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

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ABSTRACT

We investigate theoretically the combined effects of the electron–electron and the Rashba spin–orbit interactions on two electrons confined in quasi-one-dimensional semiconductor double quantum dots. We study both InSb-based structures, which are of interest due to their strong spin–orbit coupling, and also InAs-based systems, which have been recently studied experimentally. We calculate the two-electron wave functions in the effective-mass approximation and explore the interplay between the 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.

1. Introduction

Substantial efforts have been devoted to understanding and manipulating the electron spin and its dynamics aiming at potential applications in semiconductor spintronics [1–5]. In part due to the fact that quantum bit interactions are a fundamental element in quantum computing schemes, spintronic quantum dots with more than one electron have attracted increasing attention. Numerous theoretical studies of the *electronic structure* of quantum dots (QDs) with two or more electrons in the presence of the spin–orbit interaction have appeared recently [6–21]. Also, the theory of spin relaxation of two or few electrons in QDs has attracted much interest in the last five years. As a partial bibliographical source including these two aspects of the problem of spin in QDs, we mention the up-to-date review of spin–orbit effects in QDs with one and two electrons, written from an experimentalist's point of view, given in Ref. [22].

The QDs considered in the literature are usually of the quasi-two-dimensional type, with one dimension much smaller than the other two. Motivated by the recent availability of nanorod or nanowhisker QDs, in which the carriers are confined to elongated or quasi-one-dimensional (Q1D) dot combinations, we reported in two previous publications on the electronic structure and spin relaxation of one electron with spin–orbit interactions in Q1D dots [23,24]. (See references to experimental works on nanorod dots in those two papers.) In two recent experiments related to the work we present here, Fasth et al. [25] measured the strength of the spin–orbit interaction in two-electron cylindrical dots defined inside InAs-based nanowhiskers (diameter ~50 nm, length ~120 nm), and Pfund et al. [26] studied spin relaxation in a similar system. As a necessary extension of our previous work, and motivated by the current interest in spin phenomena in few-electron structures, in this paper we calculate and analyze in detail the two-electron states in narrow nanowhisker QDs. We take into account the Rashba spin–orbit coupling and the Coulomb interaction between the electrons and work in the effective mass approximation. 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. 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. Also, we investigate the combined influence on the energy levels of the electron–electron interaction, the Rashba interaction, and an applied magnetic field (through the Zeeman energy).

This paper is organized as follows. In Section 2 we introduce the effective quasi-one-dimensional Hamiltonian of two interacting electrons in the presence of the Rashba interaction and

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describe the method used to diagonalize the Hamiltonian. In Section 3 we present the results and discussion of our calculations, and in Section 4 we provide concluding remarks.

2. 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 a system with two coupled 30 nm wide dots, separated by an interdot barrier 3 nm wide. In our calculations we consider $Al_{0.1}In_{0.9}Sb$–InSb and $Al_{0.48}In_{0.52}As$–InAs structures which have a potential energy depth of 100 and 690 meV, respectively. 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 $H^0 = (p_z^2/2m^*) + V_z(z)$, displaced vertically according to their corresponding energy levels, E_n, for the InSb structure.

The nanowhisker where the double-dot structure is defined is assumed to be so thin ($\simeq 2$ nm in the transverse direction) that only the lowest transverse mode is active. Although this is indeed a very small lateral size we can still use the effective-mass approximation since the details of the transverse wave function are not relevant to the physical effects we examine here, which are related to the longitudinal degree of freedom. As we will see shortly below, the lateral wave function appears only in the determination of the effective one-dimensional interaction, which is robust against the details of the transverse averaging-out. Thus, the effective one-dimensional Hamiltonian of two interacting electrons with Rashba interaction, in the absence of a magnetic field, is written as [23]

$$H = H_1^0 + H_2^0 + H_{1dR} + V_{int}, \tag{1}$$

where $H_i^0 = (p_{z,i}^2/2m^*) + V_z(z_i)$, m^* is the conduction-band effective mass ($m^* = 0.013m_0$ for InSb and $m^* = 0.0239m_0$ for InAs, where m_0 is the bare electron 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 [23]

$$H_{1dR} = \sum_{i=1}^{2} \frac{\gamma_R}{\hbar} \left\langle \frac{\partial V_x}{\partial x} \right\rangle p_{z,i}(\sigma_{x_i} - \sigma_{y_i}), \tag{2}$$

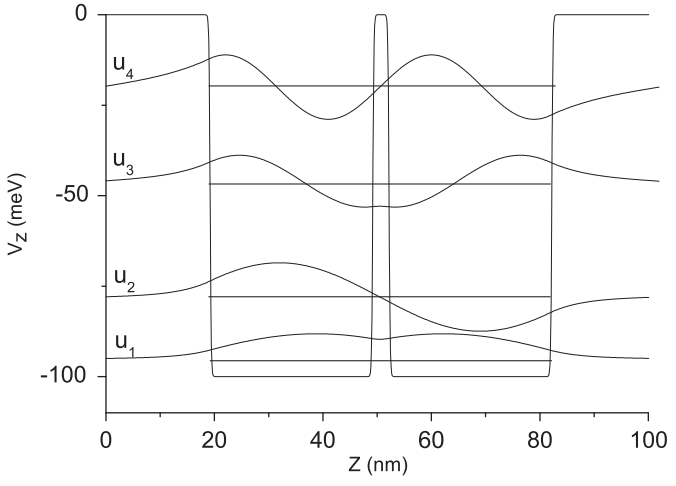

Fig. 1. The $Al_{0.1}In_{0.9}Sb$–InSb double-well confining potential in the longitudinal direction of the quasi-one-dimensional nanowhisker quantum dots. The single-particle eigenfunctions and energies are also shown.

where $\gamma_R = 500\,\text{Å}^2$ (InSb), $\gamma_R = 110\,\text{Å}^2$ (InAs) [30], σ_{x_i,y_i} are Pauli matrices, and $\langle \partial V_x/\partial x \rangle$ is an effective electric field which we will call here "the Rashba parameter", and which can be tuned to some extent by applying a lateral gate voltage [27–29].

The effective one-dimensional electron–electron Coulomb interaction is given by [31]

$$V_{int}(|z_2 - z_1|) = \int dx_1\, dx_2\, dy_1\, dy_2 \times \frac{e^2 \Phi(x_1)^2 \Phi(x_2)^2 \Phi(y_1)^2 \Phi(y_2)^2}{\varepsilon\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}}, \tag{3}$$

where $\mathbf{r}_i = (x_i, y_i, z_i)$, $i = 1, 2$, are the electron positions, and ε is the dielectric constant of the material (16.8 for InSb and 15.15 for InAs). The lateral averaging-out is done over the ground state Φ of the laterally confining potential $V_x = V_y$. Notice that for simplicity and only to the effect of calculating the effective one-dimensional Coulomb interaction, $V_x = V_y$ is assumed to be a harmonic oscillator potential, whose ground state Φ has a spatial extent of roughly 2 nm.

As a basis set for the two-electron Hilbert space we take all the u_n ($n = 1, 4$) which gives 28 two-particle basis states:

$$\begin{aligned}
&\varphi_i = u_i(z_1)u_i(z_2)|0,0\rangle,\\
&\varphi_{j+3} = (1/\sqrt{2})[u_1(z_1)u_j(z_2) + u_j(z_1)u_1(z_2)]|0,0\rangle,\\
&\varphi_{k+5} = (1/\sqrt{2})[u_2(z_1)u_k(z_2) + u_k(z_1)u_2(z_2)]|0,0\rangle,\\
&\varphi_{10} = (1/\sqrt{2})[u_3(z_1)u_4(z_2) + u_4(z_1)u_3(z_2)]|0,0\rangle,\\
&\varphi_{l+9} = (1/\sqrt{2})[u_1(z_1)u_l(z_2) - u_l(z_1)u_1(z_2)]|1,1\rangle,\\
&\varphi_{l+12} = (1/\sqrt{2})[u_1(z_1)u_l(z_2) - u_l(z_1)u_1(z_2)]|1,-1\rangle,\\
&\varphi_{l+15} = (1/\sqrt{2})[u_1(z_1)u_l(z_2) - u_l(z_1)u_1(z_2)]|1,0\rangle,\\
&\varphi_{m+17} = (1/\sqrt{2})[u_2(z_1)u_m(z_2) - u_m(z_1)u_2(z_2)]|1,1\rangle,\\
&\varphi_{m+19} = (1/\sqrt{2})[u_2(z_1)u_m(z_2) - u_m(z_1)u_2(z_2)]|1,-1\rangle,\\
&\varphi_{m+21} = (1/\sqrt{2})[u_2(z_1)u_m(z_2) - u_m(z_1)u_2(z_2)]|1,0\rangle,\\
&\varphi_{26} = (1/\sqrt{2})[u_3(z_1)u_4(z_2) - u_4(z_1)u_3(z_2)]|1,1\rangle,\\
&\varphi_{27} = (1/\sqrt{2})[u_3(z_1)u_4(z_2) - u_4(z_1)u_3(z_2)]|1,-1\rangle,\\
&\varphi_{28} = (1/\sqrt{2})[u_3(z_1)u_4(z_2) - u_4(z_1)u_3(z_2)]|1,0\rangle,
\end{aligned} \tag{4}$$

where $i = 1-4$, $j, l = 2-4$, and $k, m = 3, 4$. The two-particle spin wave functions are the usual singlet $|S\rangle = |S = 0, m_S = 0\rangle$ and triplet states $\{|T^+\rangle = |1,1\rangle, |T^0\rangle = |1,0\rangle, |T^-\rangle = |1,-1\rangle\}$.

The eigenvalue problem of the full two-electron Hamiltonian given in Eq. (1) will be solved by expanding the two-electron wave functions in the given basis set

$$\psi_i = \sum_{j=1}^{28} a_{ij}\varphi_j, \tag{5}$$

where $i = 1, \ldots, 28$, and determining the coefficients a_{ij} by numerical diagonalization. The Rashba coupling produces the general effect of mixing states with different spin wave functions, and as we will see in the next section the degree of mixing depends markedly on the structure's parameters.

In order to fully characterize the two-electron system in what could be the realistic experimental situations we will also introduce a magnetic field B 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. Consider, for example, that for a typical magnetic field of 2 T the magnetic length is about 10 times larger than the lateral size of our structure. Thus, we will assume that the magnetic field contributes only a Zeeman term to the Hamiltonian:

$$H_Z = \frac{g_0\mu_B B}{\hbar} S_z, \tag{6}$$

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where μ_B is the Bohr magneton, g_0 is the Landé factor ($g_0 = -51$ for InSb and -15 for InAs), and $S_z = S_{1,z} + S_{2,z}$ is the z-component of the total spin operator.

3. Results

We solve the eigenvalue problem of the two-electron Hamiltonian given by Eq. (1) plus the Zeeman term, Eq. (6). Our goal is to understand the interplay between the Pauli exclusion, the electron–electron Coulomb interaction, the single-particle Rashba coupling, and the applied magnetic field.

In order to gain some insight into the nature of the two-electron states, in Fig. 2 we show the probability density of the ground state and the first five excited states for the two electrons in a double-dot InSb structure (see Fig. 1) with Coulomb interaction, no Rashba coupling, and no external magnetic field. The energies of the low-lying states as functions of the external magnetic field including the Coulomb interaction (no Rashba) are given in Fig. 3(a). The six lowest two-particle states can be analyzed qualitatively taking into account the lowest two, bonding (symmetric) and antibonding (antisymmetric), orbitals, u_1 and u_2, seen in Fig. 1, and the two-spin basis set. In other words, they can be expanded fairly accurately in the reduced basis set (extracted from Eq. (4))

$$\begin{aligned}
\varphi_1 &= u_1(z_1)u_1(z_2)|0,0\rangle,\\
\varphi_2 &= u_2(z_1)u_2(z_2)|0,0\rangle,\\
\varphi_5 &= (1/\sqrt{2})[u_1(z_1)u_2(z_2) + u_2(z_1)u_1(z_2)]|0,0\rangle,\\
\varphi_{11} &= (1/\sqrt{2})[u_1(z_1)u_2(z_2) - u_2(z_1)u_1(z_2)]|1,1\rangle,\\
\varphi_{14} &= (1/\sqrt{2})[u_1(z_1)u_2(z_2) - u_2(z_1)u_1(z_2)]|1,-1\rangle,\\
\varphi_{17} &= (1/\sqrt{2})[u_1(z_1)u_2(z_2) - u_2(z_1)u_1(z_2)]|1,0\rangle. \qquad (7)
\end{aligned}$$

In Fig. 2 we see that in the ground state the two electrons occupy, as expected, different dots, due to their mutual Coulomb repulsion. It can easily be checked that ψ_1 is a linear superposition of mainly the two states φ_1 and φ_2, which can efficiently remove the probability density for having both electrons in the same dot. Incidentally, it is thus verified also that it is a spin singlet state (a general theorem for bound pairs of electrons establishes that this must be the case). The presence of the bonding orbital u_1 in φ_1 and therefore in ψ_1 introduces a non-zero probability density in the interdot barrier region, seen in the figure. The way that the energy levels are affected by the Coulomb interaction can be appreciated by comparing Fig. 3(a) to the spectrum of energies without Coulomb nor Rashba interaction given in Fig. 4(a). In particular, it can be seen that the ground state energy is shifted upwards on the order of 10 meV due to the electron–electron Coulomb repulsion.

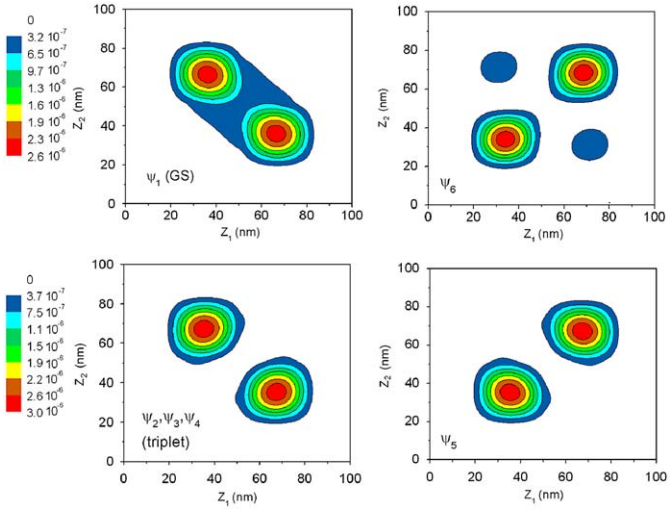

Fig. 2. (Color online). Probability density of two electrons in the double quantum dot with Coulomb interaction but without Rashba coupling. ψ_1: ground state (GS), $\psi_{i=2,\ldots,6}$: low-lying excited states. Note that in ψ_5 and ψ_6 both electrons are mainly in the *same* dot, while the other states can be seen as having one electron in each dot.

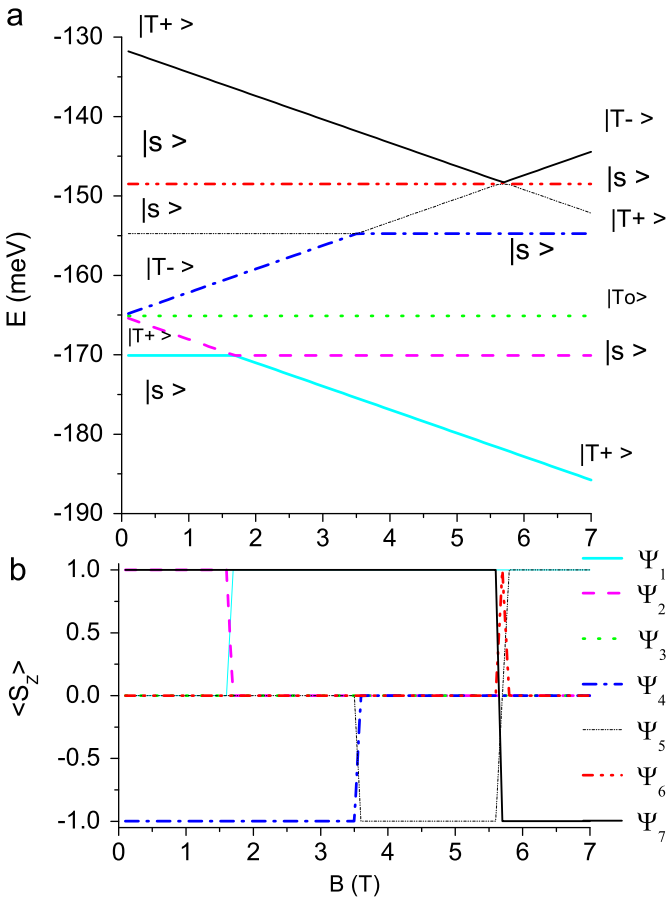

Fig. 3. (Color online). (a) Energy levels and (b) mean value of $S_z = S_{1,z} + S_{2,z}$ *versus* applied magnetic field for the two-electron eigenstates with Coulomb interaction and without Rashba coupling. Barrier width: 3 nm. $|S\rangle$: singlet state, $|T^{\pm,0}\rangle$: triplet states.

The states ψ_2, ψ_3, and ψ_4 at $B = 0$ shown in Fig. 2 also have the two electrons de-localized (i.e. sitting in different dots), but they correspond to the spin triplet and therefore their orbital wave function is antisymmetric with respect to particle exchange. These triplet states are not affected strongly by the Coulomb interaction since the Pauli exclusion principle already keeps the electrons apart in the absence of their mutual repulsion. Indeed, these three states are given essentially by the non-interacting basis states $\varphi_{11}, \varphi_{14}$, and φ_{17} (see Eq. (7)). This spatial two-electron wave function has a node at the point $(z_1, z_2) = (0, 0)$, i.e. it has a global "antibonding" character. Notice finally that the two higher energy states, ψ_5 and ψ_6, correspond to singlet states and differ significantly from the previous states, in the sense that both electrons lie mostly in the same dot in spite of the Coulomb repulsion. The eigenstate ψ_5 is similar to φ_5, but its energy is strongly shifted upwards due to the Coulomb energy cost of having both electrons in the same dot.

In Fig. 4 we plot the two-electron energy levels *versus* the applied magnetic field for the InSb-based system shown in Fig. 1,

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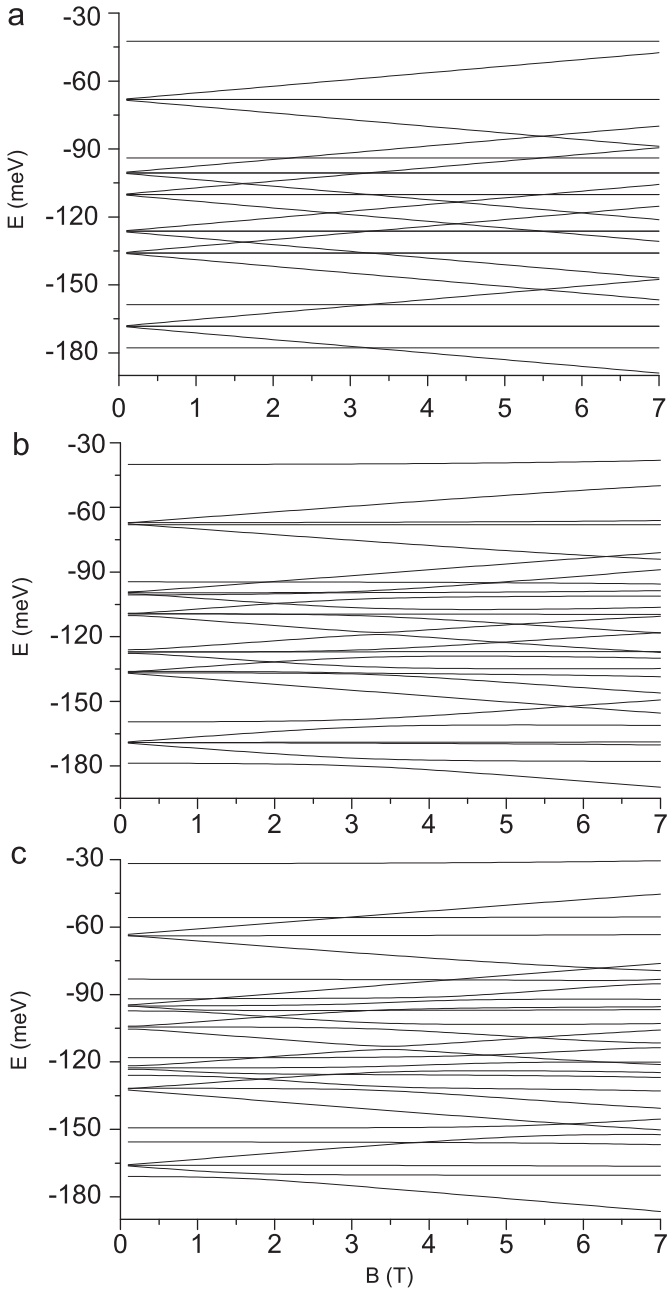

Fig. 4. Energy levels *versus* applied magnetic field for the two-electron eigenstates: (a) without Coulomb and Rashba interactions, (b) with only Rashba coupling, and (c) with Coulomb and Rashba interactions.

in the following cases: (a) no Rashba nor Coulomb interaction, (b) with Rashba interaction only (structural parameter $\langle \partial V_z/\partial x \rangle = 1\,\text{meV/Å}$), and in (c) adding Coulomb interaction.

Let us point out some basic features of the lowest energies of the two non-interacting electrons, seen in Fig. 4(a). First notice that since the spatial wave functions do not depend on the magnetic field and only the Zeeman energy does, the energies have a linear field dependence. At zero magnetic field, the ground state ψ_1 ($= \varphi_1$ from Eq. (4) or (7)) is a singlet (with energy $2E_1$), but around $B \approx 3\,\text{T}$ there is a level crossing and its spin part becomes $|1,1\rangle$ ($\psi_1 = \varphi_{11}$ after the crossing). The next four levels at $B = 0$ are degenerate and equal to $E_1 + E_2$. One of them is a singlet state (φ_5) and the other three correspond to triplet states ($\varphi_{11}, \varphi_{14}, \varphi_{17}$). The latter lose their degeneracy when $B \neq 0$, but the two states with $S_z = 0$ (φ_5 and φ_{17}) remain degenerate.

When the Rashba interaction is included (Fig. 4(b)), the two lower crossings at $B \approx 3\,\text{T}$ become avoided crossings. The same happens to other (not all) avoided crossings throughout the spectrum. 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 to some extent with a transverse electric field (gate voltage). Finally, the inclusion of the Coulomb interaction produces a more complex energy spectrum (Fig. 4(c)). For a better understanding of the combined effects of these two interactions in the energy spectrum, we extract from Figs. 4(b) and (c) the first seven eigen-energies and plot them along with their corresponding mean value of the z-projection of the spin shown in Fig. 5. Let us make the following observations:

(i) In both Figs. 5(b) and (d), it can be seen that the Rashba interaction causes ψ_2 and ψ_5 not to be spin eigenstates anymore at $B = 0$. In spite of that, following common practice, we label these states as if they were pure spin states, as one spin component dominates the admixture (this happens in general far from the avoided crossings).

(ii) Two of the level crossings in Fig. 5(a) (E_1 with E_2 and E_5 with E_6 at $B \approx 3\,\text{T}$) become avoided crossings, as the pair of states involved are coupled by the Rashba interaction.

(iii) In Fig. 5(a), there is a level crossing at $B \approx 5.6\,\text{T}$ between E_6 and E_7 which does not become an avoided crossing since the two states involved in it are not coupled by the Rashba interaction.

(iv) In Fig. 5(c), we see that the Coulomb interaction modifies the energy levels, in some cases substantially, thus shifting the position (along the magnetic-field axis) of some level crossings, and creating new ones. For example, the first avoided crossing appears at a smaller magnetic field ($B \approx 1.6\,\text{T}$) than without Coulomb. This occurs because the Coulomb interaction shifts the ground state upwards more than the neighboring triplet state $|T^+\rangle$, bringing them closer together. The following singlet state is pushed strongly upwards by the Coulomb interaction, producing a new crossing with a triplet $|T^-\rangle$ state, at $B \approx 3.7\,\text{T}$. On the other hand, the latter state is coupled by Rashba interaction to the next energy level (another singlet), thus producing an anticrossing at $B \approx 5.4\,\text{T}$. The crossing between E_6 and E_7 has been shifted slightly upward due to the effect of the Coulomb 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 interaction. The symmetry under space reversal (odd *versus* even) prevents the mixing of a state with double dot occupancy (singlet ψ_5) and a state where each dot has one electron (ψ_4), where each state has opposite space-reversal symmetry.

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 only six of the states at a given magnetic field $B = 0.5\,\text{T}$ for InSb. 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 $\langle S_z \rangle$ 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),

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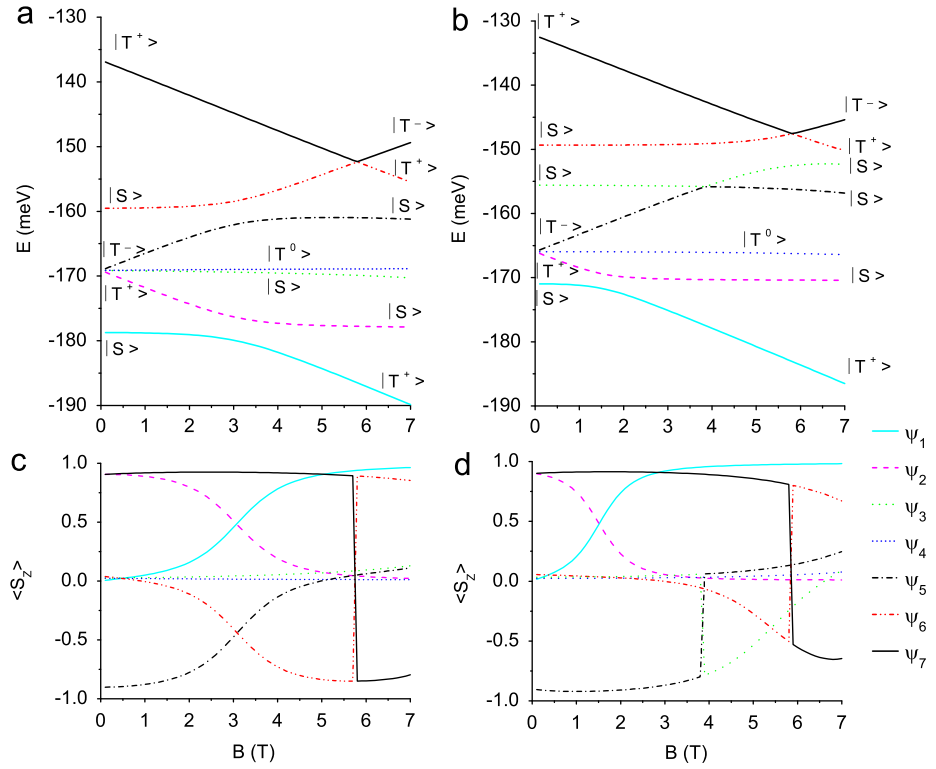

Fig. 5. (Color online). InSb: (a) and (c) seven lowest energy levels and (b) and (d) their corresponding mean value of $S_Z = S_{1,z} + S_{2,z}$ *versus* applied magnetic field for the two-electron eigenstates including Rashba interaction ((a) and (b)) and adding Coulomb interaction ((c) and (d)). The strength of the Rashba coupling is given by $\langle \partial V_X/\partial x\rangle = 1\,\text{meV/Å}$. $|S\rangle$ = singlet state, $|T^{\pm,0}\rangle$ = triplet states.

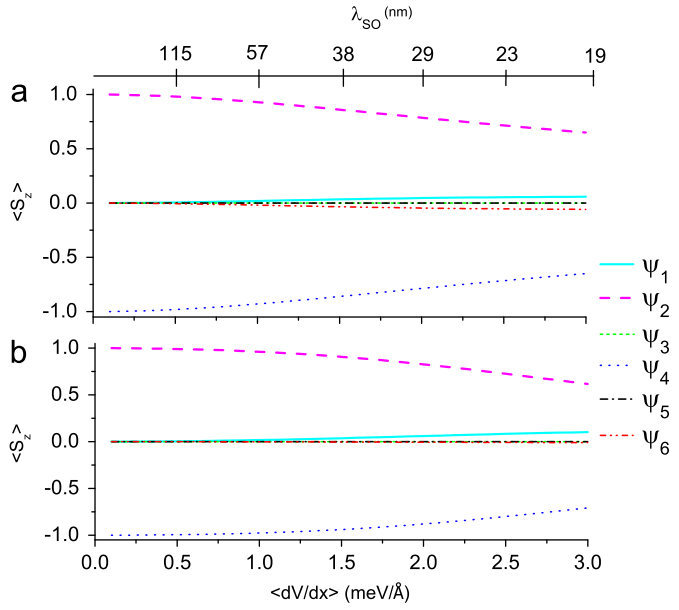

Fig. 6. (Color online). InSb: mean value of $S_z = S_{1,z} + S_{2,z}$ as a function of the Rashba parameter $\langle \partial V_x/\partial x\rangle$ for the six two-electron eigenstates. $B = 0.5\,\text{T}$. (a) Without Coulomb interaction; (b) with Coulomb interaction. λ_{SO} is the spin–orbit length.

this symmetry about the zero value is lost due to the different mixing of two-particle orbitals (φ_i) in higher and lower lying states produced by the Coulomb interaction. Fig. 6 includes an axis (top) in terms of the spin–orbit length ($\lambda_{SO} = \hbar^2/m^*\gamma_R\langle \partial V_x/\partial x\rangle$) [32], which is inversely proportional to the Rashba parameter. This length parameter helps to 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 $\lambda_{SO} \simeq 60\,\text{nm}$, the size of the two-well system.

Finally, we analyze an AlInAs–InAs-based structure with the same dimensions as the InSb double-dot system treated above. InAs-based structures have recently been studied experimentally [25,26]. In Fig. 7, we show the energy levels and the mean value of S_z of the first six two-particle eigenstates, for $\langle \partial V_x/\partial x\rangle = 0.4\,\text{meV/Å}$. Fig. 7(a) shows two anticrossings at $B \approx 1\,\text{T}$ which should be confronted with the two anticrossings seen in Fig. 5(a). First, we note that they are shifted to a lower magnetic field, due to the smaller gap between the symmetric and antisymmetric single-particle eigenstates in the InAs structure (which is then more easily overcome by the Zeeman energy). Second, we call attention to the narrower splittings at the avoided crossings, due, naturally, to a weaker Rashba coupling. The electron–electron interaction included in Fig. 7(c) has a strong impact on the energy levels, due to the close proximity of the bare energy levels. One manifestation of this influence is the large shift of the first avoided crossing, which now appears at $B \approx 0.05\,\text{T}$, down from $B \approx 1\,\text{T}$ in (a).

4. Conclusions

In this paper, we have investigated the effects of the Coulomb electron–electron interaction on energy levels and spin z projection of a two-electron system in a quasi-1D doubled quantum dots in the presence of Rashba coupling. As a function of a magnetic field applied in the longitudinal direction, some energy-level crossings become avoided crossings when the Rashba spin–orbit is turned on and their width can be controlled to some extent with a gate voltage that determines the effective field parameter $\langle \partial V_x/\partial x\rangle$. Coulomb interaction modifies the positions of the energy

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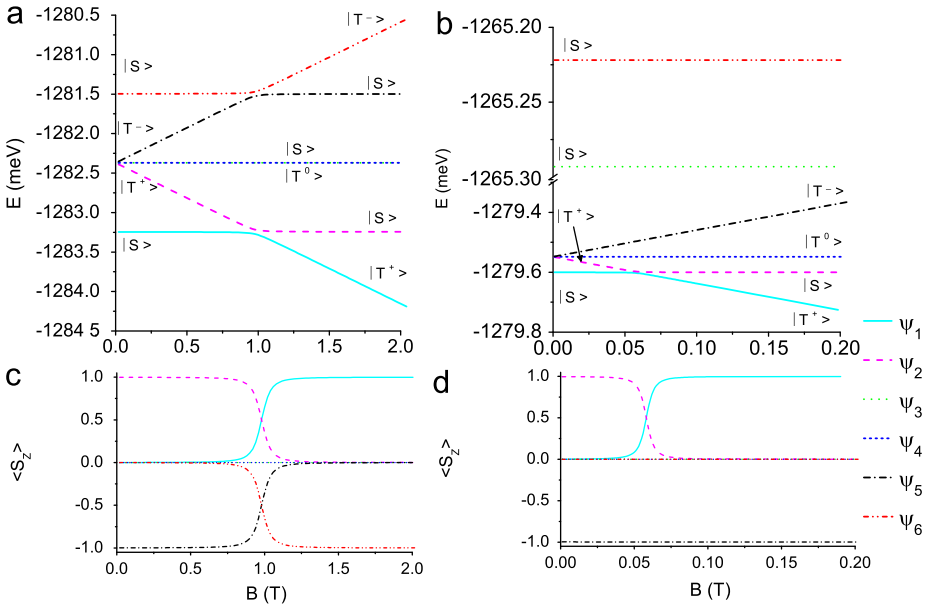

Fig. 7. (Color online). InAs: (a) and (c) lowest energy levels and (b) and (d) their corresponding mean value of $S_z = S_{1,z} + S_{2,z}$ *versus* applied magnetic field for the two-electron eigenstates including Rashba interaction ((a) and (b)) and adding Coulomb interaction ((c) and (d)). The strength of the Rashba coupling is given by $\langle \partial V_x/\partial x \rangle = 0.4\,\text{meV/Å}$. $|S\rangle$ = singlet state, $|T^{\pm,0}\rangle$ = triplet states.

levels changing the energy spectrum, producing new possible crossings or moving the original crossings to a different value of the magnetic field.

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