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Spin–orbit interaction and energy states in semiconductor quantum dots

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Abstract

We present a theoretical study of the impact of the spin–orbit interaction on electron energy states in small cylindrical quantum dots. In our calculations, we use the effective one electronic band Hamiltonian and the spin dependent boundary conditions. It has been found that the spin–orbit interaction can modify the energy spectrum of narrow gap semiconductor quantum dots. The modification consists of the energy state spin splitting that strongly depends on the dot size. The spin splitting demonstrates a non-monotonic dependence on the dot size and can provide a situation when only the lower spin split states with angular quantum number $|l| = 1$ are bound in the dot.

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The electron spin plays an important role in the design of quantum dot electron energy levels and can significantly alter the properties of the electron energy states [1–3]. A new branch of semiconductor electronics (so called spintronics [4–7]) has produced much interest in the spin-dependent energy structure of semiconductor quantum dots. In semiconductor spintronics devices, the carriers generation, recombination, and transport will be controlled by electron spin polarization as well as the electron charge. A study of the spin dependent electron confinement in semiconductor quantum dots can be an essential part of semiconductor spintronics development.

There is an additional reason to investigate the spin dependence of the electron energy state in III–V semiconductor quantum dots and nanocrystals. When the potential for electrons in III–V semiconductors is inversion asymmetric, the spin–orbit (SO) interaction removes the spin degeneracy and considerably affects the electron energy states [8,9]. It has been found that

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the Rashba SO interaction [9] can critically effect the energy states and electronic properties of III–V semiconductor quantum structures [10–22]. The Rashba spin–orbit interaction term is used successfully to interpret experimental results in various quantum well and quantum wire structures [10,11,16–22]. In this paper, we investigate the effect of the SO interaction on narrow gap semiconductor dependent quantum dot energy states. We use the effective one band spin-dependent Hamiltonian and the spin-dependent boundary conditions [12,13]. It will be demonstrated that SO interaction can change the positions of electron energy states of the quantum dots.

We consider a cylindrical quantum dot with a hard-wall confinement potential that is induced by the discontinuity of the conduction band edge of the system. This model is commonly used in calculations of the electron energy states of quantum dots embedded into a different material matrix [23]. The model allows us to solve the three-dimensional Schrödinger equation with a small number of additional approximations. It must be emphasized that basic parameters of the materials for semiconductor quantum dot structures (such as energetic gaps, effective masses, band offsets etc.) are affected by different factors (strain, for instance) and are poorly known. In modern literature of this topic, values of the parameters vary within a wide range [24–26]. In our calculations we adjust the material parameters in accordance to the literature data.

In three-dimensional semiconductor quantum structures the approximate one electron band effective Hamiltonian is given in the form

$$\hat{H} = \hat{H}_0 + \hat{V}_{\rm so}, \tag{1}$$

where

$$\hat{H}_0 = -\frac{\hbar^2}{2}\nabla_r \frac{1}{m(E,\boldsymbol{r})}\nabla_r + V(\boldsymbol{r})$$

is the Hamiltonian without SO interaction, ∇_r stands for the spatial gradient, $m(E,\boldsymbol{r})$ is the energy and position dependent electron effective mass

$$\frac{1}{m(E,\boldsymbol{r})} = \frac{P^2}{\hbar^2}\left[\frac{2}{E+E_{\rm g}(\boldsymbol{r})-V(\boldsymbol{r})} + \frac{1}{E+E_{\rm g}(\boldsymbol{r})-V(\boldsymbol{r})+\Delta(\boldsymbol{r})}\right],$$

$V(\boldsymbol{r})$ is the confinement potential, $E_{\rm g}(\boldsymbol{r})$ and $\Delta(\boldsymbol{r})$ stand, respectively, for the position dependent band gap and the spin–orbit splitting in the valence band, P is the momentum matrix element. The SO interaction $V_{\rm so}(\boldsymbol{r})$ for conducting band electrons is described by [12,13,27]

$$\hat{V}_{\rm so}(\boldsymbol{r}) = i\nabla_r \beta(E,\boldsymbol{r})\cdot[\boldsymbol{\sigma}\times\nabla_r], \tag{2}$$

where

$$\beta(E,\boldsymbol{r}) = \frac{P^2}{2}\left[\frac{1}{E+E_{\rm g}(\boldsymbol{r})-V(\boldsymbol{r})} - \frac{1}{E+E_{\rm g}(\boldsymbol{r})-V(\boldsymbol{r})+\Delta(\boldsymbol{r})}\right],$$

and

$$\boldsymbol{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$$

is the vector of the Pauli matrices.

For systems with a sharp discontinuity of the conduction band edge between the quantum dot (material 1) and the crystal matrix (material 2), the hard-wall confinement potential can be presented as

$$V(\boldsymbol{r}) = \begin{cases} 0, & \boldsymbol{r}\in 1 \\ V_0, & \boldsymbol{r}\in 2. \end{cases}$$

From integration of the Schrödinger equation with Hamiltonian (1) along the direction perpendicular to the interface ($\boldsymbol{r}_{\rm n}$) we obtain the spin dependent Ben Daniel–Duke boundary conditions for the electron wave function $\Psi(\boldsymbol{r})$

$$\Psi_1(\boldsymbol{r}_{\rm s}) = \Psi_2(\boldsymbol{r}_{\rm s}),$$
$$\left\{\frac{\hbar^2}{2m(E,\boldsymbol{r})}\nabla_r - {\rm i}\beta(E,\boldsymbol{r})[\boldsymbol{\sigma}\times\nabla_r]\right\}_{\rm n} \times \Psi(\boldsymbol{r}_{\rm s}) = {\rm const.}, \tag{3}$$

where $\boldsymbol{r}_{\rm s}$ denotes position of the system interface.

When the quantum dot has a disk shape of radius ρ_0 and thickness z_0 we treat the problem with cylindrical coordinates (ρ, ϕ, z). The origin of the system lies in the center of the disk and the z-axis is chosen along the rotation axis. Because of the system cylindrical symmetry, the wave function can be represented as

$$\Psi(\boldsymbol{r}) = \Phi(\rho,z)\exp({\rm i}l\phi), \tag{4}$$

where $l = 0, \pm 1, \pm 2, \ldots$ is the orbital quantum number. To derive the equation for $\Phi(\rho, z)$ we will use the adiabatic approximation [23,28], which represents an approximate solution in the form

$$\Phi(\rho, z) \approx R(\rho)Z(z).$$

First we consider the ground state of z-direction electron motion, and solve the one-dimensional quantum well problem. The wave function of this ground state has the form

$$Z(z) = \begin{cases} A\cos(kz), |z| < z_0/2, \\ B\exp(-\kappa|z|), |z| \geqslant z_0/2, \end{cases} \quad (5)$$

where

$$k(E, E_z) = \sqrt{2m_1(E)E_z}/\hbar,$$

$$\kappa = \sqrt{2m_2(E)(V_0 - E_z)}/\hbar,$$

$m_i(E)$ is the energy dependent electron effective mass inside ($i = 1$) and outside ($i = 2$) the dot, $E = E_\rho + E_z$ is the total electron energy that consists of the ρ and z direction motion effective energies. From the Ben Daniel–Duke boundary conditions [29] in z-direction we can obtain a transcendental equation.

$$\tan[k(E_\rho, E_z)z_0/2] = \frac{m_1(E)\kappa(E_\rho, E_z)}{m_2(E)k(E_\rho, E_z)}. \quad (6)$$

Eq. (6) gives the $E_z(E_\rho)$ dependence in an implicit form. With the wave function (5) (after proper normalization), we substitute in the three-dimensional Schrödinger equation and integrate out the z coordinate by taking the average

$$\hat{H}_\rho = \int \mathrm{d}z\, Z^*(z)\hat{H}Z(z).$$

When we neglect the kinetic energy contribution from the z-dependent part for $\rho \geqslant \rho_0$ [28] the quasi one-dimensional Schrödinger equation in the ρ-direction is given by the form

$$-\frac{\hbar^2}{2\tilde{m}_1}\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + \frac{\mathrm{d}}{\rho\mathrm{d}\rho} - \frac{l^2}{\rho^2}\right)R_1(\rho) = E_\rho R_1(\rho), \quad \rho < \rho_0,$$

$$-\frac{\hbar^2}{2m_2}\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + \frac{\mathrm{d}}{\rho\mathrm{d}\rho} - \frac{l^2}{\rho^2}\right)R_2(\rho) = (V_0 - E)R_0(\rho), \quad \rho \geqslant \rho_0, \quad (7)$$

with the spin-dependent boundary conditions

$$R_1(\rho_0) = R_2(\rho_0),$$

$$\frac{1}{\tilde{m}_1}\frac{\mathrm{d}R_1}{\mathrm{d}\rho}\bigg|_{\rho_0} - \frac{1}{m_2}\frac{\mathrm{d}R_2}{\mathrm{d}\rho}\bigg|_{\rho_0} + \frac{2\sigma(\tilde{\beta}_1 - \tilde{\beta}_2)}{\hbar^2\rho_0}R_1(\rho_0) = 0. \quad (8)$$

In Eqs. (7) and (8)

$$\frac{1}{\tilde{m}_1(E_\rho, E_z)} = \frac{1}{m_1(E)}\int_{|z|<z_0/2}\mathrm{d}z|Z(z)|^2 + \frac{1}{m_2(E)}\int_{|z|\geqslant z_0/2}\mathrm{d}z|Z(z)|^2,$$

$$\tilde{\beta}_1(E_\rho, E_z) = \beta_1(E)\int_{|z|<z_0/2}\mathrm{d}z|Z(z)|^2,$$

$$\tilde{\beta}_2(E_\rho, E_z) = \beta_2(E)\int_{|z|\geqslant z_0/2}\mathrm{d}z|Z(z)|^2,$$

and σ refers to the spin polarization along the z-axis. Eq. (7) with the boundary conditions (8) are used to obtain the solution of the problem. A formal solution of (7) is well known as follows:

$$R_1(\rho) \sim J_{|l|}(p\rho),$$

$$R_2(\rho) \sim K_{|l|}(g\rho),$$

where J_n and K_n are, respectively, the Bessel function and modified Bessel function,

$$p(E_\rho, E_z) = \sqrt{2\tilde{m}_1(E_\rho, E_z)E_\rho}/\hbar,$$

$$g(E_\rho, E_z) = \sqrt{2\tilde{m}_1(E_\rho, E_z)(V_0 - E)}/\hbar.$$

On using the boundary conditions (7), the equation that gives the energy states is found to be

$$\frac{p}{\tilde{m}_1}\left\{\frac{|l|}{p\rho_0}J_{|l|}(p\rho_0) - J_{|l|+1}(p\rho_0)\right\}K_{|l|}(g\rho_0) - \frac{g}{m_2}\left\{\frac{|l|}{g\rho_0}K_{|l|}(g\rho_0) - K_{|l|+1}(g\rho_0)\right\}J_{|l|}(p\rho_0) + 2\sigma l\frac{(\tilde{\beta}_1 - \tilde{\beta}_2)}{\hbar^2\rho_0}J_{|l|}(p\rho_0)K_{|l|}(g\rho_0) = 0. \quad (9)$$

We need the equation above, in addition to Eq. (6), to solve the problem. The total energy $E = E_z + E_\rho$ is a

complicated function of the dot parameters, the electron angular momentum, and spin. The energy states system consists of discrete levels numerated by a set of numbers $\{n, l, \sigma\}$, where n denotes nth solution of (9) with fixed l and σ. States with the same n and parallel (antiparallel) orbital momentum and spin (the same sign for l and σ) remain two-fold degenerate (the Kramers degeneracy). But levels with the same n and antiparallel orbital momentum and spin are separated from those with parallel orbital momentum and spin. The spin–orbit interaction removes the four-fold degeneracy of the energy states in the cylindrical quantum dots.

The energy of the confined electron states is found by numerically solving of the system of Eqs. (6) and (9). For cylindrical quantum dots, we use conventional notation for electron energy states: $n_\rho L_\sigma$, where n is the main quantum number of the ρ-plane motion, $L = S, P, D, \ldots$, denotes the absolute value of l, and σ refers to the electron spin direction in respect to the angular momentum direction ($+1$ if the directions are parallel and -1 otherwise). For all calculations we choose the lowest energy state in the z-direction.

In our calculations of the energy states for InAs quantum dots in a GaAs matrix we tuned the band parameters to take into account effects of strain in small InAs quantum dots. In accordance to results of Ref. [26], we use band structure parameters of InAs: energy gap is $E_{1g} = 0.52$ eV, spin–orbit splitting is $\Delta_1 = 0.48$ eV, the value of the nonparabolicity parameter is $E_{1p} = 3m_0P_1^2/\hbar^2 = 22.2$ eV, m_0 refers to the free electron effective mass. For GaAs we choose: $E_{2g} = 1.52$ eV, $\Delta_2 = 0.34$ eV, $E_{2p} = 24.2$ eV. The band offset parameter is taken as $V_0 = 0.55$ eV. It should be noted, that the larger E_{1g} makes the spin–orbit effect lower but at the same time more realistic for the strained quantum dots.

The spin splitting effect is zero for the lowest state energy $1S_{\pm1}$ follows from Eq. (9). The size dependence of the 1P level splitting $\Delta E_{1P} = E_{1P_{+1}} - E_{1P_{-1}}$ is shown in Fig. 1. The theory demonstrates noticeable spin splitting for relatively small quantum dots. The splitting is strongly dependent on the dot size and decreases rapidly when the size increases. But for dots with very small height the spin splitting is reduced. This is a result of electron wave function penetration into the barrier along the z direction. The averaged effective mass $\tilde{m}_1$ and spin–orbit interaction parameter

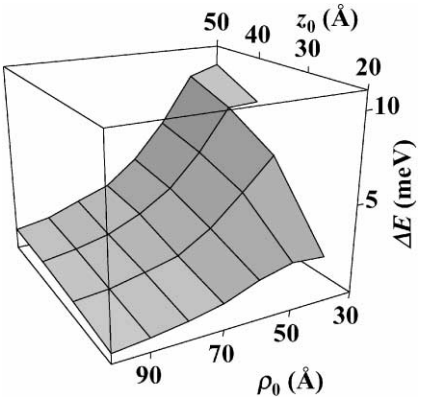

Fig. 1. Spin splitting of $|l| = 1$ levels for InAs quantum dots of different sizes.

$\tilde{\beta}_1$ are closer to those of the GaAs matrix. This makes the difference between $\tilde{\beta}_1$ and $\tilde{\beta}_2$ smaller. When z_0 increases the difference also increases and becomes z-independent after z_0 about 50 Å. This is a reason for the ΔE_{1P} dependence on ρ_0 with fixed z_0 to demonstrate the nonmonotonic behavior [28].

An interesting consequence of the spin–orbit interaction is the possibility to find quantum dot parameters, when one set of the spin split states is located below the dot top energy V_0 and another one is located above V_0. Basically, we can obtain a dot of a critical (maximal) size $\{z_{c0}, \rho_{c0}\}$ when only the $1P_{-1}$ electron states are bound. For InAs quantum dots we have calculated the following critical sizes: $\{15\,\text{Å}, 46\,\text{Å}\}, \{20\,\text{Å}, 39\,\text{Å}\}, \{30\,\text{Å}, 36\,\text{Å}\}, \{40\,\text{Å}, 32\,\text{Å}\}, \{50\,\text{Å}, 30\,\text{Å}\}$. When we reach the critical size and continue to reduce $\{z_0, \rho_0\}$, the $1P_{+1}$ levels become unbound very soon when $\{z_0, \rho_0\}$ are about few angstroms less than $\{z_{c0}, \rho_{c0}\}$. Thus, the range of InAs dot sizes when we have only the $1P_{-1}$ bound states is very narrow. In an experimental situation, it can be a random number of quantum dots with only the $1P_{-1}$ bound states. Certainly, the spin splitting impact becomes stronger for states with $|l| > 1$. It should be noted that the critical sizes mentioned above are found to be out of the adiabatic approximation validity region [28]. A detailed study of the critical dot sizes could only be performed with a more powerful numerical technique like the finite element method. Another possibility is to consider InSb quantum dots with a stronger SO interaction.

In short conclusion, we have studied theoretically the effect of the spin–orbit interaction on the energy spectrum of quantum dots. The calculation is based on a simple effective one electronic band Hamiltonian and spin-dependent boundary conditions. Our results show that the spin–orbit interaction can noticeably modify the energy states of narrow gap semiconductor InAs cylindrical quantum dots. The modification is strongly dependent on the dot sizes. The spin splitting in cylindrical quantum dots demonstrates a non-monotonic dependence on the dot size. The splitting can provide a situation when only the lower spin split electron energy states are bound in the dot.

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