Electron correlations in a quantum dot with Bychkov-Rashba coupling

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We report on a theoretical approach developed to investigate the influence of the Bychkov-Rashba interaction on a few interacting electrons confined in a quantum dot. We note that the spin-orbit coupling profoundly influences the energy spectrum of interacting electrons in a quantum dot. Interelectron interaction causes level crossings in the ground state and a jump in magnetization. As the coupling strength is increased, that jump is shifted to lower magnetic fields. Low-field magnetization will therefore provide a direct probe of the spin-orbit coupling strength in a quantum dot.

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It has long been recognized that a two-dimensional electron gas (2DEG) in narrow-gap semiconductors, particularly in InAs-based systems with its high values of the g factor, exhibit zero-field splitting due to the spin-orbit (SO) coupling.[1] This coupling is also the driving mechanism for making futuristic devices based on controlled spin transport, such as a spin transistor,[2,3] where the electron spins would precess (due to the SO coupling) while being transported through the 2DEG channel. Tuning of this precession in the proposed spin transistor would provide an additional control that is not available in conventional devices, but may be crucial for the rapidly emerging field of semiconductor spintronics.[3] Hence the upsurge of interest in recent years for a better understanding of the SO coupling in nanostructured systems.

The spin-orbit interaction in semiconductor heterostructures can be caused by an electric field perpendicular to the 2DEG. Riding on an electron, this electric field will be *felt* as an effective magnetic field lying in the plane of the 2DEG, perpendicular to the 2D wave vector k of the electron. We consider the Bychkov-Rashba (BR) Hamiltonian,[4,5]

$$\mathcal{H}_{\mathrm{BR}} = \frac{e\hbar^2}{(2m_0c)^2}(\vec{k}\times\vec{\mathbf{E}})\cdot\vec{\sigma},$$

where $\vec{\mathbf{E}}$ is the confining electric field at the 2DEG, $\vec{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$ denotes the Pauli spin matrices, and c is the speed of light. The single-electron Hamiltonian for the 2DEG with the electric field normal to the interface, $\vec{\mathbf{E}}=(0,0,E_z)$, takes the form

$$\mathcal{H} = -\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+\mathrm{i}\alpha\left(\sigma_y\frac{\partial}{\partial x}-\sigma_x\frac{\partial}{\partial y}\right),$$

where α is the SO coupling parameter which is sample dependent and is proportional to the electric field (interfacial and externally applied). Experimentally observed values of α lie in the range of $5-45$ meV nm.[1] The energy dispersion then consists of two branches:

$$\mathcal{E}^{\pm}(k) = \frac{\hbar^2}{2m^*}k^2 \pm \alpha k,$$

with an energy separation $\Delta_{\mathrm{SO}}=\mathcal{E}^{+}-\mathcal{E}^{-}=2\alpha k$ for a given k. The corresponding wave functions are

$$\Psi^{\pm}(k_x,k_y) = \chi^{\pm}(k_x,k_y)e^{\mathrm{i}k_x x+\mathrm{i}k_y y} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm\dfrac{-\mathrm{i}k_x+k_y}{k}\end{pmatrix}e^{\mathrm{i}k_x x+\mathrm{i}k_y y}.$$

The spin parts of the wave functions $\chi^{\pm}(k_x,k_y)$ are mutually orthogonal and $\langle\chi^{\pm}|\sigma_z|\chi^{\pm}\rangle=0$. Therefore in the states $\Psi^{\pm}$ the spins of the electrons lie in the xy plane and point in opposite directions. In addition,

$$\langle\chi^{\pm}|\sigma_x|\chi^{\pm}\rangle = \frac{2k_y}{k}, \quad \langle\chi^{\pm}|\sigma_y|\chi^{\pm}\rangle = -\frac{2k_x}{k},$$

i.e., the spins are *perpendicular* to the momentum (k_x,k_y). Spatial alignment of spins therefore depends on the wave vector.[1]

Spin-orbit interaction and electron-electron interactions are responsible for a variety of interesting effects in quantum dots.[6] In this paper, we present a numerically exact treatment of the BR Hamiltonian in a system of interacting electrons confined in a parabolic quantum dot (QD)[7,8] under the influence of an external magnetic field. More specifically, we explore the energy spectra and magnetization[9] of a few interacting electrons in a quantum dot in the presence of SO coupling. It should be pointed out that while a large number of theoretical work has been reported as yet in the literature for a 2DEG[10] and a QD[11,12] with spin-orbit coupling, in most cases, the electron-electron interaction has been ignored (or treated within an approximation[13]) due to its inherent complexity.

Let us begin with the single-electron states. Unlike the case of a circular quantum dot with hard walls where exact analytical results for the single-electron energy spectrum (in the presence of the SO interaction) are available, for the more realistic case of a parabolic QD, the energy spectrum can only be obtained numerically. In the presence of the BR interaction, the Schrödinger equation consists of two parts:

$$-\frac{\hbar^2}{2m^*}\nabla^2\psi^{\uparrow}+\alpha\nabla^-\psi^{\downarrow}+v_c(\mathbf{r})\psi^{\uparrow}=\varepsilon\psi^{\uparrow},$$

$$-\frac{\hbar^2}{2m^*}\nabla^2\psi^{\downarrow}-\alpha\nabla^+\psi^{\uparrow}+v_c(\mathbf{r})\psi^{\downarrow}=\varepsilon\psi^{\downarrow}, \quad (1)$$

where ψ is a two-component spinor,

$$\psi=\begin{pmatrix}\psi^{\uparrow}\\ \psi^{\downarrow}\end{pmatrix}, \quad (2)$$

$\nabla^{\pm}=\partial/\partial x\pm i(\partial/\partial y)$, and $v_c(\mathbf{r})$ is the confinement potential. We seek a solution of the form

$$\psi^{\uparrow}=f_{\uparrow}(r)e^{im_{\uparrow}\theta},$$

$$\psi^{\downarrow}=f_{\downarrow}(r)e^{im_{\downarrow}\theta},$$

which with Eq. (1) yields $m_{\uparrow}=m_{\downarrow}-1(=m)$. In the case of a parabolic confinement potential $v_c=\frac{1}{2}m^*\omega_0^2r^2$, the radial equations are

$$xf_{\uparrow}''+f_{\uparrow}'+\left(\nu-\frac{m^2}{4x}-\frac{x}{4}\right)f_{\uparrow}-\beta x^{1/2}\left(f_{\downarrow}'+\frac{m+1}{2x}f_{\downarrow}\right)=0,$$

$$xf_{\downarrow}''+f_{\downarrow}'+\left(\nu-\frac{(m+1)^2}{4x}-\frac{x}{4}\right)f_{\downarrow}+\beta x^{1/2}\left(f_{\downarrow}'-\frac{m}{2x}f_{\uparrow}\right)=0, \quad (3)$$

where $x=r^2/a^2$, $a^2=\hbar/(m^*\omega_0)$, $\nu=\varepsilon/(2\hbar\omega_0)$ and $\beta=m^*a\alpha/\hbar^2$. When $\beta=0$ (i.e., $\alpha=0$), Eq. (3) reduces to two uncoupled Laguerre equations with solutions

$$f_{\uparrow}=f_{nm}=e^{-x/2}x^{|m|/2}L_n^{|m|},$$

$$f_{\downarrow}=f_{n,m+1},$$

with the energies

$$\nu_{nm}=n+\frac{|m|+1}{2}. \quad (4)$$

In the presence of an external magnetic field B the term

$$\mathcal{H}_B=\frac{e^2B^2r^2}{8m^*c^2}-\frac{ieB\hbar}{2m^*c}\frac{\partial}{\partial\theta}+\frac{e\alpha B}{2\hbar c}r\begin{pmatrix}0 & e^{-i\theta}\\ e^{i\theta} & 0\end{pmatrix}+\frac{1}{2}g\mu_BB\sigma_z$$

has to be added to the spinor Hamiltonian $\mathcal{H}$. Here the first two terms (diagonal) are due to the interaction of the orbital motion and the magnetic field. The third (nondiagonal) term originates from the vector potential part $\vec{A}=(B/2)(-y,x,0)$ in the minimal coupling scheme $\alpha/\hbar[\vec{\sigma}\times(\vec{p}-e/c\vec{A})]_z$ of the SO interaction. The last term gives the Zeeman energies of the components of the spinors. When $\beta=0$ the functions f_{nm} will still be eigenstates of the Hamiltonian provided that we replace the single particle energies ν_{nm} with the expressions

$$\nu_{nm}^{\sigma}=n+\frac{|m|+1}{2}-\frac{\omega_c}{4\Omega}m+\sigma\frac{g\mu_BB}{4\hbar\Omega},$$

where signs $\sigma=\pm1$ correspond to the upper and lower components of the spinor. Furthermore, for the angular velocity ω_0 related to the harmonic confinement potential we have to substitute the effective angular velocity $\Omega=\omega_0(1+\omega_c^2/(4\omega_0^2))^{1/2}$ where $\omega_c=eB/(m^*c)$ is the cyclotron frequency.

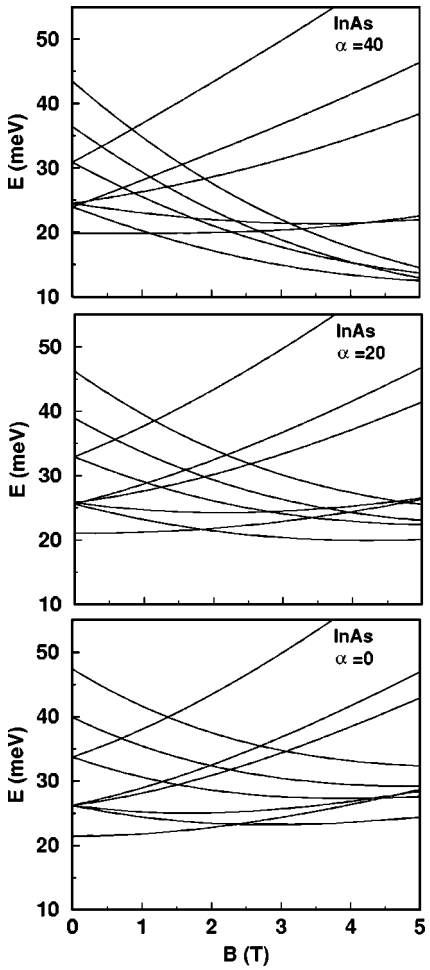

FIG. 1. Energy spectrum of a two-electron InAs quantum dot versus the applied magnetic field for different values of the Bychkov-Rashba interaction parameter α (meV nm). For clarity, at each value of the magnetic field and for a given total angular momentum, only the lowest energy is plotted. The Zeeman energy is also included.

For the $\beta\neq0$ case which is our main concern here, we use the following expansion:

$$f_{\uparrow}=\sum_{n=0}^{\infty}c_n^{\uparrow}f_{nm},\quad f_{\downarrow}=\sum_{n=0}^{\infty}c_n^{\downarrow}f_{n,m+1}.$$

For the angular momenta $m\geqslant0$ we find that the expansion coefficients satisfy the equations[11]

$$(\nu-\nu_{nm}^{\uparrow})c_n^{\uparrow}=\frac{\beta}{2}[\eta^+(n+m+1)c_n^{\downarrow}+\eta^-nc_{n-1}^{\downarrow}],$$

$$(\nu-\nu_{n,m+1}^{\downarrow})c_n^{\downarrow}=\frac{\beta}{2}[\eta^+c_n^{\uparrow}+\eta^-c_{n+1}^{\uparrow}],$$

and the equations

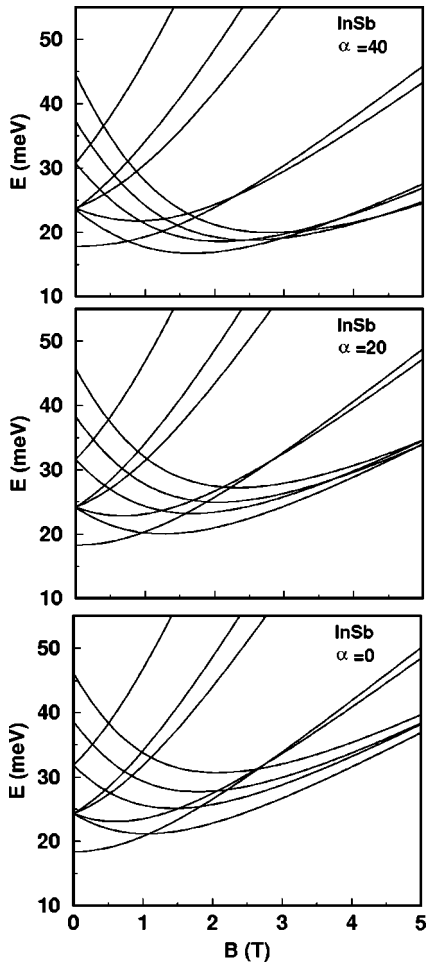

FIG. 2. The same as in Fig. 1, but for the InSb quantum dot system.

$$(\nu - \nu_{nm}^{\uparrow})c_n^{\uparrow} = -\frac{\beta}{2}[\eta^- c_n^{\downarrow} + \eta^+ c_{n+1}^{\downarrow}],$$

$$(\nu - \nu_{n,m+1}^{\downarrow})c_n^{\downarrow} = -\frac{\beta}{2}[\eta^-(n-m)c_n^{\uparrow} + \eta^+ n c_{n-1}^{\uparrow}],$$

for states with $m<0$, and $\eta^{\pm}=1\pm ea^2B/(\hbar c)$. Solutions of these eigensystems provide the single-electron energies ε and the spinor wave functions ψ [Eq. (2)], which have been investigated earlier by several authors in a variety of ways.[12]

For a system of interacting electrons we diagonalize the many-body Hamiltonian in a basis consisting of noninteracting many-body states, which in turn are constructed as antisymmetrized direct products of the two-component spinors ψ. Since the Coulomb force is independent of the spin orienation we evaluate the sum

$$\langle \psi_{\lambda_1}\psi_{\lambda_2}|V_{\mathrm{Coul}}|\psi_{\lambda_3}\psi_{\lambda_4}\rangle = \sum_{\sigma_1,\sigma_2}\langle \psi_{\lambda_1}^{\sigma_1}\psi_{\lambda_2}^{\sigma_2}|V_{\mathrm{Coul}}|\psi_{\lambda_3}^{\sigma_2}\psi_{\lambda_4}^{\sigma_1}\rangle,$$

$\lambda=(n,m)$, of four terms. An explicit expression for these terms for a parabolic QD can be found in Ref. 8.

In our numerical investigations, we choose InAs and InSb quantum dots with parameters, $m^*/m_0=0.042$, $\epsilon=14.6$, $g=14$ and $m^*/m_0=0.014$, $\epsilon=17.88$, $g=40$, respectively. InSb quantum dots are also considered here because of its high g values and a relatively large α ($\sim$14 meV nm).[14] In both systems, we choose $\hbar\omega_0=7.5$ meV. The energy spectrum of the two-electron state in InAs QD is shown in Fig. 1 for various values of the BR coupling parameter α. Similar results for InSb QD are presented in Fig. 2.

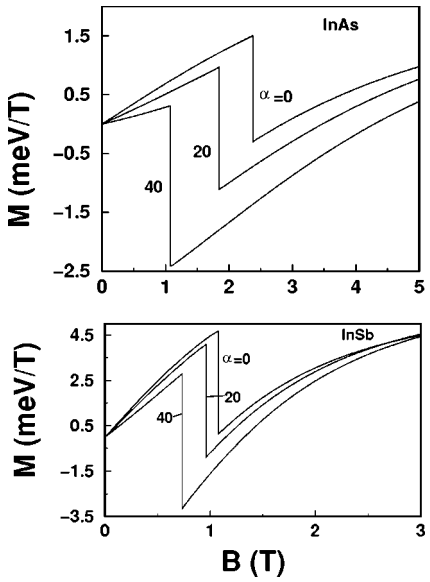

FIG. 3. Magnetization in the ground state for various values of the SO coupling strength and for the two QD systems.

The essential feature of the energy spectra at $\alpha=0$ is that with the increase in the magnetic field, the ground state moves from $J=0$ to $J=2$ ($J=m+s_z$ is the total angular momentum). This is already well established in the literature.[9] This level crossing persists for a nonzero value of α, but the crossing point shifts to lower magnetic fields. This shift of the crossing point can perhaps be observed experimentally by a variety of ways, such as capacitance spectroscopy, or by transport spectroscopy.[8]

The results for magnetization at the ground state, defined as $M=-\partial E/\partial B$, where E is the total energy of the system, of quantum dots with or without the BR interaction is presented in Fig. 3. Magnetization is a fundamental thermodynamic quantity that reflects the change of the ground state electron energy in a magnetic field,[15] thereby providing valuable information about many-electron dynamics of the QD in a magnetic field. We have established earlier that oscillations in magnetization in a few electron-quantum dots are a direct consequence of the effects related to the electron-electron interaction between the two-dimensional electrons confined in the dot.[9]. A jump in M occurs at a magnetic field where the ground state changes from one angular momentum to another (Figs. 1 and 2). Similar behavior is also expected in a nanoscopic quantum ring.[16] With increasing strength of α, this jump in magnetization at the energy-level crossing is pushed to lower magnetic fields. For the InAs QD this shift can be as large as $\sim$1.5 Tesla when α is increased from zero to 40 meV nm. Therefore, low-field magnetization measurements of quantum dots could be a direct probe of the SO coupling strength.

In closing, we have developed a theoretical approach where the SO interaction is treated via exact diagonalization of the Hamiltonian for interacting electrons confined in a parabolic QD. Coulomb interaction causes energy levels to cross and at the crossing point magnetization shows a jump. In a magnetic field the strength of the SO coupling is proportional to the field (in addition to the coupling parameter and the angular momentum). Hence, the effect of the coupling is more prominent for slopes of the higher angular momenta energy curves. As a consequence, an increase in the SO coupling strength causes the energy level crossings to move to weaker fields and the jump in magnetization shows a large shift to weaker magnetic fields. This result can be exploited to tune the SO coupling strength that might be useful for spin transport. Our theoretical approach can be extended to include a larger number of electrons in the dot. Details will be published elsewhere.

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