) prevents the mixing of a state with double dot occupancy (singlet $|\psi_3\rangle$) and a state where each dot has one electron ($|\psi_i\rangle$), where each state has opposite space-reversal symmetry. Notice that the width of the avoided crossings is determined mainly by the strength of the spin-orbit coupling, and therefore it can be adjusted with a transverse electric field (gate voltage).

In Fig. 5 we present the energy levels and the mean value of $S_z$ as functions of the magnetic field for a structure with a 5 nm interdot barrier. Notice that, compared to the case of a 3 nm interdot barrier (Fig. 4), crossings and anti-crossings shift to lower values of the magnetic field. This happens because the wider barrier decreases the bonding-antibonding gap, the wave function overlap and the associated exchange integral that determines the singlet-triplet separation at zero field. As the $S$-$T$ gap is smaller, it is more easily overcome by the Zeeman energy. For an 8 nm barrier, the bonding-antibonding gap is only slightly over half of the value for the 3 nm barrier, and the singlet-triplet crossing occurs at a field of 1.2 T, for example.

In Fig. 6 we present the mean value of $S_z$ as a function of the Rashba parameter $\langle \partial V_x / \partial x \rangle$ for all the states at a given magnetic field $B = 0.5$ T (using a barrier width of 3 nm). In this figure, we compare two cases, (a) without and (b) with Coulomb interaction, in order to exhibit better the role of spin-orbit coupling in the spin mixing. As expected, without Rashba coupling, i.e. with $\langle \partial V_x / \partial x \rangle = 0$, the spin projection of each of these states naturally takes the exact values 1, 0, and $-1$, as seen in both Figs. 6(a) and (b). An important difference between (a) and (b) is that there is a symmetry around $S_z = 0$ when the Coulomb interaction is absent. The ground state in Fig. 6(a) (thick cyan solid line) starts with $S_z = 0$ and at a certain (typically large) value of the Rashba parameter reaches a maximum. On the other hand, in Fig. 6(b), this symmetry about the zero value is lost due to the different mixing of two-particle orbitals ($\{ |\psi_i\rangle \}$) in higher- and lower-lying states produced by the Coulomb interaction. Figure 6 includes an axis (top) in terms of the spin-orbit length $\lambda_{SO} = \hbar^2 / m^* \gamma_R \langle \partial V_x / \partial x \rangle$ which is inversely proportional to the Rashba parameter. This length parameter helps visualize the strength of the Rashba coupling in comparison to the characteristic dimensions of the structure. It is interesting to point out that spin mixing is first noticeable when $\lambda_{SO} \approx 60$ nm, the size of the two-well system.

With a 5 nm barrier width, we find that the ground state has a mean value of $S_z$ roughly equal to zero up to a Rashba constant of 2.2 meV/Å in the presence of the Coulomb interaction, unlike the case in Fig. 6 where the ground state is clearly mixed for Rashba constant beyond 1.5 meV/Å.

IV. CONCLUSIONS

In this paper, we have investigated the effects of the Coulomb electron-electron interaction on the states, energy levels, and $z$-projection of the spin of two electrons confined in a quasi-1D double-quantum-dot nanowhisker.
in the presence of Rashba spin-orbit interaction. As a function of a magnetic field in the longitudinal direction, some energy-level crossings become avoided crossings when the Rashba spin-orbit is turned on. The width of the avoided crossings can be controlled with a lateral gate voltage via the intensity of the Rashba parameter \( \langle \partial V_x \rangle \). The positions of these crossings and avoided crossings as functions of the magnetic field can be selected by changing the width of the interdot barrier. Finally, we found that the Coulomb interaction reduces the spin mixing in the ground state, as well as in the excited states, and displayed this reduction as a function of the Rashba spin-orbit length.

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