

## Significant $g$ -factor values of a two-electron ground state in quantum dots with spin-orbit coupling

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The magnetization of semiconductor quantum dots in the presence of spin-orbit (SO) coupling and interactions is investigated numerically. When the dot is occupied by two electrons we find that a level crossing between the two lowest many-body eigenstates may occur as a function of the spin-orbit coupling strength. This level crossing is accompanied by a nonvanishing magnetization of the ground state. Using first-order perturbation theory as well as exact numerical diagonalization of small clusters, we show that the tendency of interactions to cause Stoner-type instability is enhanced by the SO coupling. The resulting  $g$  factor can have a significant value and thus may influence  $g$ -factor measurements. Finally we propose an experimental method by which the predicted phenomenon can be observed.

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### I. INTRODUCTION

The effect of spin-orbit (SO) coupling on the energy spectrum of quantum dots (QDs) and metallic grains has attracted notable attention in recent years.<sup>1-3</sup> Much experimental and theoretical effort has concentrated on the magnetization of mesoscopic samples. For example, measurements of the  $g$  factors of nanoparticles using tunneling spectroscopy<sup>4-6</sup> have led to several theoretical studies<sup>7,8</sup> which treated the electrons in the quantum dots as noninteracting particles. Other theoretical studies have considered interactions as well while investigating the interplay between interactions and disorder in quantum dots without SO coupling. It was shown that the combination of these effects can lead to nontrivial spin polarization.<sup>9-15</sup> In this paper we present an additional mechanism which can lead to spin polarization and nontrivial  $g$  factor, where the role typically played by disorder is taken by the SO coupling.

Usually the  $g$  factor is defined through the splitting of the Kramers doublets<sup>16,17</sup> in the presence of a weak magnetic field. Namely, the  $g$  factor of the  $i$ th single-particle level with spin  $\sigma$  is given by

$$g_{i,\sigma} = \frac{2[\epsilon_{i\sigma}^{(0)} - \epsilon_{i\sigma}^{(H)}]}{\mu_B H}, \quad (1)$$

where  $\epsilon_{i\sigma}^{(H)}$  ( $\epsilon_{i\sigma}^{(0)}$ ) is the corresponding energy level in the presence (absence) of a weak magnetic field  $H$  and  $\mu_B$  is the Bohr magneton. The spin index  $\sigma \in \{+, -\}$  is used to denote the two time-reversed states according to the sign of the  $z$  component of their average magnetic moments. In the absence of a magnetic field each level is twofold degenerate; and this degeneracy is lifted by the magnetic field, which increases the energy of one of the levels and decreases the energy of the other. Therefore,  $g_{i,\sigma}$  as defined by this formula can have either sign depending on the direction of the energy change. The ground-state energy always decreases when a magnetic field is applied; thus, the  $g$  factor of the ground state obtained by Eq. (1) is positive. Usually, the value of  $g$  does not depend on the spin index, at least to zeroth order in  $H$ , so that one can denote the  $g$  factor of the  $i$ th level as  $\pm g_i$ , with the convention that  $g_i \geq 0$ .

For free electrons the  $g$  factor is constant,  $g_i=2$  for each level  $i$ , and this value is more or less correct also for bulk measurements in various metals.<sup>1</sup> However, in experiments performed on metallic nanoparticles, values which are significantly less than the free value of the  $g$  factor were obtained.<sup>5,6</sup> Moreover, large fluctuations in the measured values were seen. These findings attracted much theoretical attention and resulted in studies which have obtained, within the framework of the random-matrix theory (RMT), a description of the  $g$ -factor probability distribution in the presence of SO coupling and disorder but in the absence of interactions.<sup>7,8</sup> In a recent work, the statistical properties of these distribution functions were related to several physical observables.<sup>18</sup> According to these results, the SO coupling influences the probability distribution of the  $g$  factors of the discrete energy levels. The distribution function was shown to be universal, where the width is expressed in terms of various physical parameters. The presence of strong SO coupling and disorder results in sample to sample fluctuations of the  $g$  factor. Moreover, the  $g$  factor is expected to fluctuate also between different levels of a specific sample, with a distribution function determined by RMT.

Indeed, recent measurements of nanoparticles have obtained  $g$  factors which seem to be consistent with RMT predictions. For example, several experimental studies of metallic three-dimensional (3D) nanoparticles have shown the reduction in the measured  $g$  factor as a function of the spin-orbit coupling strength. For aluminum nanoparticles, in which the SO coupling is negligible, the measured  $g$ -factor values are approximately those of free electrons<sup>4</sup> (i.e.,  $g \approx 2$ ), while for gold nanoparticles, in which the SO coupling is strong, the measured  $g$  factors were in the range of 0.28–0.45.<sup>5</sup> Furthermore, by extracting several  $g$  factors from each sample, Petta and Ralph<sup>6</sup> succeeded to present an impressive confirmation of the theoretical RMT distribution function.

Nevertheless, according to Eq. (1) the  $g$ -factor measurement should compare the specific single-particle energy level before and after the magnetic field is applied. However, practical experiments usually differ from that approach in two points. First, measurements are usually related to the total

energy of the system and not to that of a specific level. Second, the measurement of the energy is sometimes indirect, as is the case in tunneling spectroscopy.

These two points can be ignored if one neglects the interaction between particles. For a noninteracting system with an odd number of electrons  $n_e=2p+1$ , the change in the total ground-state energy due to magnetic field is equivalent to that of the highest filled level.  $n_e-1$  electrons populate  $p$  Kramers pairs, where in each pair one level increases and the other decreases in the presence of a magnetic field, so that their total contribution vanishes. The only contribution to the  $g$  factor comes from the single electron occupying one level of pair  $p+1$ , so that if we define the  $g$  factor of the ground state with  $n_e$  electrons by

$$g(n_e) = \frac{2[E_{\text{gs}}^{(0)}(n_e) - E_{\text{gs}}^{(H)}(n_e)]}{\mu_B H}, \quad (2)$$

where  $E_{\text{gs}}^{(H)}(n_e)$  represents the total ground-state energy in the presence of a magnetic field  $H$ , then  $g(2p+1)=g_{p+1}$ . In addition, when the number of electrons  $n_e$  is even, the total ground-state energy is not expected to change when a magnetic field is applied since all the filled levels divide into pairs, in which the movement of one level is compensated by the other (to first order in  $H$ ). Therefore, for an even number of electrons, a calculation of the  $g$  factor using Eq. (2) gives  $g(2p)=0$ .

The second point, regarding the indirect energy measurement, requires an interpretation of the experimental results. For example, using tunneling spectroscopy one measures the gate-voltage value for which a conductance peak of a QD occurs. At such an event the energies of the QD with  $n_e-1$  and  $n_e$  electrons and the gate voltage  $V_g$  are related by the equation  $eV_g = E_{\text{gs}}(n_e) - E_{\text{gs}}(n_e-1)$ . When a magnetic field is applied, the position of the peak will change as a function of  $H$ . Therefore, by denoting the measured  $g$  factor by  $\tilde{g}$ , one can analyze the peak motion in order to determine the  $g$  factor by calculating

$$\tilde{g} = \frac{2[eV_g(0) - eV_g(H)]}{\mu_B H} = g(n_e) - g(n_e-1). \quad (3)$$

Since either  $n_e$  or  $n_e-1$  is even, its corresponding  $g$  factor vanishes and thus  $\tilde{g}$  is equivalent to the other  $g$  factor. Namely,  $\tilde{g}=g(n_e)$  or  $\tilde{g}=-g(n_e-1)$ . Actually, since each peak is split in the presence of a magnetic field into two peaks having an opposite magnetic-field dependence, extracting  $\tilde{g}$  from successive peaks results in the set of the single-particle  $g$  factors, i.e.,  $g_1, -g_1, g_2, -g_2, \dots$

As mentioned above, measurements done using tunneling spectroscopy have indeed obtained  $g$  factors which can be interpreted using RMT predictions. Nevertheless, as we have discussed, Eq. (2) is equivalent to Eq. (1) only for systems of noninteracting particles. Once interactions between electrons are important, it should be emphasized that Eq. (2) is a definition of a many-particle  $g$  factor, which depends on the total magnetization of the ground-state wave function. For example, one can obtain spin contribution to the  $g$  factor larger than 2, which is a phenomenon that cannot happen for a single-particle  $g$  factor.<sup>9-15</sup> Indeed, by adding an interaction

term to the RMT Hamiltonian, an increase in the  $g$ -factor fluctuations was reported.<sup>19,20</sup> It was shown that the interactions result in a possibility of getting nontrivial spin values in the ground state and accordingly in an optional enhancement of the  $g$  factor to values greater than 2.

Although the theoretical studies of Refs. 19 and 20 were performed for an odd-electron occupation, their results suggest the possibility of a nontrivial spin polarization for the even-electron case as well. If, for any reason the  $g$  factor of an even-electron ground state indeed differs from zero, then *the quantity measured in tunneling spectroscopy may not equal the single-level  $g$  factor nor the many-particle  $g$  factor.* In such case it should be related to the difference between two many-particle  $g$  factors, as shown in Eq. (3)

In principle, the above description of the  $g$  factor holds for both metallic and semiconductor dots. However, in semiconductor dots the strength of the SO coupling can be tuned by the use of a gate voltage.<sup>21,22</sup> Furthermore, several significant implications of SO effects in semiconductors, such as spin-polarized field effect transistor<sup>23</sup> and spin Hall effect,<sup>24,25</sup> have recently attracted notable attention.

With this in mind, we investigate in the current paper the ground-state magnetization properties of semiconductor QDs with SO coupling where interactions between the electrons are considered. We show that the interplay between the SO coupling and the electron-electron interactions may result in a level crossing (LC) between the two lowest many-body levels. When these states are close in energy, the magnetic field splits them into two polarized states with a finite magnetization. As a result, there is a possibility to have a significant  $g$  factor in the two-particle ground state. Finally, we propose an experimental method which can be used in order to observe the predicted phenomenon.

We note that we have neglected so far the orbital effect and its influence on the magnetization of nanoparticles. For 3D nanoparticles this is reasonable.<sup>8</sup> On the other hand, for two-dimensional (2D) systems the orbital effect is expected to play an important role. For example, due to the orbital effect, the single-particle  $g$  factor can exceed the value of 2. In addition, the  $g$  factors of two levels belonging to the same Kramers pair  $g_{i,+}$  and  $g_{i,-}$  might be different. As a result, the  $g$  factor of the doubly occupied ground state, which can be simply written when the electrons are noninteracting as  $g(2)=g_{1,+}+g_{1,-}$ , may not vanish. However, this contribution to  $g(2)$  which is the quantity of interest in this work, is linear in the magnetic field  $H$  and thus can be neglected for the weak fields used in such measurements.

The rest of the paper is organized as follows. In Sec. II we describe the model Hamiltonian we use in order to incorporate, besides the magnetic field, both SO coupling and interactions between electrons. In Sec. III we present results for a system with noninteracting particles, which are shown to reproduce some known ground-state properties. In addition, we find that there are specific values of the SO coupling strength in which the Kramers doublet remains degenerate even when a magnetic field is applied. The effects of interplay between SO and electron-electron interactions are considered in Sec. IV. Our results point out that a finite magnetization can be obtained for systems with an even-particle occupancy. In Sec. V we discuss the experimental relevance of this finding,

i.e., the possibility that it might affect practical  $g$ -factor measurements.

## II. MODEL

In order to model the semiconductor QD we use a tight-binding description of a finite 2D lattice with  $A$  columns and  $B$  rows (the number of sites is denoted by  $N=AB$ ), with open boundary conditions, which is occupied by  $n_e$  electrons. As a result of a coupling between the spin degree of freedom and the orbital motion, a finite probability for spin flips during hopping processes exists. Separating the interactions from the free part, one can write the Hamiltonian as  $\hat{H}_{\text{QD}}=\hat{H}_0+\hat{H}_{\text{int}}$ , where the free part in the absence of disorder can be divided to a hopping term and a Zeeman term; i.e.,  $\hat{H}_0=\hat{H}_{\text{hop}}+\hat{H}_B$ . The hopping part of the Hamiltonian is

$$\hat{H}_{\text{hop}}=-\sum_{m,n,\sigma,\sigma'}(V_x\hat{a}_{m,n,\sigma}^\dagger\hat{a}_{m,n+1,\sigma'}+V_y\hat{a}_{m,n,\sigma}^\dagger\hat{a}_{m+1,n,\sigma'}+\text{H.c.}), \quad (4)$$

where  $\hat{a}_{m,n,\sigma}^\dagger$  ( $\hat{a}_{m,n,\sigma}$ ) is the creation (annihilation) operator of an electron with spin  $\sigma$  in the lattice site placed in row  $m$  and column  $n$ . The matrices  $V_x$  and  $V_y$  are given by the Ando model,<sup>26</sup> which is the discrete version for the Rashba spin-orbit coupling,<sup>27</sup> as

$$V_x=\begin{pmatrix} V_1 & V_2 \\ -V_2 & V_1 \end{pmatrix}, \quad V_y=\begin{pmatrix} V_1 & -iV_2 \\ -iV_2 & V_1 \end{pmatrix}, \quad (5)$$

where  $V_1$  ( $V_2$ ) is the hopping matrix element for events which conserve (flip) the spin. The overall hopping amplitude  $t=\sqrt{V_1^2+V_2^2}$  is taken as the energy unit of the problem. In other words, all energies are expressed in terms of  $t$ .

The strength of the SO coupling can be expressed by the ratio between the absolute value of the spin-flip amplitude and that of the total hopping element. Using a dimensionless parameter  $\lambda=\frac{V_2}{\sqrt{V_1^2+V_2^2}}=V_2/t$ , we examine the entire range of  $\lambda$  between very weak ( $\lambda\rightarrow 0$ ) and very strong ( $\lambda\leq 1$ ) spin-orbit couplings. Realistic values for  $\lambda$  are between 0 and 0.5.<sup>26,28</sup> As mentioned above, these values can be controlled by tuning the gate voltage.<sup>21,22</sup>

We now add a perpendicular magnetic field to our 2D sample, and we choose a gauge in which the vector potential is  $A=-Hy\hat{x}$ . The Zeeman term in the Hamiltonian is thus diagonal in spin space and can be written as

$$\hat{H}_B=\mu_B H \sum_{m,n,\sigma} \sigma \hat{a}_{m,n,\sigma}^\dagger \hat{a}_{m,n,\sigma}, \quad (6)$$

where  $\sigma=\pm 1$ .

With the gauge chosen, one has to modify the hopping elements in the  $\hat{x}$  direction according to the Peierls substitution<sup>29</sup> and write  $V_x\rightarrow V_x e^{-i\theta m}$ . In this expression  $m$  is the row number and  $\theta$  is the phase that can be written as  $\theta=\frac{2\pi Hs^2}{\phi_0}$ , where  $s$  is the lattice constant and  $\phi_0=hc/e$  is the magnetic-flux quantum. Thus,  $\theta$  is a dimensionless parameter that measures the magnetic flux throughout a lattice unit cell in units of the quantum flux  $\phi_0$ .

The Zeeman energy can be related to the hopping phase  $\theta$  and to the hopping amplitude  $t$  by the following considerations. One can express the absolute value of the Zeeman energy as  $\mu_B H=\mu_B \phi_0 \frac{\theta}{2\pi s^2}$ . Substituting the physical constants  $\mu_B \phi_0=\frac{\pi \hbar^2}{m_0}$ , where  $m_0$  is the electron mass, and using the relation  $t=\frac{\hbar^2}{2m_{\text{eff}}s^2}$ , where  $m_{\text{eff}}$  is the effective mass at the bottom of the band, one gets  $\mu_B H=\frac{\theta \hbar^2}{2m_0 s^2}=\theta t \frac{m_{\text{eff}}}{m_0}$ . The factor  $\frac{m_{\text{eff}}}{m_0}$  depends on the specific type of the QD; and in general,  $m_{\text{eff}}\approx m_0$  for metallic grains while  $m_{\text{eff}}< m_0$  for semiconductor ones. In the current study we use 2D geometry which is suitable for modeling typical semiconductor QDs. Moreover, the Ando model which incorporates the spin-orbit coupling was originally proposed for surfaces of III-V compound semiconductors.<sup>26</sup> Thus we set for the rest of this paper  $\frac{m_{\text{eff}}}{m_0}\approx \frac{1}{15}$ , as in the case of GaAs. However, we have checked that tuning this value does not lead to a qualitative change in the main results. Finally, since all energies are measured in units of  $t$ , the strength of the Zeeman term  $\mu_B H/t$  determines exactly the hopping phase.

At last, the interactions term in the Hamiltonian is

$$\hat{H}_{\text{int}}=U \sum_{m,n} \hat{a}_{m,n,\uparrow}^\dagger \hat{a}_{m,n,\uparrow} \hat{a}_{m,n,\downarrow}^\dagger \hat{a}_{m,n,\downarrow}, \quad (7)$$

which represents a Hubbard interaction with strength  $U$ .

The Hamiltonian  $\hat{H}_{\text{QD}}$  is exactly diagonalized using the Lanczos procedure for lattices of up to  $15\times 14$  sites occupied by 1 or 2 electrons, and its lowest eigenstates are numerically found. In order to calculate the spin polarization of the QD we apply a weak magnetic field along the  $\hat{z}$  axis and calculate the expectation value of  $\hat{S}_z$  for the lowest levels. For the  $g$ -factor calculations, we compare the ground-state energies with and without the magnetic field for each sample and use Eq. (2). The strength of the magnetic field we apply is  $\mu_B H/t\sim 10^{-4}-10^{-3}$ ; and for an experimental system in which the mean level spacing is 0.1–1 meV, it is equivalent to a magnetic field of 10–1000 G, in correspondence with realistic measurements.

## III. NONINTERACTING ELECTRONS

We start with noninteracting particles by taking  $U=0$ . Without the magnetic field, all single-particle states (and in particular the ground state) are doubly degenerate (the Kramers degeneracy).<sup>16,17</sup> When a magnetic field is applied, it splits this degeneracy and one gets to zeroth order in the magnetic field,  $\langle S_z^{(1)}\rangle=-\langle S_z^{(2)}\rangle$ , where  $\langle S_z^{(m)}\rangle$  denotes the expectation value of the operator  $\hat{S}_z$  in the  $m$ th eigenfunction ( $m=1$  being the ground state). For  $\lambda\rightarrow 0$ ,  $|\langle S_z\rangle|\rightarrow \frac{1}{2}$ . When the SO coupling increases, a general decrease in  $|\langle S_z\rangle|$  can be expected, and this trend can be seen in the upper panel of Fig. 1.

However, one can see that the value of  $\langle S_z\rangle$  switches abruptly between these two levels near  $\lambda=0.12$ . This is a sign of a LC, which can be seen by looking at the energy difference between these levels (lower panel of Fig. 1). The switching of  $\langle S_z\rangle$  occurs exactly when the energy difference



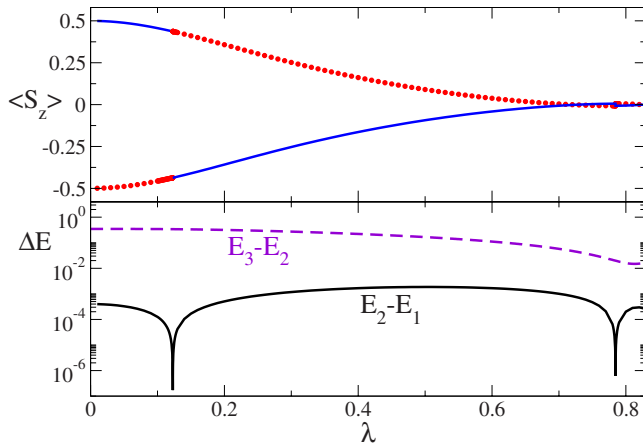


FIG. 1. (Color online)  $\langle S_z \rangle$  of the lowest two single-particle levels (upper panel) and  $\Delta E$ , the energy difference between them (lower panel; notice the semilogarithmic scale), calculated for a system of  $8 \times 7$  sites in the presence of a magnetic field of strength  $\mu_B H = 2 \times 10^{-4} t$  as a function of the SO coupling strength. The value of  $\langle S_z \rangle$  switches abruptly between the two levels (one level is shown by symbols and the other by a line) near  $\lambda = 0.12$ , where the energy difference vanishes, implying a level crossing between the lowest two levels. The energy of the third level, however, remains much higher (lower panel, dashed line).

vanishes. We note that such crossings occur also for large values of  $\lambda$ .

It is important to notice that the LC presented here occurs between states which belong to the same Kramers pair (i.e., states which are the time reversal of each other). The energy difference between states of different pairs is much larger, and although it is reduced by the SO coupling it is usually much larger than the contribution of the weak magnetic field we apply ( $\mu_B H/t$  of the order of  $10^{-4}$ ) to the energy (see the dashed line in the lower panel of Fig. 1). As a result, crossings between states which originate from different pairs are much less probable.

In Sec. IV we study the case of doubly occupied systems. For noninteracting electrons, based on the results of the current section, it is clear that a LC between the lowest two doubly occupied states is improbable since their Slater determinants contain single-particle states from different Kramers pairs. Nevertheless, as will be shown in Sec. IV, the electron-electron interaction can change this picture qualitatively.

#### IV. INTERPLAY BETWEEN INTERACTIONS AND SPIN-ORBIT COUPLING

We now turn to study the effect of interactions on the behavior of the  $g$  factor in the presence of SO coupling. Calculating the ground-state energies of the two lowest doubly occupied many-body states, one finds that there is a LC between these states at a certain value of the SO coupling (denoted in the following by  $\lambda_c$ ), as can be seen in the upper panel of Fig. 2. In the vicinity of  $\lambda_c$ , the expectation value of  $\hat{S}^2$  switches smoothly between these states, as is shown in the lower panel of Fig. 2.

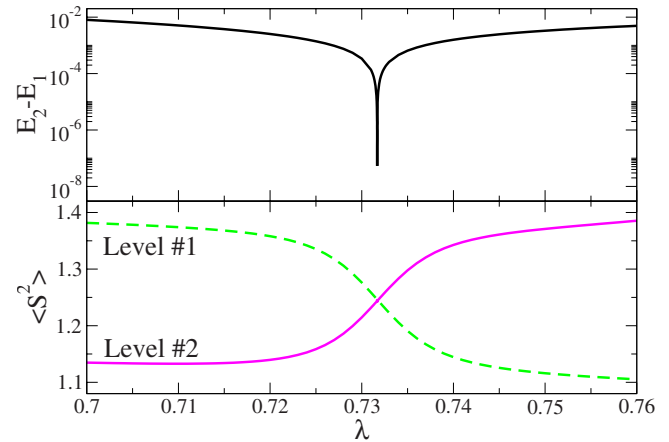


FIG. 2. (Color online) Typical results of the level crossing of the two lowest doubly occupied states. The results shown were obtained for a system of  $8 \times 7$  sites with  $U = 3t$ . Upper panel: the energy difference  $E_2 - E_1$  is shown as a function of the spin-orbit coupling strength  $\lambda$  (notice the semilogarithmic scale). The dip shows the crossing point. Lower panel: the switch of  $\langle \hat{S}^2 \rangle$  between these two states, which is centered at the same place.

As noted in Sec. III, such LC does not exist for noninteracting two-electron states since it involves levels belonging to different single-particle Kramers pairs. Moreover, in the cases when there is a LC in the noninteracting system, i.e., between single-particle levels belonging to the same Kramers pair, the  $g$  factor vanishes at the LC point (to zeroth order of  $H$ ; it has however a linear magnetic-field dependence from orbital effects). On the other hand, in the case of interacting electrons we find that both states involved in the LC have a significant magnetization of zeroth order in  $H$ . The magnetization properties, i.e.,  $\langle \hat{S}_z \rangle$  and the  $g$  factor, do not present a smooth switching as for  $\langle \hat{S}^2 \rangle$  in the vicinity of the LC. Instead, when the energies of the two states become close enough to each other so that the energy associated with the magnetic field becomes important, both states develop a spin polarization as can be seen in Fig. 3. This leads to an enhancement of  $\langle \hat{S}_z \rangle$  in the crossing region and to significant values of the  $g$  factor.

The significant values obtained for the  $g$  factor are crucially related to the degeneracy point (the LC). Far from this point, when the two lowest many-particle states are not degenerate, each of these states  $\psi_1$  and  $\psi_2$  is the time reversal of itself, i.e.,  $\mathcal{T}(\psi_1) = \psi_1$  and  $\mathcal{T}(\psi_2) = \psi_2$ , where  $\mathcal{T}$  is the time-reversal operator. This immediately implies that  $\langle \hat{S}_z \rangle = 0$  for both states, and the corresponding  $g$  factors vanish as well. This picture changes in the vicinity of the degeneracy point, where the magnetic field breaks the degeneracy by polarizing both states. This of course results in a finite value of the  $g$  factor. Such nonvanishing  $g$ -factor values can thus be seen as long as the energy associated with the magnetic field is larger than the level separation. Accordingly, as the magnetic field is enhanced, the peaks in  $\langle \hat{S}_z \rangle$  and  $g$  get wider.

The dependence of the energy on the magnetic field is shown in Fig. 4, with a comparison between the LC regime and an arbitrary point. In the latter, a quadratic dependence

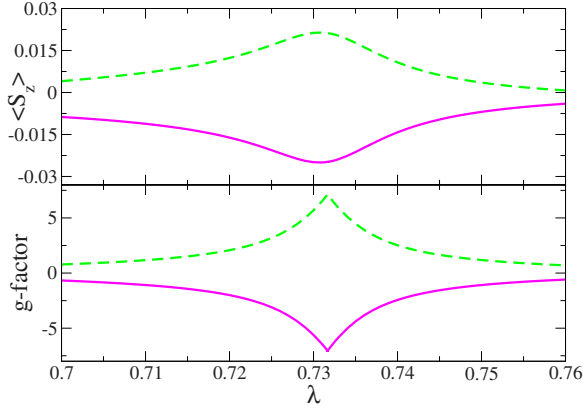


FIG. 3. (Color online) Typical results of the spin polarization  $\langle \hat{S}_z \rangle$  (upper panel) and the  $g$  factor, calculated using Eq. (2) (lower panel), of the two lowest doubly occupied states in the regime of the level crossing between them. The results shown were obtained for a system of  $8 \times 7$  sites with  $U=3t$  and  $\mu_B H=10^{-4}t$ .

of the ground-state energy on the magnetic field is clearly seen. On the other hand, near the LC point each of these states has a significant magnetization, and the dependence of the energy on the magnetic field is linear, with a finite value of the  $g$  factor.

These phenomena can be given a simple interpretation. Kinetic-energy considerations make it advantageous to put the two electrons in the same orbital level and create an unpolarized ground state. Repulsive interactions, however, cause a polarized ground state to be preferred since the Pauli principle then tends to separate the electrons. Usually, the kinetic energy wins. However, SO coupling tends to reduce the single-particle level spacing, so at some point the interactions win and a Stoner-type instability emerges.<sup>30,31</sup> In order to support this intuitive picture, we have calculated the energy difference between the two lowest many-body levels using first-order perturbation theory in the interaction strength. As can be seen in Fig. 5, the interaction tends to

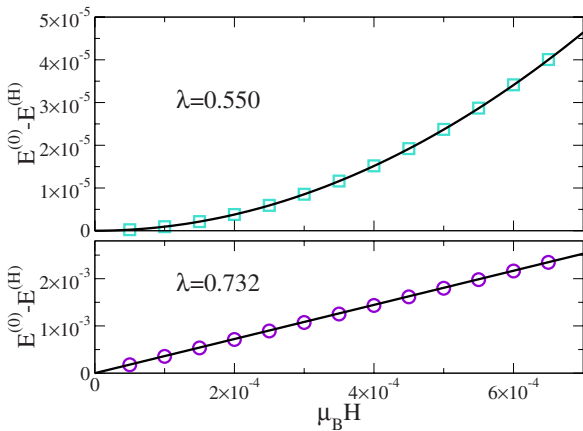


FIG. 4. (Color online) The dependence of the energy on the magnetic field is compared between the regime of a level crossing (lower panel) and another arbitrary point (upper panel). The results shown by symbols were obtained for a system of  $8 \times 7$  sites with  $U=3t$ , and the solid lines represent quadratic (upper panel) and linear (lower panel) fits.

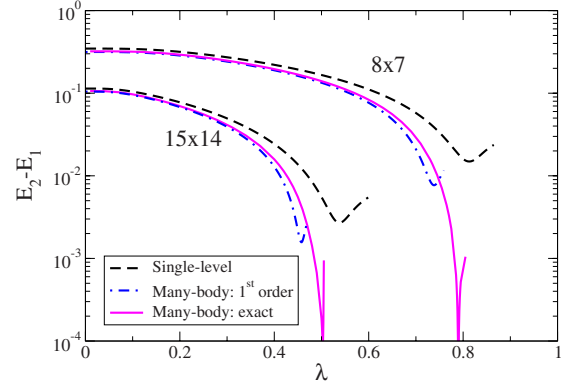


FIG. 5. (Color online) The dependence of the energy difference between the two lowest many-body levels on the SO strength for systems of  $8 \times 7$  and  $15 \times 14$  sites. The results shown are of the noninteracting case (dashed curve) and of interacting electrons with  $U=t$  calculated exactly (solid line) or by using first-order perturbation theory (dashed-dotted line). Notice the semilogarithmic scale.

decrease the energy difference between the lowest two many-body levels. When the electrons are noninteracting, the levels approach each other with increasing SO coupling, yet the minimal distance between them is much larger than the magnetic energy. The presence of interactions enhances this tendency toward the situation in which a LC is possible.

From these results one can conclude that whereas the  $g$  factor of a doubly-occupied system can be neglected for most values of  $\lambda$ , it nevertheless has a significant value near  $\lambda_c$ . When the system size increases, the instability and the  $g$ -factor peak occur for smaller values of the SO coupling, as is shown in Fig. 5. In Sec. V we argue that such  $g$ -factor values might be significant even for realistic sample sizes and physical parameters, and thus they should not be neglected when analyzing experimental data.

## V. EXPERIMENTAL RELEVANCE AND DISCUSSION

In order to check whether the  $g$ -factor peak presented in Sec. IV occurs for realistic systems, one must study how the system size modifies this behavior. When the system is enlarged, one must be careful to leave the other physical parameters unchanged. The strength of the interactions is usually described by the parameter  $r_s$ , which is defined through the ratio between the potential and the kinetic energies. The kinetic energy per electron in 2D samples goes like the electron density  $n=n_e/N$ . For Coulomb interactions one has  $E_p \sim n \iint (U_C/r) dx dy$  per electron, where  $U_C$  is the Coulomb interaction strength between sites separated by one lattice constant. Since  $r \sim n^{-1/2}$  one gets  $E_p \sim U_C \sqrt{n}$  and thus  $r_s \sim U_C / \sqrt{n}$ . However, for Hubbard interactions  $E_p \sim n \iint U \delta(x-x_0) \delta(y-y_0) dx dy = nU$ , so that  $r_s \sim U$ . Therefore, in order to keep  $r_s$  constant, the value of  $U$  should stay unchanged when the system size increases.

In Fig. 6 we show the dependence of the  $g$  factor on  $\lambda$  for various system sizes ranging from  $8 \times 7$  to  $15 \times 14$ . As can be seen, the enhancement of the  $g$  factor occurs for all of the curves, with some quantitative changes in the position and the height of the peak. Although a substantial enlargement of

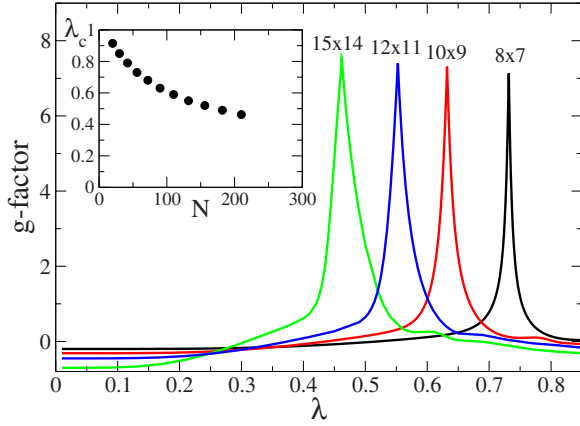


FIG. 6. (Color online) The  $g$  factor of the doubly occupied ground state as a function of the SO coupling strength  $\lambda$  for lattice sizes of  $8 \times 7$ ,  $10 \times 9$ ,  $12 \times 11$ , and  $15 \times 14$  (size increases from right to left) with  $U=3t$ . Inset: the dependence of  $\lambda_c$  on the number of sites.

the system is not numerically possible because of the limitations of the exact diagonalization technique, the trend is clearly seen. The value of  $\lambda_c$  which is found to decrease with increasing system size (see the inset of Fig. 6) suggests that for a sufficiently large system size the crossing occurs for a moderate value of the SO coupling, which may be experimentally relevant. In addition, the modest increase in the peak height suggests that a significant peak may be observed for realistic system sizes.

Finally, we would like to discuss the implications of the  $g$ -factor peak on  $g$ -factor measurements. Once a finite magnetization of the doubly occupied ground state is possible, it can affect experiments done by, e.g., tunneling spectroscopy. Such measurement presents the result for the difference between two  $g$  factors, as given by Eq. (3). If the even-electron state has a nonvanishing  $g$  factor, such as in the vicinity of the LCs we have presented, the measured quantity  $\tilde{g}$  may not be equal to the  $g$  factor of the state with an odd number of electrons to which it is usually attributed.

In such cases, a signature of the LC may be seen experimentally. In the regular case (as opposed to the LC scenario), the two levels which belong to the same Kramers doublet have the same  $g$  factor up to a sign, and the dependence of the two energies on the magnetic field is symmetric. However, in the region of a LC, the two levels receive contributions from different even-particle states. Explicitly, with a magnetic field, the  $p$ th Kramers pair is split to levels with different  $g$  factors:  $g(2p-1)-g(2p-2)$  and  $g(2p)-g(2p-1)$ . Thus, if  $g(2p)$  or  $g(2p-2)$  (or both) is not negligible, the magnetic-field dependence will not be symmetric. Furthermore, since the strength of the spin-orbit coupling can be tuned by using a gate voltage,<sup>21,22</sup> different shapes of the magnetic-field dependence may be obtained for a specific sample with different values of the gate voltage. An example is presented in Fig. 7. As one can see, the clearest nonsymmetric behavior is obtained for  $\lambda \approx \lambda_c$  (right panel), but such dependence can be seen for a region in its vicinity as well (middle panel). Far enough from this region (left panel) the symmetric dependence reappears.

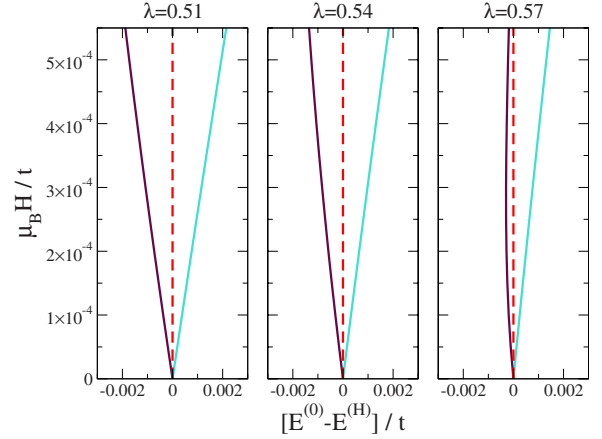


FIG. 7. (Color online) The magnetic-field dependence of the first Coulomb peaks ( $n_e=1,2$ ) for a lattice of  $11 \times 10$  with  $U=3t$  (for which  $\lambda_c \approx 0.59$ ).

We have also tried to verify that the reported phenomenon occurs for states with even electron numbers larger than 2 as well. However, the treatment of such cases is more difficult since the size of the Hilbert space ( $\binom{2AB}{n_e}$ ) quickly passes the computational limit when  $n_e$  increases. Therefore, the numerical simulation is limited to much smaller lattices; and although they show features similar to the LC and the enhanced  $g$  factors reported for the two electron ground state, the question whether a LC occurs for larger lattices as well needs further investigation. As a possible method for that calculation we suggest the particle-hole version of the density-matrix renormalization-group algorithm,<sup>32</sup> which is suitable for such finite Fermi systems.<sup>33</sup> In addition, since as mentioned above the interplay between interactions and disorder can also result in a nontrivial spin polarization, the combination of both disorder and SO coupling with interactions can enhance this finding. These two points deserve a separate investigation.

To conclude, we have shown that the combination of interactions and spin-orbit scattering can lead to a magnetization of states having an even number of electrons. This effect was explained using first-order perturbation theory by the tendency of interactions to drive a Stoner instability, which is enhanced by the SO coupling. By studying the behavior when the system size increases, it seems that such result may be experimentally observed even for realistic sizes of QDs. Therefore it might be relevant for understanding  $g$ -factor measurements. Based on our explanation of the results, we believe that similar phenomena might be observed in metallic nanoparticles as well. However, a numerical investigation for 3D systems is quite difficult.

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