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Effect of electron-electron interactions on the magnetization of quantum dots

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The low-temperature magnetization of parabolic quantum dots is calculated and is shown to be a sensitive probe of interaction effects. The interaction causes the ground state to occur at certain magic values of the total angular momentum, the strength of the magnetic field determining which of them is selected. Increasing the magnetic field causes the ground-state angular momentum to jump from one magic value to another and this causes the discontinuities in the magnetization. The effects of spin lead to extra discontinuities at low magnetic field. The magic angular momenta for the spin-polarized case are derived by a simple physical argument.

The electron-electron interaction in quantum dots subjected to a magnetic field leads to interesting effects which are highly elusive. For example, Maksym and Chakraborty[1] (MC) have shown that the ground state of electrons in a magnetic field occurs only at certain *magic* values of the total angular momentum, and that transitions from one magic value to another should occur as the magnetic field is increased. This cannot be probed by infrared spectroscopic techniques because far-infrared radiation couples to the center-of-mass motion and hence is insensitive to the interaction when the confinement is parabolic.[1-3] Nevertheless, there are probes that are sensitive to the interaction and MC showed that the heat capacity is one of them. In the present work the magnetization is found to be another, which can in principle be measured. (Störmer and co-workers[4] have measured the magnetization of a two-dimensional electron gas.) It is shown that the field dependence of the magnetization is oscillatory with discontinuities that occur when the ground-state angular momentum changes. In addition, the effect of spin is considered, and it is shown that this leads to rich behavior in the low-field regime, where both the spin and angular momentum of the ground state vary discontinuously with magnetic field. Finally, the key physics is explained in terms of a simple model that includes only the states in the zeroth Landau level, and the rule for determining the magic values of angular momentum in the spin-polarized case is given.

The starting point for calculating the magnetization is the calculation of the energy eigenvalues of the electrons interacting in a parabolic dot. This is done by numerically diagonalizing the Hamiltonian

$$\mathcal{H}=\sum_{n,l,s}\mathcal{E}_{nl}c^{\dagger}_{nls}c_{nls}+\sum_{\substack{n_1\ldots n_4\\ l_1\ldots l_4\\ s,s'}}\mathcal{A}_{n_1l_1,n_2l_2,n_3l_3,n_4l_4}c^{\dagger}_{n_1l_1s}c^{\dagger}_{n_2l_2s'}c_{n_3l_3s'}c_{n_4l_4s}\ ,$$

where $\mathcal{E}_{nl}$ are single-electron energies and $\mathcal{A}$ is the Coulomb matrix element

$$\mathcal{A}=\tfrac{1}{2}\int d\mathbf{r}_1\,d\mathbf{r}_2\,\phi^{*}_{n_1l_1}(\mathbf{r}_1)\phi^{*}_{n_2l_2}(\mathbf{r}_2)\times V(\mathbf{r}_1-\mathbf{r}_2)\phi_{n_3l_3}(\mathbf{r}_2)\phi_{n_4l_4}(\mathbf{r}_1)\ .$$

The single-electron energies are obtained from[5,6] $\mathcal{E}_{nl}=(2n+1+|l|)\hbar\Omega-\frac{1}{2}l\hbar\omega_c$, where $\Omega=(\frac{1}{4}\omega_c^2+\omega_0^2)^{1/2}$, $\omega_c=eB/m^*$, and $\hbar\omega_0$ is the confinement energy. The single-electron wave function (ignoring the normalization constant) is written as[3] $\phi_{nl}=r^{|l|}\exp(-il\theta)L_n^{|l|}(r^2/2a^2)\exp(-r^2/4a^2)$, where the effective magnetic length a is given by $a^2=\hbar/(2m^*\Omega)$. The quantum number $-l$ is the angular momentum and the quantum number n is related to the Landau quantum number $N=n+(|l|-l)/2$ (referred to as Fock-Darwin-level index in Ref. 3). In the absence of confinement this becomes the usual Landau-level index and the single-electron energies become $(N+\frac{1}{2})\hbar\omega_c$, but in the presence of confinement, $\mathcal{E}_{nl}$ is a function of both N and l. The relevance of these quantum numbers is that they are used to select the basis states for the numerical diagonalization. The basis includes all contributions of single-electron states that are compatible with the desired total angular momentum, subject to the constraint that the sum of the single-electron N values does not exceed the specified maximum. The exact eigenstates have the property that they can be factorized into a product of a function of the center of mass and a function of relative motion,[1,2] and this method of truncating the basis ensures that the same holds for the numerically generated eigenstates.

Once the many-body eigenvalues and eigenstates are available, the magnetization can be calculated in one of two ways. The first is to evaluate matrix elements of the magnetization operator $\mathcal{M}=(-e/2m^*)\sum_{i=1}^{n_e}\mathbf{r}_i\times(\mathbf{p}_i+e\mathbf{A}_i)$, where n_e is the number of electrons. The second is to differentiate the eigenvalues with respect to the magnetic field B. While these two procedures would give the same result if the basis was infinite, the results obtained from a truncated basis differ and the results given by the differentiation procedure are superior. The reason is that

the magnetization operator couples states whose n quantum numbers differ by ± 1, as well as states with the same n. Therefore accurate evaluation of magnetization requires a larger basis than accurate calculation of the energy eigenvalues. The differentiation procedure is superior because calculating the magnetization by differentiation of the eigenvalues obtained in the truncated basis is equivalent to including the omitted states by first-order perturbation theory and then calculating matrix elements of the magnetization operator. This can be proved by considering dE/dB explicitly:

$$\frac{dE}{dB}=\left\langle\frac{d\psi_0}{dB}|\mathcal{H}|\psi_0\right\rangle+\langle\psi_0|d\mathcal{H}/dB|\psi_0\rangle+\left\langle\psi_0|\mathcal{H}|\frac{d\psi_0}{dB}\right\rangle, \tag{1}$$

where ψ_0 is a state formed from the truncated basis and E is its energy. The derivatives of ψ_0 can be estimated by first-order perturbation theory:

$$\frac{d\psi_0}{dB}\approx\frac{\psi_0(B+\delta B)-\psi_0(B)}{\delta B}$$
$$\approx\sum_j\phi_j\frac{\langle j|d\mathcal{H}/dB|0\rangle}{E_j-E_0}+\sum_{\alpha\neq 0}\psi_\alpha\frac{\langle\alpha|d\mathcal{H}/dB|0\rangle}{E_\alpha-E_0}, \tag{2}$$

where the ψ_α come from the diagonalization within the truncated basis and the ϕ_j are the remaining basis states. Substituting (2) into (1) shows that differentiation of the energies automatically generates a first-order contribution from the omitted basis states; hence differentiation is the superior calculational method. In practice the calculations are done at finite temperature; that is, the numerically generated eigenvalues are used to compute the free energy, which is then differentiated to get the magnetization. All the Zeeman terms for each spin are included in the calculation of the free energy.

The results are shown in Figs. 1 and 2. The top panel of each figure gives the magnetization as a function of B, calculated both with and without interaction for three electrons (Fig. 1) and four electrons (Fig. 2). The remaining panels show the ground-state total-angular-momentum quantum number J and the ground-state spin S. All results are for GaAs quantum dots with $\hbar\omega_0=4$ meV. The calculations were done with the maximum value of N taken to be 1; that is, one electron was allowed to have $N>0$ and the other electrons had $N=0$. This truncation is surprisingly accurate, even at low magnetic fields. The absolute value of the magnetization is insensitive to the upper value of the N sum, and the only effect of increasing it is that the position of the discontinuities changes. This is illustrated in the inset in Fig. 1, where the results of allowing the upper limit of the N sum to rise to 2 are shown. The curves coincide on either side of the discontinuity but the position of the discontinuity is shifted by about 0.15 T. This level of accuracy is typical for fields greater than about 2.5 T; at lower fields the positions of the discontinuities are estimated to be accurate to ± 0.4 T. Physically, the discontinuities correspond to changes of the ground state J, or both J and S, as can be seen by comparing the three panels of the figure. When the system is spin polarized, the sequence of magic J values is the same as found in Ref. 1. Qualitatively the discontinuities resemble the structure discussed by Sivan and Imry[7] but their ori-

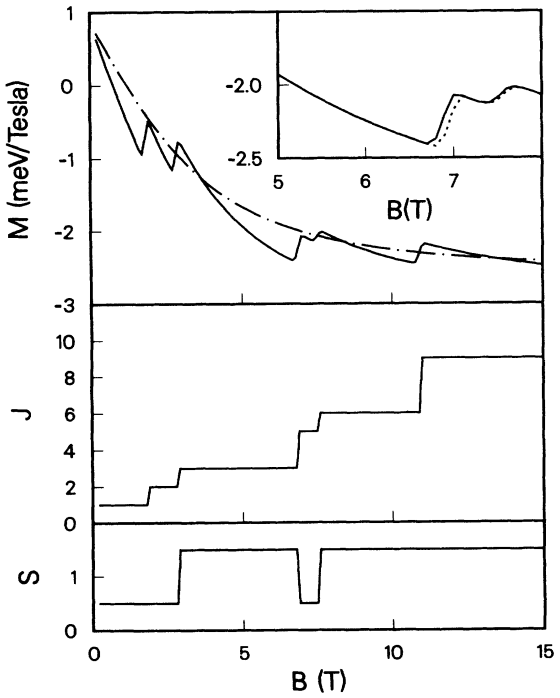

FIG. 1. Magnetization $\mathcal{M}$ (meV/Tesla) at $T=0.1$ K of a parabolic quantum dot containing three electrons ($N=1$), the ground-state angular momentum J, and the ground-state spin S. The dash-dotted line corresponds to the noninteracting case. A comparison of the results for the $N=2$ case (dotted line) is given in the inset.

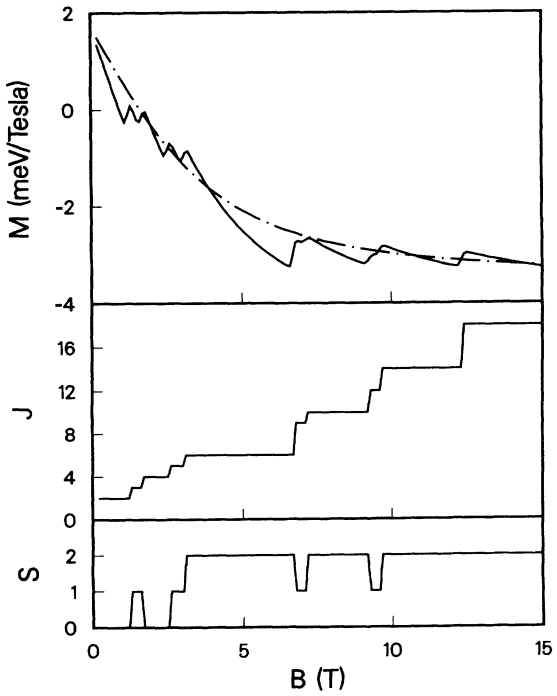

FIG. 2. The same as Fig. 1, but for the four-electron system.

gin is quite different; the latter are an edge-state effect that occurs when several Landau levels are occupied. In contrast, the discontinuities found here occur even when a Landau level is partly full, and are clearly a consequence of the interaction. The magnetization for noninteracting electrons has no discontinuities because the lowest-two single-electron levels are unaffected by level crossings as the field is increased [curves of $\mathcal{E}_{nl}(B)$ for the parameters used here are given in Ref. 8]. Hence systems of up to four noninteracting electrons in the lowest spin state stay in the same angular-momentum state throughout the field range, so the magnetization curve is smooth. All the discontinuities in this case are a consequence of the interaction. For five or more noninteracting electrons the magnetization would be affected by negative l levels crossing positive l levels; however, the position of these crossings would be drastically affected by the interaction. In addition, there are relatively few of them when the electron number is small (for five electrons in the lowest spin state there is only one) and they tend to occur at low field. In contrast, the discontinuities due to the interaction occur at a regular sequence of J values throughout the field range. Because of the small magnetization per dot, experimental observation of the discontinuities would require measurements on an array of dots, and so would be affected by statistical fluctuations in electron number. Nevertheless, the discontinuities should be observable when the fluctuations are small because the discontinuities for different numbers of electrons occur at different magnetic fields.

There are two aspects to the physics underlying the results shown in Figs. 1 and 2. The first is the question of how the interaction affects the magnetization, and the second is the reason why the ground-state angular momentum changes with magnetic field. Both aspects can easily be understood by considering the simplified case of a spin-polarized system with electrons restricted to occupying $N=0$ states. In this case the expression for the total energy simplifies considerably because the interaction energy can be diagonalized independently of the confinement energy. In addition, the confinement energy in this case is only a function of J, so the total energy of each state takes the form

$$E=(n_e+J)\hbar\Omega-\tfrac{1}{2}J\hbar\omega_c+\frac{e^2}{4\pi\epsilon\epsilon_0 a}\lambda(J)+g^*\mu_B BS_z\,,$$

where the first two terms are the confinement energy, the third is the interaction energy, the fourth is the Zeeman energy, $\lambda(J)$ is a dimensionless eigenvalue that depends only on J, and g^* is the effective g factor. For GaAs, g^* is small, so the Zeeman term only affects the magnetization at the 1% level, and the physics is determined by the first three terms. Differentiating them yields two contributions to magnetization:

$$\mathcal{M}=-\frac{\hbar e}{2m^*}\left[(J+n_e)\frac{\omega_c}{2\Omega}-J\right]-\frac{e^2}{8\pi\epsilon\epsilon_0}\frac{e}{(\hbar m^*)^{1/2}}\frac{\omega_c}{(2\Omega)^{3/2}}\lambda(J)\,.$$

These two terms behave very differently in the low- and high-field limits. When $B=0$, the confinement term is $\hbar eJ/2m^*$, and as B increases, it smoothly decreases and approaches $-\hbar en_e/2m^*$ as $B\to\infty$. In contrast, the interaction term approaches 0 both when $B\to 0$ and when $B\to\infty$. For the parameters used here this term contributes at the 1% level when $B<2.5$ T, and $\sim 15\%$ when $B=10$ T; it is most significant when $2.5<B\lesssim 10$ T. The field dependence of the magnetization at fixed J is essentially determined by the first term, and if J was independent of B, the magnetization of the interacting system would be qualitatively similar to that of the noninteracting system. The major effect of the interaction is that the ground state J changes with magnetic field. Every time this happens the magnetization curve *shifts to a different track,* and this causes the discontinuities shown in Figs. 1 and 2.

The jumps in the ground state J occur because at the magic J values there are basis states in which electrons are kept very effectively. The ground state always occurs at one of these J values and the competition between interaction and confinement determines[1] the optimum J. Physically, the preference for certain J values can be understood in a number of equivalent ways; the simplest is to consider the diagonal elements of the Hamiltonian. These have the form $\sum\bar{\mathcal{A}}_{ll'}n_l n_{l'}$, where n_l is the number operator and $\bar{\mathcal{A}}_{ll'}=\mathcal{A}_{0l0l'0l'0l}-\mathcal{A}_{0l0l'0l'0l'}$. The quantity $\bar{\mathcal{A}}_{ll'}$ is the difference between the Hartree energy and the exchange energy of a pair of electrons with angular momenta l and l'. It is plotted in Fig. 3 as a function of l' for the case when $l=5$, and this illustrates its behavior for typical values of l and l'. When $l=l'$, $\bar{\mathcal{A}}_{ll'}=0$ then increases as $|l-l'|$ is increased, and then it decreases again. Thus it is energetically favorable to have $|l-l'|$ either large or small for all pairs of electrons; however, large values can only occur when the total angular momentum is large. The optimal way of making $|l-l'|$ small is to put all the electrons on adjacent orbitals, but this can only be done when J satisfies $J=n_e(n_e-1)/2+kn_e$, where $k=0,1,2,\ldots$. For three electrons this leads to the *magic* angular momenta 3, 6, 9, 12, . . . , while for four electrons it gives 6, 10, 14, 18,.... These are exactly the values found in numerical calculations for the spin-polarized case. These calculations also confirm that basis states in which all

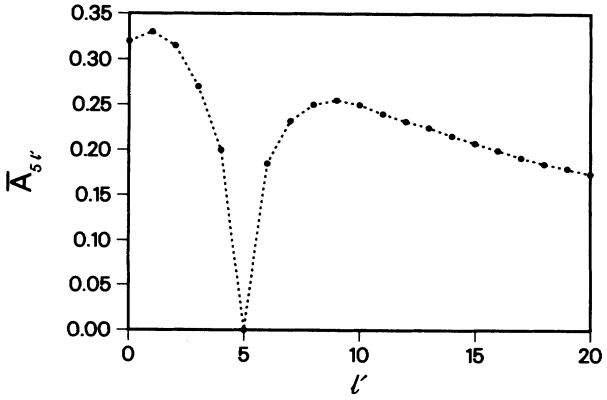

FIG. 3. The l' dependence of $\bar{\mathcal{A}}_{5l'}$ (units: $e^2/4\pi\epsilon\epsilon_0 a$). The points give values of $\bar{\mathcal{A}}$ and the dashed line is to guide the eye.

electrons occupy adjacent orbitals occur with high probability; for example, 53.5% for three electrons at $J=9$ and 48.8% for four electrons at $J=14$. In this physical picture the magic angular momenta are favored because the exchange term efficiently reduces the energy of basis states in which all electrons sit on adjacent orbitals. An alternative way of looking at the situation is to consider the motion of a pair of electrons about its center of mass. In this picture small relative angular momenta occur with very small probability if the electrons occupy adjacent orbitals. This leads to a reduction in energy because the large-angular-momentum matrix elements of the Coulomb interaction are the smallest.

The remaining item to consider is spin. From Figs. 1 and 2 it is clear that spin effects are important at fields $B \lesssim 10$ T, and that the system is spin polarized at higher fields. It is perhaps surprising that the occurrence of full spin polarization in the range $10 \leq B \leq 15$ T is a *consequence* of the interaction. The reason is that the confinement energy is not negligible in this field range. An increase of spin polarization must be accompanied by an increase of J because of the exclusion principle. Since the confinement energy increases with J, flipping a spin costs energy, and full spin polarization does not occur until the Zeeman term is large enough to overcome this energy penalty. (The three-electron noninteracting system is spin polarized up to 20 T, but for four electrons a transition from $S=0$ to $S=1$ occurs at about 19 T.) The other effect of spin is that it causes extra discontinuities in the magnetization. Each spin state has its own sequence of magic J values, and each magic J value corresponds to a possible ground state at that spin. Only some of these J values lead to discontinuities because the lowest-energy state at a given spin is not always the absolute ground state. In the case of three electrons at $S=\frac{1}{2}$, the magic J values for states formed from the zeroth Landau level are 2, 5, 8, 11, . . . , but only 2 and 5 lead to discontinuities because $S=\frac{3}{2}$ states have lower energies than the remaining $S=\frac{1}{2}$ states. In addition, $J=1$ occurs at low magnetic fields, where the contribution of $N=1$ states is important. The four-electron case is more complicated. Although magic J sequences exist, not every member of them occurs at all strengths of the confining potential. For example, the magic J values for states formed from the zeroth Landau level at $S=1$ are 5, 9, 13, 17, . . . , and some of these occur in Fig. 2. However, $J=9$ does not occur if the confinement is very weak and for moderate values of confinement $J=13$ shifts to $J=12$. Because of this sensitivity to the confinement, it is difficult to give a rule that determines the magic J values for an arbitrary number of electrons at an arbitrary spin. In contrast to the spin-polarized case, it seems that the magic J values have to be determined numerically.

In summary, the low-temperature magnetization of quantum dots provides a sensitive probe of the effect of the electron-electron interaction on the ground state. The key physics can be understood in terms of a simple model in which only the zeroth-Landau-level states are taken into account.

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