Magnetization of interacting electrons in anisotropic quantum dots with Rashba spin–orbit interaction

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Abstract
Magnetization of anisotropic quantum dots in the presence of the Rashba spin–orbit interaction has been studied for three and four interacting electrons in the dot for non-zero values of the applied magnetic field. We observe unique behaviors of magnetization that are direct reflections of the anisotropy and the spin–orbit interaction parameters independently or concurrently. In particular, there are saw-tooth structures in the magnetic field dependence of the magnetization, as caused by the electron–electron interaction, that are strongly modified in the presence of large anisotropy and high strength of the spin–orbit interactions. We also report the temperature dependence of magnetization that indicates the temperature beyond which these structures due to the interactions disappear. Additionally, we found the emergence of a weak sawtooth structure in magnetization for three electrons in the high anisotropy and large spin–orbit interaction limit that was explained as a result of merging of two low-energy curves when the level spacings evolve with increasing values of the anisotropy and the spin–orbit interaction strength.

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Magnetization of quantum confined planar electron systems, e.g. quantum dots (QDs), the so-called artificial atoms [1–3], and quantum rings [4] is an important probe that manifests entirely on the properties of the energy spectra. This is a thermodynamical quantity that for the QDs has received some experimental attention [5–7], particularly after the theoretical prediction that the electron–electron interaction is directly reflected in this quantity [8]. In addition to the large number of theoretical studies reported in the literature on the electronic properties of isotropic quantum dots, there has been lately some studies on the anisotropic quantum dots, both theoretically [10,11] and experimentally [12]. Theoretical studies of the magnetization of elliptical QDs have also been reported [13]. Effects of the Rashba spin–orbit interaction (SOI) [14] on the electronic properties of isotropic [15] and anisotropic quantum dots [16] have been investigated earlier. An external electric field can induce the Rashba spin–orbit interaction [17] which couples different spin states and introduces level repulsions in the energy spectrum [15,16,18]. This coupling is an important ingredient for the burgeoning field of semiconductor spintronics, in particular, for quantum computers with spin degrees of freedom as quantum bits [19,20]. Three-electron quantum dots are particularly relevant in this context [21,22]. Electronic properties of parabolic quantum dots, including magnetization, was reported recently in the case of the ultrastrong Rashba SO coupling limit [23]. Here we report on the magnetic field dependence of the magnetization of an anisotropic QD containing several interacting electrons, particularly three and four, in the presence of the Rashba SOI. Our present work clearly demonstrates how magnetization of the QDs uniquely reflects the influence of anisotropy and the Rashba SOI, both concurrently as well as individually as the strengths of the SOI and the anisotropy are varied independently. The temperature dependence of magnetization is also studied here, where we noticed the gradual disappearance of the interaction induced structures in magnetization with increasing temperature. Another important feature that we found in our present study is the emergence of a weak sawtooth structure in three-electron magnetization result in the high anisotropy and large spin–orbit interaction limit that we explain as a result of merging of two low-energy curves when the level spacings evolve with increasing parameters. With the help of the theoretical insights presented here, experimental studies of magnetization will therefore provide valuable information on the inter-electron effects, the Rashba spin–orbit coupling and the degree of anisotropy of the quantum dots.

At zero temperature the magnetization $M$ of the QD is defined as $M = - \frac{\partial E_g}{\partial B}$ where $E_g$ is the ground state energy of the system [8,9]. We have studied the magnetic field dependence of $M$ by evaluating the expectation value of the magnetization operator $\hat{M} = - \frac{\partial \hat{H}}{\partial \hat{B}}$, where $\hat{H}$ is the system Hamiltonian. Since the Coulomb...
interaction is independent of $\mathbf{B}$, $\hat{\mathbf{m}}$ would be just a one-body operator, i.e., we can ignore the interaction part from the Hamiltonian. The Hamiltonian of a single-electron system subjected to an external magnetic field with the vector potential $\mathbf{A} = (-\mathbf{B}, 0)$, the confinement potential, and the Rashba SOI is

$$\mathcal{H} = \frac{\hbar}{2m_e} \left( \mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 + \frac{\hbar}{2m_e} \left( \omega_y^2 x^2 + \omega_y^2 y^2 \right) + \frac{\hbar}{\alpha c} \left( \sigma \times \left( \mathbf{p} - \frac{e}{c} \mathbf{A} \right) \right)_z + \frac{1}{2} \hbar g_e \alpha \mathbf{B} \sigma_z.$$

The first term of the Hamiltonian is the kinetic energy, which can be written as

$$K = \frac{1}{2m_e} \left( \mathbf{p}_x^2 + \mathbf{p}_y^2 + \frac{eB}{c} \mathbf{y} \cdot \mathbf{p}_x \right) + \frac{\hbar^2 B^2}{4c^2} (y^2 + x^2).$$

The SOI part (third term) is

$$H_{SO} = \frac{\hbar}{\alpha c} \left[ \sigma_x \left( \mathbf{p}_x - \frac{eB}{2c} \mathbf{x} \right) - \sigma_y \left( \mathbf{p}_y + \frac{eB}{2c} \mathbf{y} \right) \right],$$

while the second and the last term correspond to the confinement potential and the Zeeman term, respectively. We then need to evaluate the expectation value of the magnetization operator

$$\hat{\mathbf{m}} = -\frac{\hbar i}{\hbar} \partial_\mathbf{B} = -\frac{1}{2m_e} \left( \mathbf{p}_x - \frac{eB}{2c} (y^2 + x^2) \right) + \frac{\hbar}{\alpha c} (\sigma_x \sigma_y - \sigma_y \sigma_x) - \frac{1}{2} \hbar g_e \sigma_z.$$
\[ M = \sum_m \frac{\partial E_m}{\partial B} \mathrm{e}^{-E_m/\kappa T} / \sum_m \mathrm{e}^{-E_m/\kappa T}. \]  

where the partial derivatives were evaluated, as explained above, as the expectation values of the magnetization operator in the interacting states labelled by \( m \). In elliptical confinements, the mutual Coulomb interaction is handled by the numerical scheme elucidated previously [24], i.e., we diagonalize the many-body Hamiltonian in the basis consisting of non-interacting many-body states, which are constructed by the SO coupled single-particle spinors. These spinors are in turn, as the result of the diagonalization of the SO Hamiltonian, expressed as superpositions of the fundamental 2D oscillator spinors:

\[ | i \rangle = | \uparrow \rangle = | n_s \rangle \langle n_s |, \quad | j \rangle = | \downarrow \rangle = | n_s \rangle \langle n_s |. \]

Here \( n_s \) and \( n_s \) are the oscillator quantum numbers and \( | s \rangle \) stands for the spinors

\[ | 1 \rangle = | \uparrow \rangle \) stands for \( | 0, 0 \rangle \) and \( | 1 \rangle = | \downarrow \rangle \) stands for \( | 0, 1 \rangle \).

We see that in the end the magnetization evaluation reduces to a many-fold summation of the matrix elements:

\[ \langle n_s, n_s | j | n_s, n_s \rangle = -\frac{e}{2m_e c^2} (n_s, n_s; s_1|y|n_s, n_s; s_2) \]

\[ -\frac{e^2 B}{4m_e c^2} < n_s, n_s; s_1|y^2 + x^2|n_s, n_s; s_2) \]

\[ + \frac{ae^2}{2\hbar} < n_s, n_s; s_1|e_x n_s, n_s; s_2) \]

\[ -\frac{1}{2}\Delta n_p(n_s, n_s; s_1|e_p n_s, n_s; s_2), \]

which is now susceptible to direct numerical evaluation.

In our numerical investigations, we chose the InAs quantum dot that shows strong Rashba spin–orbit effects [15,16,24]. In this case, the relevant parameters are: \( e = 15.15, g = -14, m_e = 0.042 \). The energy spectra for three electrons are shown in Figs. 2, 4 and 6 for various values of the SO coupling strength \( \alpha \) and for different values of the anisotropy. For \( B = 0 \) the ground states are two-fold degenerate no matter how strong the SO coupling or how anisotropic the QD becomes. Interestingly, contrary to our expectations, at non-zero magnetic fields most of the level crossings of the energy spectra do not turn into anticrossings when the SO coupling is turned on. Only for a strong value of the Rashba parameter \( \alpha (\alpha = 40) \) [Fig. 6(a) and (b)] the level crossings transform to level repulsions. However, when the QD becomes more anisotropic those level repulsions reappear as level crossings [Fig. 6(c) and (d)].

The energy spectra of anisotropic InAs QD for four electrons are displayed in Figs. 8 and 10 in the absence and presence of Rashba SOI, respectively. Clearly the four electron energy spectra are more dense compared to three electron (or less number of electrons in the dot) energy spectra and exhibit additional level crossings, which are reflected to the corresponding magnetization results (Figs. 7 and 9). Those level crossings move to higher magnetic field as the eccentricity of the dot increases and this feature becomes more prominent when the SOI is turned on (Fig. 10).

Our three electron results for the magnetic field dependence of the magnetization for anisotropic QDs are presented in Figs. 1, 3 and 5. The results are calculated both with and without (red curves) the Coulomb interaction between the electrons for various values of the SO coupling strength and for various values of anisotropy. A major difference between the non-interacting system and the interacting system can be found in the magnetization

\( M \) is the background dielectric constant.

We have also studied the finite-temperature behavior of the magnetization, following the thermodynamical model discussed earlier [25]. Since we are investigating the system with a fixed number of electrons, we use the canonical ensemble. The temperature dependence of magnetization was therefore evaluated from the thermodynamic expression

\[ \langle \alpha \rangle = \frac{\langle H \rangle}{\langle \beta \rangle} = \frac{\sum_m \mathrm{e}^{-E_m/\kappa T} \langle H_m \rangle}{\sum_m \mathrm{e}^{-E_m/\kappa T}}. \]

where the temperature dependence of magnetization was therefore evaluated for the Hamiltonian with the Coulomb interaction \( V_c = e^2/\epsilon r \) included as in our earlier work [24], but now for three and four interacting electrons. Here \( \epsilon \) is the background dielectric constant.

We see that in the end the magnetization evaluation reduces to a many-fold summation of the matrix elements:

\[ \langle n_s, n_s | j | n_s, n_s \rangle = -\frac{e}{2m_e c^2} (n_s, n_s; s_1|y|n_s, n_s; s_2) \]

\[ -\frac{e^2 B}{4m_e c^2} < n_s, n_s; s_1|y^2 + x^2|n_s, n_s; s_2) \]

\[ + \frac{ae^2}{2\hbar} < n_s, n_s; s_1|e_x n_s, n_s; s_2) \]

\[ -\frac{1}{2}\Delta n_p(n_s, n_s; s_1|e_p n_s, n_s; s_2), \]

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\[ M = \sum_m \frac{\partial E_m}{\partial B} \mathrm{e}^{-E_m/\kappa T} / \sum_m \mathrm{e}^{-E_m/\kappa T}. \]
results: while there is no structure present in the non-interacting cases (red curves), there are prominent structures for the interacting systems. As it was predicted in earlier theoretical works [8] (and confirmed in our present work), the electron–electron interaction causes saw-tooth structure in the magnetic field dependence of the magnetization, which is a consequence of the change in the ground state energy from one magic angular momentum to another (in the case of isotropic QDs) [2]. Another interesting behavior of magnetization that should be pointed out here is that with increasing strength of the Rashba SO parameter $\alpha$ the jump in magnetization at the level crossings in the energy spectra moves to lower magnetic fields, while increasing anisotropy of the QD pushes the jump in magnetization to higher magnetic fields. For InAs elliptical QDs this shift is at most $\sim 1$ T, when $\alpha$ is increased from 0 to 40 meV nm and $\omega_y$ is varied from 4.1 to 10 meV. Therefore, low-field magnetization measurements of the QDs could be a direct probe of the SO coupling strength. In general, the sawtooth structure shifts to higher magnetic fields when one squeezes the dot, while stretching of the dot results in a shift in the opposite direction.

The main feature of the temperature dependence of magnetization is that as the temperature is increased the saw-tooth structure of the magnetization curve gradually disappears (Figs. 1 and 3 for three electrons and Figs. 7 and 9 for four electrons). The jump in magnetization slowly vanishes even in the absence of increasing temperature for an anisotropic QD [Fig. 5 (a) and (b)] which is a result of large SO coupling. However, an emergent small jump in magnetization is again visible (at $T=0$ K) for strong anisotropic QDs and large SOI [Fig. 5(c) and (d)] which is clearly the result of two low-lying energy levels crossing near 1.2 T.

**Fig. 7.** Temperature dependence of magnetization of a four-electron anisotropic dot without the Rashba SOI ($\alpha=0$). The results are for $\omega_x=4$ meV and (a) $\omega_y=4.1$ meV, (b) $\omega_y=6$ meV, (c) $\omega_y=8$ meV, and (d) $\omega_y=10$ meV.

**Fig. 8.** Energy levels of a four-electron anisotropic dot without the Rashba SOI ($\alpha=0$). The results are for $\omega_x=4$ meV and (a) $\omega_y=4.1$ meV, (b) $\omega_y=6$ meV, (c) $\omega_y=8$ meV, and (d) $\omega_y=10$ meV.

**Fig. 9.** Same as in Fig. 7, but for $\alpha=20$ meV nm.

**Fig. 10.** Same as in Fig. 8, but for $\alpha=20$ meV nm.
[Fig. 6(c) and (d)] (marked by circles). Another emergent jump in magnetization also appeared in Fig. 3(a) around 0.35 T again as a result of energy level crossing. In the four-electron results most of the magnetization features are preserved. As it was expected, they express many more saw-tooth structures due to the Coulomb interaction than those were in the three-electron problem. In addition, we notice that the jump in magnetization for four electrons appears at higher magnetic fields compared to three-electron magnetization for the same parameters. For example, at $T = 0$ in the presence of SO coupling ($\alpha = 20\%$) the point of jump in the magnetic field dependence of the magnetization is beyond 3 T for four-electron [Fig. 9(d)] whereas for three-electron the jump occurs at 2.2 T [Fig. 3(d)]. Similar work for a larger system is computationally very challenging, here we present the magnetization results and energy spectra only for $\alpha = 20\text{ meV}$. nm.

To summarize: we have reported here detailed and accurate studies of the magnetization of anisotropic quantum dots with interacting electrons in the presence of the Rashba SOI for finite values of the magnetic field. The Coulomb interaction in the presence of the spin-orbit coupling exhibits a very strong effect on magnetization, particularly in the presence of strong anisotropy by introducing large saw-tooth structures in the magnetic field dependence of the magnetization, which is weakened by increasing temperature. Interestingly, there is also the emergence of this structure in the high anisotropy and large SOI limit that is explained as due to merging of two low-energy curves when the level spacings evolve with increasing parameters. Armed with the theoretical insights presented here, an experimental probe of the quantum dot.

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