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Energy levels of a parabolically confined quantum dot in the presence of spin-orbit interaction

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We present a theoretical study of the energy levels in a parabolically confined quantum dot in the presence of the Rashba spin-orbit interaction (SOI). The features of some low-lying states in various strengths of the SOI are examined at zero and nonzero magnetic fields. It is shown that the spin-polarized electronic states can be more easily achieved in a weakly confined dot when SOI is greater than a critical value of the confinement strength. The presence of a magnetic field enhances the possibility of the spin polarization and the SOI leads to different energy dependence on magnetic fields applied. Furthermore, in high magnetic fields, the spectra of low-lying states show basic features of Fock–Darwin levels as well as Landau levels.

I. INTRODUCTION

The state-of-the-art material engineering and nanofabrication techniques have made it possible to realize advanced semiconductor devices at atomic scales, such as quantum dots in which the electron motion along all directions is quantized and conducting electrons are confined within the nanometer distances. In such a system, few electrons are confined within a point-like structure so that it can behave as an artificial atom and, consequently, be used as electronic and optical devices such as memory chip, quantum computer, quantum cryptography, quantum-dot laser, etc. In recent years, the electronic, transport, optical, and optoelectronic properties of spin-degenerate quantum dots have been intensively investigated.

On the other hand, the progress made in realizing spin-polarized electronic systems on the basis of diluted magnetic semiconductors and narrow-gap semiconductor nanostructures has opened up a field of spin-electronics (or spintronics). As has been pointed out in a good review edited by Wolf and Awschalom, due to the unique nature of the spin-orbit interaction (SOI) in electronic materials, quantum transport of electrons in a spin-polarized system differs fundamentally from that in a spin-degenerate device. Thus, the spin-dependent effects can offer mechanisms and schemes for information storage and for increasing the speed of data processing. As a result, the electronic devices, such as spin-transistor, spin-waveguide, spin-filter, etc., have been proposed. Moreover, optical methods for injection, modulation and detection of spin-polarized electrons will eventually become the target for the development of spin-polarized nano-optoelectronic devices. At present, one of the major challenges for the application of the spintronic systems as working devices is to optimize the spin lifetimes of the carriers in the devices. It has been realized that in contrast to the diluted magnetic semiconductors in which the SOI is induced by the presence of an external magnetic field, spin-splitting of carriers can be achieved in narrow-gap semiconductor nanostructures even in the absence of the magnetic field. Experimental data have indicated that in narrow-gap semiconductor based quantum wells, such as InAlAs/InGaAs heterostructures, the higher-than-usual zero-magnetic-field spin-splitting (or spontaneous spin-splitting) can be realized by the inversion asymmetry of the microscopic confining potential due to the presence of the heterojunction. This kind of inversion asymmetry corresponds to an inhomogeneous surface electric field and, hence, this kind of spin-splitting is electrically equivalent to the Rashba spin-splitting or Rashba effect. From the fact that InGaAs-based quantum dots are normally fabricated using InAlAs/InGaAs heterojunctions, one would expect that the Rashba spin-splitting can be observed in these quantum dot systems and spin-polarized quantum dots can therefore be achieved. Practically, the spin-split quantum dots can be made from, e.g., an InAlAs/InGaAs heterostructure with a negative bias applied to the side gate.

In contrast to a spin-split quantum well structure in which the Rashba effect can be easily identified by, e.g., the magnetotransport experiments via measuring the Shubnikov–de Hass oscillations, the spintronic effects in a quantum dot cannot be easily observed using conventional transport measurements. Normally, optical measurements, such as optical absorption and transmission, cyclotron-resonance, etc., can be used to determine the energy

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II. APPROACHES

The device system under investigation is a typical quantum dot formed on top of a narrow-gap semiconductor heterojunction (such as an InGaAs/InAlAs-based heterostructure) grown along the Z direction, and the lateral confinement is formed in the XY plane. A perpendicular magnetic field \( B \) is applied along the growth direction of the quantum dot. We consider the situation where the SOI is mainly induced by the presence of the InGaAs/InAlAs heterojunction due to the Rashba effect. In such a case, the lowest order of the SOI can be obtained from, e.g., a k-p bandstructure calculation.\(^{12}\) It should be noted that when the SOI is induced by the Rashba effect due to the presence of the heterojunction and when the magnetic field is applied along the \( Z \) direction, the electronic subband structure along the growth direction (or the \( Z \) axis) depends very little on the SOI. Therefore, under the effective-mass approximation, the electronic structure along the XY plane and in the \( Z \) direction in a quantum dot can be treated separately. Including the contribution from SOI, the single-electron Hamiltonian describing the electronic system in the XY plane can be written as

\[
H = \frac{1}{2m^*} (p - eA)^2 + \frac{\alpha}{\hbar} (\sigma \times (p - eA))_z + V_c(r),
\]

where the Zeeman term is neglected for simplicity. Here, \( m^* \) is the electron effective mass in the XY plane, \( p = (p_x, p_y) \) with \( p_x = -i\hbar \partial / \partial X \) is the momentum operator, \( A = (Y, -X, 0)B/2 \) is the vector potential induced by the magnetic field which is taken in the symmetric gauge here for convenience, and \( V_c(r) \) is the confining potential of the quantum dot along the XY plane with \( r = (X^2 + Y^2)^{1/2} \). Furthermore, \( \alpha \) is the Rashba parameter which measures the strength of the SOI. Due to the Pauli spin matrices \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \), this Hamiltonian is a \( 2 \times 2 \) matrix. After rewriting this Hamiltonian in the cylindrical polar coordinate, we find that the solution of the corresponding Schrödinger equation is in the form of \( \Psi(X,Y) = e^{im\theta} \psi(r) \), where \( m \) is a good quantum number and \( \theta \) is an azimuthal angle to the \( X \) axis. Thus, the eigenfunction \( \psi(r) \) and eigenvalue \( E \) of the system can be determined by solving

\[
\begin{align*}
H_0 - E & \quad \quad e^{-i\theta} H_+ [\psi_1(r)] = 0, \\
- e^{i\theta} H_- & \quad \quad H_0 - E [\psi_2(r)] = 0,
\end{align*}
\]

with

\[
H_0 = - \frac{\hbar^2}{2m^*} \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} - \frac{m^2}{r^2} \right) + V^*(r) + \frac{m}{2} \hbar \omega_c,
\]

and

\[
H_\pm = \alpha \left( \frac{\partial}{\partial r} - \frac{m}{r} + \frac{r}{2l^2} \right).
\]

Here, \( \omega_c = eB/m^* \) is the cyclotron frequency, \( l = (\hbar/eB)^{1/2} \) is the radius of the ground cyclotron orbit, and \( V^*(r) \) is the effective trapping potential. It should be noted that the solution of Eq. (2) does not depend on \( \theta \), because the eigenfunction and eigenvalue can be obtained, in principle, by solving

\[
[(H_0 - E)^2 + H_+ H_-] \psi_i(r) = 0,
\]

where \( i = 1, 2 \). Eq. (3) is a fourth-order differential equation. There is no simple and analytical solution to this equation. In this article, we therefore attempt a tractable approach to solve the problem.

For the case of a parabolically confined quantum dot, we have the confining potential \( V_c(r) = m^* \omega_c^2 r^2 / 2 \) where \( \omega_c \) is the characteristic frequency of the confinement. For convenience, we define \( \Omega = \sqrt{3 \omega_c^2 + \omega_o^2} \) and \( a = (2\hbar/m^* \Omega)^{1/2} \). After setting \( r^2 = a \tilde{r}^2 \) and assuming \( \psi_i(r) = e^{-i\tilde{r}^2/2} C_i(\tilde{r}) \), Eq. (2) readily becomes

\[
\begin{align*}
(h_0 + \mathcal{E}) & \quad \quad - e^{-i\theta} h_+ [C_1(\tilde{r})] = 0, \\
- e^{i\theta} h_- & \quad \quad h_0 + \mathcal{E} [C_2(\tilde{r})] = 0,
\end{align*}
\]

where \( h_0 = \chi^2 \partial^2 / \partial \tilde{r}^2 + (|m| - x + 1) \partial / \partial x + (|m| + m) / 2x - (1 - \omega_c / \Omega) / 2 \), \( \mathcal{E} = E \hbar \Omega - m \omega_c / 2 \), \( \chi = \alpha \sqrt{a} \) \( \hbar \), and \( a = (\alpha \hbar / \sqrt{3 m^* \Omega}) \). In this article, we are interested in finding the energy spectrum of a quantum dot in the presence of the SOI and of a magnetic field. We assume that the electron wave functions are in the form

\[
C_1(\tilde{r}) = \sum_{N = 0}^{\infty} C_{m,N} L_N^m(\tilde{r}),
\]

and

\[
C_2(\tilde{r}) = \sum_{N = 0}^{\infty} D_{m,N} L_N^m(\tilde{r}),
\]

with \( L_N^m(\tilde{r}) \) being the associated Laguerre polynomial. Thus, introducing \( C_1(\tilde{r}) \) into Eq. (4) and carrying out the normalization, we obtain two coupled equations which determine the energy \( E \) and the coefficients \( C_{m,N} \) and \( D_{m,N} \):

\[
(E - E_0^{m,N}) C_{m,N} - A_m \hbar \Omega \int_{0}^{1} \tilde{r} L_N^m(\tilde{r}) D_{m,N+1,1}^{m,N}/2 = 0
\]

where \( E_0^{m,N} = \frac{m^* \omega_c^2 a^2}{2l^2} \).
and
\[(E-E_{m,N}^0)D_{m,N}+A_{\alpha}h\Omega \Delta_{N,N'}^m C_{m-1,N'+1}^m/2=0,\]
where \(E_{m,N}^0=m\hbar \omega_c/2+2(N+|m|+1)\hbar\Omega/2\) is the energy of a parabolically confined quantum dot in the absence of the SOI:
\[I_{N,N'}^m=\omega N(N+1)\delta_{N,N'} N_{N',N},\]
when \(m\geq 1\) for \(I_{N,N'}^m\) and \(m<0\) for \(I_{N,N'}^m\) and, otherwise,
\[I_{N,N'}^m=(\omega N+1)(N+|m|+1)\delta_{N,N'} N_{N',N},\]
with \(\omega=\omega_c/\Omega\). These results suggest that the SOI in a quantum dot can result in band mixing and shifting. Using sequence relations given by Eqs. (5) and (6), the electron energy \(E\) as well as the coefficients \(C_{m,N}\) and \(D_{m,N}\) can be determined.

III. NUMERICAL RESULTS AND DISCUSSION

In the present study, we examine the dependence of the energy levels and the occupation of electrons to different states on the strength of the SOI and of the magnetic field in a few-electron quantum dot system. We take the Rashba parameter to be \(\alpha=\omega_c/\Omega\) in eV m, in conjunction with recent experimental data realized in InAlAs/InGaAs heterostructures.\(^7,15\) The size effects of the dot are also considered. For weakly and strongly confined dots, we take the typical values of the confining potential as \(V_c=h\omega_0=1\) and \(10\) meV, respectively. The condition of electron number conservation is applied to determine the Fermi energy of the system. For demonstration of how electrons occupy to the different energy levels in the presence of SOI, we assume there are ten electrons in the dot. Moreover, in the present study the effect of the SOI on lifetimes of an electron in different states is not taken into consideration.\(^21\) The inclusion of the many-body effects induced by Coulomb interaction in a quantum dot is a higher order effect to affect the energy spectrum, although the Coulomb interaction can result in an exchange enhancement which may affect the results qualitatively.\(^22\) Later, we discuss the effect of the SOI on energy levels of the low-lying states at zero and nonzero magnetic fields. For convenience of the discussion, we label the energy states with quantum numbers \(\{N,m,\chi\}\), where \(\chi=\uparrow\) or \(\downarrow\) (\(\chi=\uparrow\) or \(\downarrow\)) referring to the down (up) spin branch of the energy states.

A. \(B=0\)

The low-lying energy states in weakly \((V_c=1\) meV\) and strongly \((V_c=10\) meV\) confined quantum dots are shown in Figs. 1 and 2, respectively, as a function of the Rashba parameter \(\alpha\) in the absence of a magnetic field. At \(B=0\), the SOI lifts the spin-degeneracy of the electronic states with the same orbital momenta and, as a result, a twofold Kramers degeneracy can be observed. In the absence of SOI or \(\alpha=0\), energies with the same quantum number \(\{N,m\}\) are degenerate and, therefore, two electrons are located in a state with \(\{N,m\}\) and five lowest states are occupied by ten electrons. With increasing \(\alpha\), energies of the down (up) spin states decrease (increase) and more electrons are located in the lower-energy spin-down states with different \((N,m)\) numbers.

For a weakly confined dot (see Fig. 1), SOI plays an important role in modifying the electron energies and the occupancy of electrons to different states. It should be noted that for an InGaAs-based quantum dot with a weak confinement, the SOI can lead to a situation where the energy of a state with \(\{N+1,m,d\}\) or \(\{N,m+1,d\}\) can be lower than that with \(\{N,m,u\}\). As a result, the state \(\{N+1,m,d\}\) or \(\{N,m\)
+1, d} which is empty at \( \alpha = 0 \) can become occupied due to the SOI, whereas the state \( \{N,m,u\} \) which is occupied at \( \alpha = 0 \) can be empty at \( \alpha \neq 0 \). We find that there exists a critical value of the strength of the SOI \( \alpha_c \) above which the system is fully spin-polarized. For example, in Fig. 1 at relatively large values of \( \alpha \geq \alpha_c \sim 10^{-10} \text{ eV m} \), all ten electrons are in the spin-down states, which implies that the system is fully spin-polarized. For comparison, we note that at \( \alpha = 5 \times 10^{-11} \text{ eV m} \) only seven electrons are in the spin-down branches. An important conclusion we draw from these theoretical results is that the SOI induced by the Rashba effect in a quantum dot is able not only to lift the spin-degeneracy of electrons and to alter the electronic subband energies but also to play an important role in varying the spin-polarization of the device system.

For a strongly confined dot (see Fig. 2), the energy gaps among different \((N,m)\) states are enhanced significantly and these gaps are mainly determined by the confinement of the dot. As a consequence, when \( \alpha < 1.5 \times 10^{-10} \text{ eV m} \) the SOI-induced strong band-mixing effects that we saw in Fig. 1 are significantly weakened. We find that in order to achieve a strong spin-polarization in the system, a relatively large value of \( \alpha \) is required. Namely, the value \( \alpha_c \) increases with increasing the strength of the quantum confinement for a dot. The results shown in Figs. 1 and 2 indicate that a strong effect of the SOI and a strongly spin-polarized system can be observed in a weakly confined quantum dot.

**B. B \neq 0**

When a perpendicular dc magnetic field is applied to a quantum dot, the nature of the spin-dependent energy spectrum can become even richer in terms of physics due to the coupling of the magnetic field to the confining potential of the dot and to the potential induced by SOI. It should be noted that in the present study, in order to examine the net contribution to the energy spectrum of a dot from the SOI, we have neglected the effects induced by the Zeeman splitting. In Figs. 3 and 4 we plot the low-lying energy levels as a function of the Rashba parameter for different magnetic fields \( B = 1 \) and \( 3 \text{ T} \), respectively, at a fixed quantum dot confinement \( V_c = 1 \text{ meV} \). In the absence of the Zeeman splitting, the SOI induced by the Rashba effect at \( B \neq 0 \) can lift the magnetic degeneracy of electrons. Namely, the states with the \( \pm |m| \) number can have different energies. We find that in this situation, the occupancy of electrons to different states has some unique features. On one hand, the presence of the magnetic field can increase the energy gaps among the states with the quantum number \((N,m)\). Thus, similar to a strongly confined dot, the magnetic field may increase the critical value \( \alpha_c \) above which the system is fully spin-polarized. This effect can be seen at a relatively low-\( B \)-field (see Fig. 3) where \( \alpha_c \sim 7.25 \times 10^{-11} \text{ eV m} \) is found. On the other hand, when the magnetic field predominates the electronic energy spectra, the energy states with the negative magnetic quantum number \( m \) and the spin-down branches are more preferable for an electron to stay. As a result, the presence of a \( B \) field can increase the spin-polarization of a quantum dot. This effect is more pronounced in the presence of a higher magnetic field (see Fig. 4 where \( \alpha_c \sim 6.75 \times 10^{-11} \text{ eV m} \)) so that the states with positive quantum number \( m \) and spin-up orientation have higher energies relative to the \( \{0, -|m|, \uparrow\} \) states. Furthermore, after comparing the \( \alpha_c \) values obtained in Figs. 1, 3, and 4, we note that the presence of the magnetic field can result in a lower value of \( \alpha_c \) and, consequently, the stronger spin-polarization can be achieved in a dot in the presence of the SOI and of a magnetic field.

In Fig. 5, we show the spectra of low-lying states as a function of the magnetic field at a fixed Rashba parameter \( \alpha = 10^{-11} \text{ eV m} \) for a weakly confined dot \( V_c = 1 \text{ meV} \). We find that in such a case, because \( \alpha \) is relatively small, the

![FIG. 3. Energy of low-lying levels vs the Rashba parameter at B = 1 T and V_c = 1 meV. The presence of the magnetic field reduces the spin-polarization and a fully spin-polarized ten-electron dot is achieved at \( \alpha > \alpha_c \sim 7.25 \times 10^{-11} \text{ eV m} \).](image-url)

![FIG. 4. Energy of low-lying states vs \( \alpha \) at B = 3 T and V_c = 1 meV. In the lower panel, \( \{0, -|m|, \uparrow\} \) states are assembled in different groups and the dashed line refers to the energy of the \( \{0, \uparrow\} \) level. A fully spin-polarized ten-electron dot is achieved at \( \alpha > \alpha_c \sim 6.75 \times 10^{-11} \text{ eV m} \).](image-url)
of quantum dots. Fig. 5 indicate that the crossover of the energy states with those with negative magnetic quantum number $m$. The inset shows the results obtained at low-$B$ fields.

In the presence of a perpendicular magnetic field, we have found that a coefficient $A_a$ affects the energy levels of a parabolically confined quantum dot. A nonperturbative approach to deal with SOI in a quantum dot has been developed. The main theoretical results obtained from this study are summarized as follows.

We have demonstrated that SOI in a quantum dot can change not only the energy levels of the system but also the spin-polarization of the device. It has been found that there exists an critical value of the strength of the SOI $\alpha_c$ above which an $N$-electron system can be fully spin-polarized. In the absence of a magnetic field, $\alpha_c$ increases with increasing confining potential of the dot.

In the presence of a perpendicular magnetic field, we enter a regime with different competing energies, where magnetic potential, confining potential of the dot and potential induced by the SOI are coupled. As a result, the presence of the magnetic field can result in much richer features of the system. When the cyclotron energy is larger than the confining potential of a dot, there is a hybridization of the Landau levels from the spatial confinement.

IV. CONCLUDING REMARKS

In this article, we have examined how the Rashba SOI affects the energy levels of a parabolically confined quantum dot. A nonperturbative approach to deal with SOI in a quantum dot has been developed. The main theoretical results obtained from this study are summarized as follows.

We have demonstrated that SOI in a quantum dot can change not only the energy levels of the system but also the spin-polarization of the device. It has been found that there exists an critical value of the strength of the SOI $\alpha_c$ above which an $N$-electron system can be fully spin-polarized. In the absence of a magnetic field, $\alpha_c$ increases with increasing confining potential of the dot.

In the presence of a perpendicular magnetic field, we enter a regime with different competing energies, where magnetic potential, confining potential of the dot and potential induced by the SOI are coupled. As a result, the presence of the magnetic field can result in much richer features of the spintronics properties in a quantum dot. The energy spectra and the value of $\alpha_c$ in a dot depend strongly on the strength of the magnetic field. In different $B$-field regimes, the energy levels of spin-modified states have different dependence of the magnetic field.

We have found that a coefficient $A_a=(\alpha h)\sqrt{2m^*/h\Omega}$ with $\Omega=(\Delta_{0}^{2}+\omega_{c}^{2})$ plays a role in switching the SOI. When $A_a>1$ a strong effect of the SOI on energy levels can be observed, whereas the effects of SOI can be neglected when $A_a<1$. Thus, (1) the strong spin-polarization can be

![Fig. 5. Dependence of the energy levels on the strength of the magnetic field at a fixed confinement $V_z=1$ meV and a fixed $\alpha=10^{-11}$ eV m. Here $E_1, E_2$, and $E_3$ groups include respectively the states with $\{0,0,-|m|,1\}, \{1,-|m|,1\}, \{N=1,N+1,1,1\}, \{N=2,0,-|m|,1\},$ and $\{N=-2,N+2,1,1\}$. The higher index groups can be generated via the rule of the least sum of the quantum numbers. The inset shows the results obtained at low-$B$ fields.](image1)

![Fig. 6. Magnetic field dependent level scheme with $V_z=10$ meV at $a=1 \times 10^{-11}$ eV m. The magnetic field induced energy gaps characterize the level assemblies. The energy levels are just Fock–Darwin states with Rashba SOI.](image2)
achieved in a weakly confined dot at zero and nonzero magnetic fields; (2) the characteristics of the Fock–Darwin scheme and the Landau-type levels are revealed when the magnetic field is strong enough; and (3) the effective SOI in the system decreases with increasing magnetic field and confining potential of the dot.

On the basis that the energy levels in spin-degenerate quantum dot systems have been well studied using optical and optoelectronic measurements, we believe these experimental techniques can also be used to examine the energy spectra of a quantum dot with SOI. We therefore hope that the theoretical results obtained in this study can be verified experimentally.

Although the present work deals with single-particle properties of a quantum dot in the presence of SOI, some many-body effects induced by Coulomb interaction can be investigated on the basis of these results. For example, using the energy spectrum and wave function obtained from this study, we can calculate the collective excitation modes and fast-electron optical spectrum using, e.g., a random-phase approximation. However, for the case of a spin-split quantum dot, these further studies require numerical calculations considerably and we therefore do not attempt them in the present work.

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