

Spin-orbit splitting in semiconductor quantum dots with a parabolic confinement potential

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We present a theoretical study of the effect of spin-orbit interaction on the electron energy spectrum of cylindrical semiconductor quantum dots. The study is based on a simple effective one-band approximation. The dependence of energy levels on parameters of the dots and the applied external magnetic field is studied. Contributions of the bulk inversion asymmetry (the Dresselhaus term) and the system inversion asymmetry (the Rashba term) to the spin splitting of the electron energy states are discussed. The spin splitting of electron states with nonzero angular momentum is demonstrated theoretically for InSb and InAs small quantum dots at zero magnetic field. We find a “crossing” of the electron energy states with the same angular momentum and different spin polarizations in a nonzero magnetic field.

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Experimental and theoretical investigations of spin-dependent confinement and transport in semiconductor quantum heterostructures have attracted considerable attention in recent years (see Refs. 1–7, and references therein). The increasing interest in this topic stems from two facts. First, advances in semiconductor technology have made it possible to create structures which possess electrical properties that are highly sensitive to electron spin. So-called “spintronics” devices can be controlled by the electron-spin polarization.^{8,9} Second, one can use a quite general physical approach to clarify unusual spin-dependent phenomena in low-dimensional semiconductor quantum structures.^{1–5,10–13}

Electron spin can significantly impact the electronic properties of quantum structures through different mechanisms. Among possible spin-dependent interactions there is an interaction between orbital angular and spin momenta of an electron known as spin-orbit (SO) interaction.^{14,15} Despite its relativistic nature, SO interaction can play an observable role in the energy-band structure of many semiconductors. When the potential through which the carriers move is inversion asymmetric, spin-orbit interaction removes the spin degeneracy even without an external magnetic field. While the SO interaction impact on the electron quantum confinement in semiconductor quantum wells and quantum wires has been extensively studied theoretically and experimentally (see for instance Refs. 1, 2, 10, and 11), SO interaction in semiconductor quantum dots (QD’s) has largely been uninvestigated.¹⁶

In a zinc-blende crystal with bulk inversion asymmetry (BIA), energy bands are split for a given direction of the electron wave vector.^{14,17–19} Additional spin splitting in semiconductor quantum structures may also occur owing to the structure confinement potential inversion asymmetry (SIA).^{15,19} Since SO interaction has been used successfully in experimental result interpretations for various quantum well and quantum wire structures, it also appears to provide a well-defined contribution to the spin properties of QD’s. Clearly, SO interaction depends heavily on the quantum sys-

tem geometry as well as the effective external and internal fields. With advanced semiconductor technology, QD’s are easily realizable within a wide range of dot geometrical shapes and built-in fields.²⁰ Therefore, the spin-dependent phenomenon in those structures is of worthwhile interest.

The goal of this paper is to start a theoretical discussion of how SO interaction can affect the electron energy states and magnetic properties of QD’s. Spin-orbit interaction is described by two contributions to the effective one-band spin dependent Hamiltonian. One of them arises from the bulk Hamiltonian, and was first considered by Dresselhaus (BIA).^{14,17} The second contribution, known as the Rashba term, represents the spin-orbit interaction of an electron moving in a QD confinement potential (SIA).^{4,15} The Coulomb interaction between electrons is neglected for simplicity. However, a recent investigation²¹ indicated that the effect of electron-electron interaction in systems with strong confinement can enhance the SO interaction. The following discussion clearly reveals that principal consequences of the SO interaction can be described with the used simplifications.

This study next considers SO interaction in semiconductor cylindrical quantum dots with a quasi-two-dimensional confinement for electrons.^{16,22,23} Widely used to describe QD energy states, this model can successfully describe the electronic properties of circular disk-shaped quantum dots (artificial atoms)^{24,25} as well as QDs formed in two-dimensional electron-gas systems by external electric^{16,26} and strain fields.²⁷ In cylindrical coordinates, we consider a quasi-two-dimensional effective parabolic lateral confinement potential^{28,29}

$$V_c(\rho) = \frac{1}{2} m \omega_0^2 \rho^2, \quad (1)$$

where $\hbar \omega_0$ is the characteristic confinement energy, ρ is the radius vector, and the electron effective mass is given by⁴

$$\frac{1}{m(E)} = \frac{1}{m(0)} \frac{E_g(E_g + \Delta)}{(3E_g + 2\Delta)} \left[\frac{2}{E + E_g} + \frac{1}{E + E_g + \Delta} \right]; \quad (2)$$

here E denotes the electron energy in the conduction band, $m(0)$ is the conduction-band-edge effective mass, and E_g and Δ are the main band gap and the spin-orbit band splitting respectively.

Consider a situation in which the z axis is normal to the disk and parallel to the $[100]$ direction (the most frequently used orientation), and assume that the z -direction potential is symmetric. The SO interaction is comprised of the two parts mentioned above. In an axial magnetic field of the symmetric gauge for the vector potential $\mathbf{A}=(B_\rho/2)\mathbf{e}_\phi$, (where ϕ is the azimuthal angle) the Dresselhaus (BIA) term can be written explicitly in cylindrical coordinates when the dot lateral size (ρ_0) is sufficiently larger than the dot height (z_0),^{12,13,17}

$$V_{\text{so}}^D(\rho, \phi) = \beta \left\{ \Sigma_\phi \left(\mathbf{k}_\phi + \frac{e}{2\hbar} B \rho \right) + \Sigma_\rho \mathbf{k}_\rho \right\}, \quad (3)$$

when

$$\Sigma_\phi = \begin{pmatrix} 0 & ie^{i\phi} \\ -ie^{-i\phi} & 0 \end{pmatrix},$$

$$\Sigma_\rho = \begin{pmatrix} 0 & e^{i\phi} \\ e^{-i\phi} & 0 \end{pmatrix}.$$

$\mathbf{k}_\phi = -i(1/\rho)\partial/\partial\phi$, $\mathbf{k}_\rho = -i\partial/\partial\rho$, and e is the electron elementary charge. The parameter β can be represented as

$$\beta \approx \gamma_c \left(\frac{\pi}{z_0} \right)^2,$$

where γ_c is the material-specific constant.¹⁷

The Rashba (SIA) term in the cylindrical coordinates is given by^{4,10,12,13}

$$V_{\text{so}}^R(\rho, \phi) = \sigma_z \alpha \frac{dV_c(\rho)}{d\rho} \left(\mathbf{k}_\phi + \frac{e}{2\hbar} \beta \rho \right), \quad (4)$$

where σ_z is the Pauli z matrix, and α is the Rashba spin-orbit coupling parameter.⁴

By including the Zeeman term, an approximate effective Hamiltonian can be obtained in the form

$$\begin{aligned} H = & -\frac{\hbar^2}{2m(E)} \left[\frac{\partial}{\rho\partial\rho} \rho \frac{\partial}{\partial\rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial\phi^2} \right] - \frac{i}{2} \hbar \omega_c(E, B) \frac{\partial}{\partial\phi} \\ & + \frac{1}{8} m(E) \omega_c^2(E, B) \rho^2 + V_c(\rho) + V_{\text{so}}^D(\rho, \phi) + V_{\text{so}}^R(\rho, \phi) \\ & + \frac{1}{2} \sigma_z \mu_B g(E) B, \end{aligned} \quad (5)$$

where

$$\omega_c(E, B) = \frac{eB}{m(E)}$$

is the electronic cyclotron frequency,

$$g(E) = 2 \left[1 - \frac{1}{m(E)} \frac{\Delta}{3(E_g + E) + 2\Delta} \right] \quad (6)$$

is the effective Landé factor of the semiconductor,³⁰ $\mu_B = e\hbar/2m_0$ is the Bohr magneton, and m_0 is the free-electron mass.

An analysis of the problem begins by considering a situation in which the dot height is adequately large (that condition is evaluated below), so that the Dresselhaus term is neglected. Under this circumstance, the energy eigenfunction of Hamiltonian (5) takes the well-known form

$$\Psi_{n,l,\sigma} = \frac{1}{\sqrt{2\pi}} \exp(il\phi) R_{n,l,\sigma}(\rho),$$

with a radial part $R_{n,l,\sigma}(\rho)$ that satisfies

$$\left[\frac{d^2}{d\rho^2} + \frac{1}{\rho} \frac{d}{d\rho} - \frac{l^2}{\rho^2} + \frac{m^2(E) \Omega_\sigma^2(E, B) \rho^2}{\hbar^2} + \Pi_{l\sigma}(E, B) \right] R_{n,l,\sigma}(\rho) = 0, \quad (7)$$

where

$$\Omega_\sigma^2(E, B) = \omega_0^2 + \frac{\omega_c^2(E, B)}{4} + \sigma \alpha \frac{m(E) \omega_0^2}{\hbar} \omega_c(E, B), \quad (8)$$

$$\begin{aligned} \Pi_{l\sigma}(E, B) = & \frac{2m(E)}{\hbar^2} \left\{ E - \frac{\hbar l}{2} \omega_c(E, B) \right. \\ & \left. - \sigma \left[\frac{\mu_B}{2} g(E) B + l \alpha m(E) \omega_0^2 \right] \right\}, \end{aligned}$$

and $\sigma = \pm 1$ refers to the electron-spin polarization along the z axis. The solution to Eq. (7) has been known for a long time (see, for example, Ref. 23). The electron energy levels are given by

$$\begin{aligned} E_{n,l,\sigma} = & \hbar \Omega_\sigma(E_{n,l,\sigma}, B) (2n + |l| + 1) + l \frac{\hbar \omega_c(E_{n,l,\sigma}, B)}{2} \\ & + \sigma \left[\frac{\mu_B}{2} g(E_{n,l,\sigma}) B + l \alpha m(E_{n,l,\sigma}) \omega_0^2 \right], \end{aligned} \quad (9)$$

and the corresponding normalized radial wave functions are given by

$$\begin{aligned} R_{n,l,\sigma}(\rho) = & \frac{\sqrt{2}}{\rho_\sigma} \left[\frac{n!}{(n+|l|)!} \right]^{1/2} \exp\left(-\frac{\rho^2}{2\rho_\sigma^2}\right) \\ & \times \left(\frac{\rho^2}{\rho_\sigma^2} \right)^{|l|/2} L_n^{|l|} \left(\frac{\rho^2}{\rho_\sigma^2} \right), \end{aligned} \quad (10)$$

where $\rho_\sigma = (\hbar/m\Omega_\sigma)^{1/2}$, and $L_n^{|l|}$ is the generalized Laguerre polynomial.³¹

Equation (9) shows the dependence of the electron energy on the quantum numbers $\{n, l, \sigma\}$ and the external magnetic field B by taking into account the nonparabolicity of the semiconductor dispersion relation [Eq. (2)].

TABLE I. QD parameters.

Semiconductor	$m(0)/m_0$	E_g (eV)	Δ (eV)	α (\AA^2)	$\hbar\omega_0$ (eV)	$r_0(0)$ (\AA)
InSb	0.014 ^a	0.24 ^a	0.81 ^a	500	0.025 ^b	148
InAs	0.04 ^c	0.42 ^a	0.38 ^a	110	0.019 ^c	100
In _{0.55} Al _{0.45} As	0.076 ^d	1.45 ^d	0.34 ^d	4.4	0.043 ^e	48

^aReference 32.

^bReference 33.

^cReference 34.

^dReference 35.

^eReference 36.

Consider how the Rashba spin-orbit interaction impacts the energy spectrum of narrow-gap semiconductor QD's. The main value of interest is the spin splitting in the electron energy:

$$\Delta E_{n,l}(B) = E_{n,l,+1}(B) - E_{n,l,-1}(B). \quad (11)$$

First we analyze a situation without an external magnetic field. The dispersion relation [Eq. (9)] in this case can be written as

$$E_{n,l,\sigma} = \hbar\omega_0 \left[2n + 1 + |l| \left(1 + \sigma \mathcal{S}(l) \frac{\alpha}{r_0^2} \right) \right],$$

where $r_0(E) = \sqrt{\hbar/m(E)\omega_0}$ is an effective QD lateral size and $\mathcal{S}(l)$ is the sign of l . The spin splitting

$$\Delta E_{n,l}(0) = \hbar\omega_0 \frac{2l\alpha}{r_0^2} \quad (12)$$

is a weak function on n [due to effects of nonparabolicity that come to Eq. (9) with $r_0(E_{n,l,\sigma})$]. The dependence of $\Delta E_{n,l}(0)$ on l is of primary concern in this study, and we examine the lowest-energy levels when $n=0$. The spin-orbit interaction separates states with the same orbital momentum and different spin directions. However, states with parallel spin and l (antiparallel spin and l) remain twofold degenerate. This is the well-known Kramers degeneracy. Doubly degenerate electron states with parallel directed spin and l have

the highest energy. This level hierarchy obviously depends on the sign of the Rashba constant.

Our calculations for InSb, InAs, and In_xAs_{1-x}Gs QDs are presented as practical examples. The band parameters and the estimated geometrical parameters of the dots are taken from the available literature, and are listed in Table I. Figure 1 presents the amount of spin splitting for QD's as a function of the orbital quantum number l at $n=0$ and zero magnetic field. According to this figure, the Rashba spin-orbit splitting can have a well-pronounced magnitude for QD's with relatively small effective sizes.

The Rashba spin splitting at zero magnetic field leads to an unusual behavior of the QD energy spectrum when a magnetic field is present. Figure 2 displays the calculated spectrum of InSb QD's as a function of the magnetic field B for a set of $\{n,l,\sigma\}$ with $n=0$ and $l=0,\pm 1,\pm 2,\pm 3$ using the parameters of Table I. For comparison, inset *a* shows the spectrum of InSb QD's with the same parabolic confinement potential but without spin-orbit interaction. The spin-orbit interaction provides a "crossing" of the energy levels with the same orbital momentum but different spins when $\Delta E_{n,l}(B_{cr})=0$ (see inset *b* in Fig. 2). Using the linear approximation for the dispersion relation [Eq. (9)] allows us to derive the conditions for the crossing of energy levels. A straightforward consequence of solution (10) is that the area covered by the electron in state $|n,l\rangle = R_{n,l,\sigma}$ in a low magnetic field is $S_{n,l} = \pi \langle l,n | \rho^2 | n,l \rangle = \pi \rho_0^2 (2n + |l| + 1)$.³⁷ Using dispersion relation (9) and this expression reveals that, at the point of the crossing,

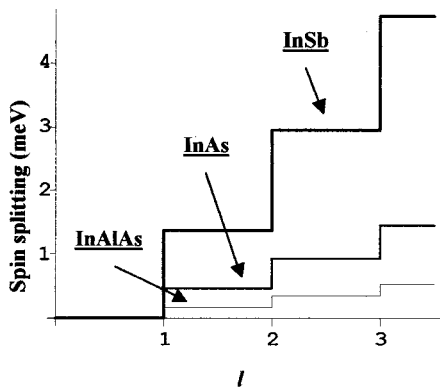


FIG. 1. The Rashba spin splitting vs the orbital angular momentum for $n=0$ at zero magnetic field for InSb, InAs, and In_{0.55}Al_{0.45}As QD's.

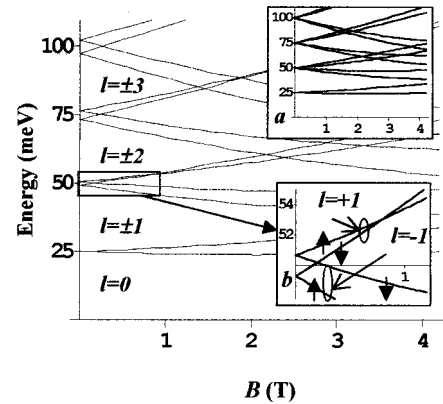


FIG. 2. Energy states for an InSb QD with Rashba spin-orbit interaction ($n=0$; inset *a* shows a spectrum without spin-orbit interaction; the arrows in inset *b* show electron-spin polarizations).

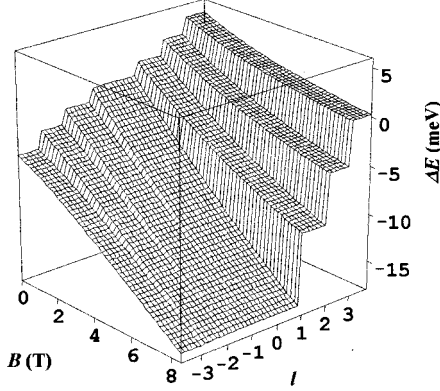


FIG. 3. Dependence of the spin splitting for InSb QD's on external magnetic field and orbital momentum (only the Rashba spin-orbit interaction is included).

$$\frac{\Phi_{n,l}}{\Phi_0} = -l(2n + |l| + 1) \left[\frac{\hbar g}{2m_0\omega_0\alpha} + (2n + |l| + 1) \right]^{-1}, \quad (13)$$

where $\Phi_{n,l} = B_{\text{cr}} S_{n,l}$ is the magnetic flux corresponding to the effective $\{n, l, \sigma\}$ state area at the crossing point and Φ_0 is the magnetic flux quantum. Equation (13) becomes very simple when $g \rightarrow 0$.³⁸ For such a case, $\Phi_{n,l}/\Phi_0 = -l$. For narrow-gap semiconductors, the magnitude of g in quantum structures has not yet been totally clarified.³⁹ Nevertheless, if g is a negative number with $|g| > 2(2n + |l| + 1)m_0\omega_0\alpha/\hbar \equiv g_0(2n + |l| + 1)$, it follows from Eq. (13) that the crossing exists for positive l . For the case of InSb QD's considered here, $g_0 \approx 3.2$.

Figure 3 shows how the Rashba spin splitting depends on the external magnetic field and l for InSb QD's. The calculated spin splitting follows the general tendency described above. The calculated magnitudes of the spin splitting and the magnetic fields at level crossing (B_{cr}) allow us to discuss more realistic theoretical models of the phenomena, and to verify the effect experimentally.

Next consider a situation when the effective sizes of the quantum dot are such that the Dresselhaus term must be considered as well. In this situation, Eq. (5) can be solved by following the scheme proposed in Refs. 10 and 40. The solution can be represented in the spinor form

$$\Psi(\rho, \phi) = \sum_{n,l} e^{il\phi} R_{n,l}^0(\rho) \left[A_l^n \begin{pmatrix} 1 \\ 0 \end{pmatrix} + B_l^n \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right], \quad (14)$$

where $\{R_{n,l}^0(\rho)\}$ is the solution [Eq. (10)] of Eq. (5) when $\alpha = \beta = g = 0$. Coefficients A_l^n and B_l^n are given by the system of equations

$$\begin{aligned} (E_{n,l+1,+1}^0 - E)A_l^n + \alpha \frac{em\omega_0^2}{\hbar} B \sum_m G_l^{nm} A_l^m \\ + i\beta \sum_m \left\{ (l-1)I_l^{nm} - P_l^{nm} + \frac{e}{2\hbar} B J_l^{nm} \right\} B_{l-1}^m = 0, \\ (E_{n,l-1,-1}^0 - E)B_l^n - \alpha \frac{em\omega_0^2}{\hbar} B \sum_m G_l^{nm} B_m^l \\ - i\beta \sum_m \left\{ (l+1)K_l^{nm} + D_l^{nm} + \frac{e}{2\hbar} B L_l^{nm} \right\} A_{l+1}^m = 0, \end{aligned} \quad (15)$$

where

$$\begin{aligned} G_l^{nm} &= \int_0^\infty \rho^3 d\rho R_{n,l}^0(\rho) R_{m,l}^0(\rho), \\ I_l^{nm} &= K_{l-1}^{mn} = \int_0^\infty d\rho R_{n,l}^0(\rho) R_{m,l-1}^0(\rho), \\ J_l^{nm} &= L_{l-1}^{mn} = \int_0^\infty \rho^2 d\rho R_{n,l}^0(\rho) R_{m,l-1}^0(\rho), \\ P_l^{nm} &= \int_0^\infty \rho d\rho R_{n,l}^0(\rho) \frac{d}{d\rho} R_{m,l-1}^0(\rho), \\ D_l^{nm} &= \int_0^\infty \rho d\rho R_{n,l}^0(\rho) \frac{d}{d\rho} R_{m,l+1}^0(\rho), \end{aligned}$$

and

$$\begin{aligned} E_{n,l,\sigma}^0(E, B) &= \hbar \left(\omega_0^2 + \frac{\omega_c^2(E, B)}{4} \right)^{1/2} (2n + |l| + 1) \\ &+ l \frac{\hbar \omega_c(E, B)}{2} + \sigma \left[\frac{\mu_B}{2} g(E) B + l \alpha m(E) \omega_0^2 \right]. \end{aligned}$$

System of equations (15) can be written in the vector form: $\mathbf{A}_l = \hat{\mathbf{M}} \mathbf{B}_{l-1}$ and $\mathbf{B}_l = \hat{\mathbf{N}} \mathbf{A}_{l+1}$.⁴⁰ The energy spectrum of the QD has to be numerically calculated from the following equation:

$$\det(\hat{\mathbf{I}} - \hat{\mathbf{M}}\hat{\mathbf{N}}) = \det(\hat{\mathbf{I}} - \bar{\mathbf{N}}\bar{\mathbf{M}}) = 0. \quad (16)$$

The chosen basic set $\{R_{n,l}(\rho)\}$ provides a very quick convergence for the roots of Eq. (16), with an increasing number n . For $n_{\text{max}} \sim 15$, the net error for the lowest four energy levels is $< 10^{-4}$ for InSb QD's in a magnetic field near the crossing points.

First we assume that $\alpha = 0$ describes the spin splitting produced by the Dresselhaus term only. Calculation results indicate that, at zero magnetic field, the spin splitting remains for all states with $|l| \geq 1$. However, in contrast to the Rashba splitting, the Dresselhaus splitting between pairs of twofold degenerate levels is proportional to $\beta^2/\hbar \omega_0 \rho_0^2$ and

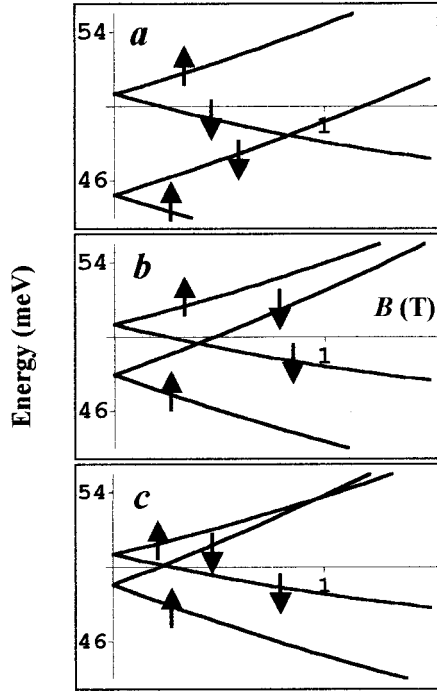


FIG. 4. $\{0, \pm 1, \sigma\}$ energy states for InSb QD's with Rashba and Dresselhaus spin-orbit interactions: (a) $z_0 = 35 \text{ \AA}$, (b) $z_0 = 46 \text{ \AA}$, and (c) $z_0 = 70 \text{ \AA}$. The other parameters are the same as in Fig. 2.

does not depend on the sign of γ_c constant. The Kramers degeneracy also remains for $\{n=0, |l| \geq 1, \sigma\}$ levels.

When the Rashba term is included in Eqs. (15), the total (Dresselhaus and Rashba) spin splitting sign heavily depends on the dot height. For InSb quantum dots with the same parameters as in Fig. 3 and $z_0 = 35 \text{ \AA}$, $\gamma_c = 160 \text{ eV \AA}^3$ (Ref. 17) at zero magnetic field, the BIA term dominates in the total spin splitting for $\{0, \pm 1, \sigma\}$ states that is about $\sim 5.5 \text{ meV}$. Since β depends heavily on the dot height, the SIA term becomes dominant for $z_0 \geq 50 \text{ \AA}$. In addition, at $z_0 \approx 80 \text{ \AA}$, the Dresselhaus term can be neglected.

Consider the eventual changes of spin splitting at zero magnetic field for "thin" quantum dots, in which the energy-state crossing demonstrates a different behavior. Figure 4 presents the calculation results for $\{0, \pm 1, \sigma\}$ states of InSb quantum dots at a magnetic field near the crossing point. In contrast to Fig. 2(b), for the dot size $z_0 = 35 \text{ \AA}$, the Dresselhaus splitting is strong enough to remove the crossing between states with the same l at low magnetic fields [Fig. 4(a)]. When the dot height increases, the Dresselhaus splitting weakens [Fig. 4(b)], and then ($z_0 \geq 45 \text{ \AA}$) the crossing appears at relatively large magnetic fields. For $z_0 = 70 \text{ \AA}$, the electron energy-level positions are extremely close to those when only the Rashba term is included [Fig. 4(c)].

In planar semiconductor systems (e.g., in quantum wells), the electron energy spectrum is insensitive to the sign of α . In quantum dots, however, it is sensitive. Therefore, BIA and SIA contributions to the total spin splitting can either sum up or subtract from each other, depending on the sign of α but independent on the sign of γ_c . In our calculation above we

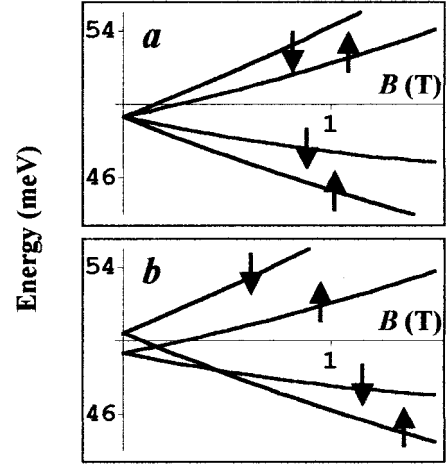


FIG. 5. $\{0, \pm 1, \sigma\}$ energy states for InSb QD's with Rashba ($\alpha = -500 \text{ \AA}^2$) and Dresselhaus spin-orbit interactions: (a) $z_0 = 46 \text{ \AA}$ and (b) $z_0 = 70 \text{ \AA}$. The other parameters are the same as in Fig. 2.

described the first situation when $\alpha > 0$. To our knowledge, the absolute signs of those constants remain a controversial issue (see Ref. 2 and references therein). As an example, Fig. 5 $\{0, \pm 1, \sigma\}$ presents energy-state positions for $\alpha < 0$. For a negative α we found a cancellation of the Rashba-Dresselhaus terms when $z_0 = 46 \text{ \AA}$ and $B \rightarrow 0$ [Fig. 5(a)]. In addition, increasing the dot height leads to the appearance of a crossing. However, in contrast to the positive α case, the crossing between electron energy states has $l = -1$ [Fig. 5(b)]. Therefore, a possible measurement of the α -dependent characteristics of quantum dots can determine the sign of α , and provide additional information about the effective spin-orbit interaction.

In conclusion, we presented a study of the effect of spin-orbit interaction on the electronic spectrum of narrow-band semiconductor quantum dots. Calculations were made on the basis of an effective one-dimensional spin-dependent Hamiltonian within the envelope-function approximation. For the parabolic confinement potential model a well-pronounced spin splitting was found for QD's with parameters of InSb and InAs.

Our results further demonstrate that the magnitude and sign of the effect depend on the effective size of the QD, and can gain a measurable value for relatively small QD's of narrow-gap semiconductors. For relatively thin cylindrical quantum dots, the Dresselhaus mechanism of the spin splitting is dominant. However, with increasing dot height, the Rashba term becomes dominant.

The main goal of the paper is to call attention to spin-splitting effects for QD's. In our calculation, a simple model and conventional parameters of the semiconductor band structures are used. A real three-dimensional calculation should be performed. However, the major finding is as follows: the spin splitting at zero magnetic field and the l -state crossing with external magnetic field are clear physical phenomena which are independent of the model. Therefore, the crossing of electron energy levels with different spins may lead to unusual magnetic properties of QD's.

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