Magnetization of Quantum Dots: A Measure of Anisotropy and the Rashba Interaction

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The magnetization of anisotropic quantum dots in the presence of the Rashba spin-orbit interaction has been studied for three interacting electrons in the dot. 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 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 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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The magnetization of quantum confined planar electron systems, e.g. quantum dots (QDs), or artificial atoms is an important probe that reflects entirely on the properties of the energy spectra. This is a thermodynamical quantity that for the QDs has received some experimental attention, particularly after the theoretical prediction that the electron-electron interaction is directly manifested in this quantity. 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 and experimentally. Theoretical studies of the magnetization of elliptical QDs have also been reported. Effects of the Rashba spin-orbit interaction (SOI) on the electronic properties of isotropic and anisotropic quantum dots have been investigated earlier. An external electric field can induce the Rashba spin-orbit interaction which couples the different spin states and introduces level repulsions in the energy spectrum. 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. Three-electron quantum dots are particularly relevant in this context. Here we report on the magnetic field dependence of the magnetization of an anisotropic QD containing three interacting electrons in the presence of the Rashba SOI. Our present work clearly indicates how the 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 magnetization 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. We have studied the magnetic field dependence of $M$ by evaluating the expectation value of the magnetization operator $\hat{m} = -\frac{\partial H}{\partial B}$, where $H$ is the system Hamiltonian. Since the Coulomb interaction is independent of $B$, $\hat{m}$ 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 $A = \frac{1}{2}B(-y,x)$, the confinement potential, and the Rashba SOI is

$$
\mathcal{H} = \frac{1}{2m_e} \left( \mathbf{p} - eA \right)^2 + \frac{1}{2}m_e \left( \omega_x^2 x^2 + \omega_y^2 y^2 \right) + \frac{\alpha}{\hbar} \left[ \sigma \times \left( \mathbf{p} - eA \right) \right]_z + \frac{\alpha}{2} \mu_B B \sigma_z.
$$

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

$$
K = \frac{1}{2m_e} \left( p_x^2 + p_y^2 + \frac{eB}{c} (yp_x - xp_y) + \frac{e^2B^2}{4c^2} (y^2 + x^2) \right).
$$

The SOI part (third term) is

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

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

\[ \hat{m} = \frac{\partial H}{\partial B} = -\frac{1}{2m_e c} \left( (yp_x - xp_y) + \frac{eB}{2c}(y^2 + z^2) \right) + \frac{e\alpha}{2\hbar} (\sigma_x x + \sigma_y y) - \frac{1}{2}g\mu_B \sigma_z, \]

with respect to the interacting electron states. We should, however, point out that the energy spectra in the present studies were evaluated for the Hamiltonian with the Coulomb interaction \( V_c = e^2/\epsilon r \) included, as in our earlier work\(^{22}\) but now for three interacting electrons. Here \( \epsilon \) is the background dielectric constant.

We have also studied the finite-temperature behavior of the magnetization, following the thermodynamical model discussed earlier\(^{23}\). Since we are investigating the system with a fixed number of electrons, we use the canonical ensemble. The temperature dependence of the magnetization was therefore evaluated from the thermodynamic expression

\[ M = \sum_m \frac{\partial E_m}{\partial B} e^{-E_m/kT} / \sum_m e^{-E_m/kT}, \]

where the partial derivatives were evaluated, as explained above, as the expectation values of the magnetization operator in the interacting states labeled by \( m \). In elliptical confinements, the mutual Coulomb interaction is handled by the numerical scheme elucidated previously\(^{22}\), 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

\[ |n_x, n_y; s_z\rangle = |n_x, n_y\rangle |s_z\rangle. \]

Here \( n_x \) and \( n_y \) are the oscillator quantum numbers and \( |s_z\rangle \) stands for the spinors

\[ |+1\rangle = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \]

\[ |-1\rangle = |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \]

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

\[ \langle n_x', n_y'; s_z' | \hat{m} | n_x, n_y; s_z \rangle = -\frac{e}{2m_e c} \langle n_x', n_y'; s_z' | (yp_x - xp_y) | n_x, n_y; s_z \rangle - \frac{e^2B}{4m_e c^2} < n_x', n_y', s_z' | y^2 + x^2 | n_x, n_y; s_z \rangle + \frac{e\alpha}{2\hbar} \langle n_x', n_y', s_z' | \sigma_x x + \sigma_y y | n_x, n_y; s_z \rangle - \frac{1}{2}g\mu_B \langle n_x', n_y', s_z' | \sigma_z | n_x, n_y; s_z \rangle, \]

which is now susceptible to direct numerical evaluation.

In our numerical investigations, we chose the InAs quantum dot that shows strong Rashba effects\(^{15,16,22}\). In this case, the relevant parameters are: \( \epsilon = 15.15, g = -14, m_e = 0.042 \). The energy spectra are shown in Fig. 2, Fig. 4, and Fig. 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 is 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), (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), (d)].

![Graph showing temperature dependence of magnetization](image-url)
FIG. 2: Energy levels of a three-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. 3: Same as in Fig. 1 but for $\alpha = 20$ meV.nm.

Our results for the magnetic field dependence of the magnetization for anisotropic QDs are shown in Fig. 1, Fig. 3 and Fig. 5, 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 the non-interacting system and the interacting system can be found in the magnetization 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 (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). An 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 $\sim 1$ Tesla, when $\alpha$ is increased from zero to 40 meV.nm and $\omega_y$ is varied from 4.1 - 10 meV. Therefore, low-field magnetization measurements of the QDs could be a direct probe of the SO coupling strength.

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 (Fig. 1 and Fig. 3). An important point to notice here is that the jump in magnetization slowly vanishes even in the absence of increasing temperature for an anisotropic QD [Fig. 5 (a), (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), (d)] which is clearly the result of two low-lying energy levels crossing near 1.2 Tesla [Fig. 6 (c), (d)] (marked by circles).

In the absence of the SO coupling the magnetization is invariant under the time reversal, which implies that the derivative of energy with respect to the magnetic field must vanish at $B = 0$. This means a vanishing magnetization at $B = 0$. However, non-zero SO coupling
breaks the time-reversal symmetry and in that case the derivative of energy with respect to the magnetic field can be discontinuous at $B = 0$, which would imply non-vanishing magnetization at $B = 0$ [Fig. 4 and Fig. 6].

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. 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. Any further extension of the present work for a larger system would be computationally very challenging, but we expect that the novel features observed in the present work will be displayed in that case. That would be the subject of our future publications. Armed with the theoretical insights presented here, an experimental probe of magnetization in anisotropic quantum dots will undoubtedly provide valuable information about the inter-electron strength, the strength of the QD anisotropy, as well as the SOI strength in the quantum dot.

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