Quantum Dots in a Magnetic Field: Role of Electron-Electron Interactions

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The eigenstates of electrons interacting in quantum dots in a magnetic field are studied. The interaction has important effects on the magnetic-field dependence of the energy spectrum. However, when the confinement potential is quadratic, the optical excitation energies of the many-body system are exactly the same as those of a single electron. This makes the interaction effects difficult to observe directly but they could be seen by measuring the thermodynamic properties of the electrons. This is illustrated with the calculations of the electronic heat capacity.

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Rapid advances in semiconductor technology have led to the fabrication of zero-dimensional structures called quantum dots. Essentially, they are little islands of two-dimensional electrons which are laterally confined by an artificial potential. Alternatively, they can be thought of as artificial atoms where the confining potential replaces the potential of the nucleus. Typical dot sizes are about 100 nm and each dot typically contains between 2 and 200 electrons.[1-4] While several current experiments[1,3,4] have focused attention on various properties of quantum dots in a magnetic field, their theoretical understanding is still in its infancy. In particular, the effect of the electron-electron interaction has not yet been investigated although Bryant[5] has emphasized its importance in the case of zero field. The purpose of this Letter is to present a detailed study of quantum dots in which both the magnetic field and the electron-electron interaction are fully taken into account. First, numerical calculations of the electron states are used to show that the electron-electron interaction is highly important and leads to unusual magnetic-field dependence of the ground state and its excitations. Next it is shown that, when the confining potential is quadratic, far-infrared (FIR) spectroscopy is insensitive to interaction effects because the center of mass (cm) and relative motions then separate in the same way as for the free electrons. This explains recent experimental results which show that the effect of the interaction is apparently very small.[1] Finally, results for the heat capacity are presented to suggest that the effect of the interaction could be probed by measuring the thermodynamic properties of the electrons.

The first step in calculating the electron states is to find the eigenstates of a single electron. It is believed that the dots currently studied experimentally confine the electrons by a potential that is quadratic to a good approximation when the electron number n_e is small.[1,6] Therefore the calculations reported here have been done for the case of ideally two-dimensional electrons, in a circular dot, confined by a radial potential of the form $\frac{1}{2}m^*\omega_0^2r^2$ with a magnetic field B perpendicular to the plane of the dot and m^* is the electron effective mass. The corresponding single-electron states were first derived by Fock[7] and Darwin[8] and later studied in detail by Dingle.[9] Apart from a normalization constant they have the form

$$\varphi(\mathbf{r})=r^{|l|}\exp(-il\theta)L_n^{|l|}(r^2/2a^2)\exp(-r^2/4a^2)\,,$$

where $L_n^{|l|}$ is a Laguerre polynomial, $a^2=(\hbar/m^*)(\omega_c^2+4\omega_0^2)^{-1/2}$, and $\omega_c=eB/m^*$. The single-electron energies depend on the two quantum numbers n and l,

$$E_{nl}=(2n+1+|l|)\hbar(\tfrac{1}{4}\omega_c^2+\omega_0^2)^{1/2}-\tfrac{1}{2}l\hbar\omega_c\,,$$

but in the limit, when $\omega_0\rightarrow 0$, they reduce to $E_{nl}=[n+\frac{1}{2}+(|l|-l)/2]\hbar\omega_c$ and depend only on the quantum number $N=n+(|l|-l)/2$. Physically, N is the Landau-level index and $-l$ is the angular momentum quantum number. Without the confining potential the energies of the positive l states would be independent of l but in its presence they increase with l. This is the key difference between the behavior of free and confined electrons. It is reponsible for much of the new physics reported here.

To calculate the states of the interacting electrons it is supposed that B is strong enough to keep them spin polarized. This assumption allows the interplay between the effects of confinement and interaction to be studied without including extra complications. The role of spin is briefly discussed later in this Letter. In the spin-polarized case the constant Zeeman term can be ignored so the Hamiltonian is

$$\mathcal{H}=\frac{1}{2m^*}\sum_{i=1}^{n_e}(\mathbf{p}_i+e\mathbf{A}_i)^2+\frac{1}{2}m^*\omega_0^2\sum_{i=1}^{n_e}r_i^2+\frac{1}{2}\frac{e^2}{4\pi\epsilon\epsilon_0}\sum_{i\neq j}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}\,,\qquad(1)$$

where $\epsilon\epsilon_0$ is the dielectric constant. The interaction between electrons in different dots is neglected but this should be a good approximation because the dot spacings are typically larger than dot sizes. The neutralizing positive background present in real systems is also ignored. For an infinite system it cancels the divergence caused by the Coulomb repulsion but for a single dot all the matrix elements of the Coulomb interaction are finite. In the case of a periodic array of dots with a large spacing of the background cancellation merely leads to a constant shift of the energy levels for the single dot. The eigenstates of the system are eigenstates of the total angular momentum, which is conserved by the electron-electron interaction. They can be classified by a quantum number J, which is the sum of the single-electron l values. The states are calculated by numerically diagonalizing the Hamiltonian. Landau-level mixing is taken into account but is found not to influence the physics. Its effect is estimated quantitatively from trial computations where an extra Landau level is included. For the parameters considered here the low-lying energy levels converge to 7% ($n_e=4$) or 2% ($n_e=3$) when only two Landau levels are taken into account. The convergence of the ground state is better and its optical excitation energies agree to within 10% ($n_e=4$) or 2% ($n_e=3$) with the expected cm excitations (see below). For higher electron numbers or lower B the effect of Landau-level mixing would be more important.

The energy levels of the three and four electron systems are shown in Fig. 1. They have been calculated using parameters appropriate to GaAs and a value of 4 meV for $\hbar\omega_0$. The energies are given relative to what would be the lowest Landau level, that is, the constant of $\hbar(\frac{1}{4}\omega_c^2+\omega_0^2)^{1/2}$ per electron is not included. Each frame of the figure shows total energies plotted against J at magnetic fields representative of *low*- and *high*-field behavior. Clearly there are always two sets of broadened levels separated by a gap. In the limit of zero confining potential these would be the lowest two Landau levels. The general trend is that the energies increase with J because the single-electron energies increase with l. This is most clearly seen at $B=2$ T; at high field the increase is much weaker. Calculations for five and six electrons show the same physics but they are not so well converged.

The main difference between high- and low-field behavior is the angular momentum of the ground state. At $B=2$ T this occurs at the lowest available J, that is, the smallest angular momentum compatible with placing all the electrons in $N=0$ states. For example, for three electrons the ground state is at $J=3$ which is formed from the l values $0+1+2$. If the electrons did not interact, the ground state would have the lowest available J provided B is so high that only $N=0$ is relevant. Because of the interaction, however, the ground-state J increases with B. This effect is caused by the interplay of the single-electron energies and the interaction energy. It can be understood in terms of a simple calculation in which only the $N=0$ states are taken into account. In this case the single-electron contribution to the energy is simply $\hbar[(\frac{1}{4}\omega_c^2+\omega_0^2)^{1/2}-\frac{1}{2}\omega_c]J$ (relative to the lowest Landau level), but the interaction contribution has to be obtained by numerical diagonalization. Figure 2 shows these two contributions together with their sum. The single-electron contribution increases linearly with J because electrons in high angular momentum states see a higher confining potential. In contrast, the interaction term decreases because electrons with higher angular momenta move in orbitals of larger radii, thereby reducing their Coulomb energy. The net result is that the total energy as a function of J has a minimum. At low field this occurs at the lowest available J because the single-electron energy increases steeply with J. At high field the increase is much weaker so the minimum occurs at a higher J value. Since each J value has its own set of energy levels, changing the field has a dramatic effect on the excitation spectrum as well as the ground state.

The ground state does not take all possible values of J because the interaction energy does not change continuously with J. Instead it contains steplike structures which occur at particular J values (see arrows in Fig. 2) and are possibly analogous to the energy cusps in the fractional quantum Hall effect.[10] Because the total en-

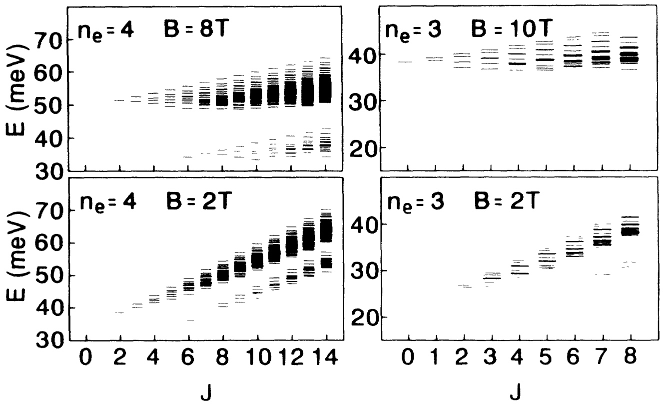

FIG. 1. Energy levels as a function of J for three and four electrons in a GaAs quantum dot. Each frame corresponds to a different magnetic field as indicated.

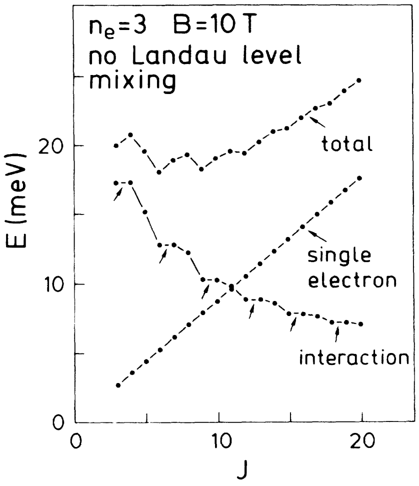

FIG. 2. Contributions to the total energy as a function of J. The points give energy values and the lines are to guide the eye. Arrows indicate the steps in the interaction energy.

ergy is the sum of the single-electron and interaction terms, the steps lead to minima in the total energy as a function of J and the ground state always occurs at one of these. For example, in Fig. 2 the global minimum occurs at $J=6$ but there is another minimum close to it at $J=9$. If the field was increased to 10.4 T, this would become the global minimum; further increasing the field would cause the global minimum to occur at $J=12$ and so on. Using the well-known formula $\nu = n_e(n_e-1)/2J$ (which is obeyed by the Laughlin states[10]), one can convert the sequence of favored J values to effective filling factors. We find that the three electron states go through the sequence of ν values $1, \frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \ldots$ and the four electron states go through $1, \frac{3}{5}, \frac{3}{7}, \frac{1}{3}, \ldots$. It is remarkable that even denominators occur in addition to the usual odd ones.[11] We emphasize that the multiple minima in the ground-state energy only occurs in the presence of confinement: With no confinement the steps in the interaction term persist but the single-electron term vanishes, consequently there are no minima at finite J.

The rich structure of the energy spectra shown in Fig. 1 is in complete contrast with current experimental results on FIR absorption. These have just two features whose energies seem to correspond to single-electron excitations. To explain this apparent contradiction it is necessary to consider the perturbation due to the electromagnetic radiation. Typical wavelengths are 50 μm while typical dot sizes are 100 nm so the dipole approximation holds to a high degree of accuracy. In other words, the electrons see a perturbing vector potential which is independent of position within the dot, or equivalently, a position-independent electric field $\mathbf{E}_0 \times \exp(-i\omega t)$. The perturbing Hamiltonian therefore has the form $\mathcal{H}' = \sum_{j=1}^{n_e} e\mathbf{E}_0 \cdot \mathbf{r}_j \exp(-i\omega t)$. This depends only on the sum of the electron coordinates; hence, it can be expressed in terms of the cm coordinate $\mathbf{R} = \sum_i \mathbf{r}_i / n_e$ and the total charge $Q = n_e e$, that is, $\mathcal{H}' = Q\mathbf{E}_0 \cdot \mathbf{R} \exp(-i\omega t)$. To understand the effect of this it is convenient to rewrite the Hamiltonian (1) in terms of the cm and $3(n_e-1)$ coordinates relative to it. These are most conveniently chosen to be $\mathbf{r}_i' = \mathbf{r}_i - \mathbf{R}$, where i ranges from 1 to $n_e - 1$. The coordinate of the n_eth electron is then given by $\mathbf{r}_{n_e} = \mathbf{R} - \sum_{i=1}^{n_e-1} \mathbf{r}_i'$ and the Hamiltonian becomes

$$\mathcal{H} = \frac{1}{2M}(\mathbf{P} + Q\mathbf{A})^2 + \tfrac{1}{2} M\omega_0^2 R^2 + \mathcal{H}_{\mathrm{rel}},$$

where $\mathbf{P} = \sum_{i=1}^{n_e} \mathbf{p}_i$, $\mathbf{A}$ is the vector potential of the cm, and $M = n_e m^*$. The last term $\mathcal{H}_{\mathrm{rel}}$ is a function of only the relative coordinates and contains all the effects of the interaction. The Hamiltonian clearly separates in the same way as established long ago[12] for the case of no confining potential. This is a very special property of quadratic confinement—if the potential was different, the cm motion would couple to the relative motion. It follows that FIR radiation excites the cm but does not affect the relative motion. Further, the cm Hamiltonian has the same form as the Hamiltonian of a single confined electron. In addition, it has *exactly* the same energy eigenvalues because ω_c in the expression for E_{nl} depends only on the charge-to-mass ratio $Q/M = e/m^*$. Consequently, FIR absorption experiments see only features at the single-electron energies.[13]

How then is it possible to observe the effects of the electron-electron interaction? There seem to be two possibilities. One is to change the shape of the dot to force coupling of the cm and relative motions. It is possible that this is responsible for some level-crossing effects observed in recent experiments.[4] The second possibility is that the interaction should affect thermodynamic properties, for example, the electronic heat capacity C_v (which is observable[14]).

To test this idea the magnetic-field dependence of C_v has been calculated. As usual, this is found from the temperature derivative of the mean energy. For simplicity Landau-level mixing is neglected, but this does not leave out any essential physics. Figure 3 gives C_v, excluding the Zeeman contribution (which is a small, slowly varying background). For interacting electrons C_v (solid lines) is clearly very different from that of noninteracting electrons (dotted lines). In particular, when the electrons interact C_v oscillates as a function of B and has minima that are associated with crossovers from one ground-state J value to another. (The dashed lines in Fig. 3 indicate the ground-state J.) The oscillations in C_v are a many-body effect, unlike the low-field oscillations in C_v for a two-dimensional electron gas.[15] Their origin is best understood by considering the curves for $T=1$ K. At this very low temperature the dominant contribution to C_v comes from two competing ground states. This causes the doublet structure around the crossovers and can be understood in terms of the B dependence of the gap between the corresponding ground

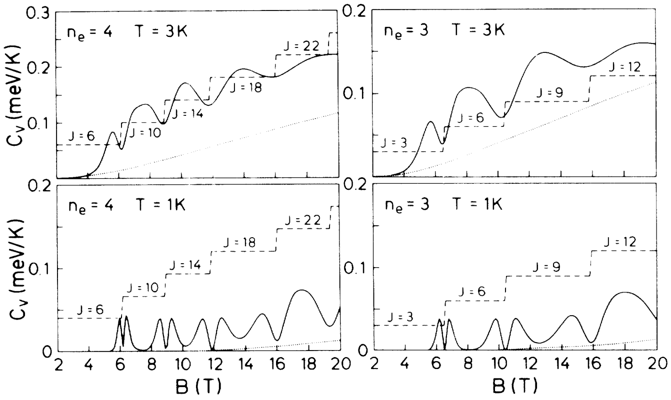

FIG. 3. Heat capacity C_v as a function of magnetic field for three and four electrons in a GaAs quantum dot. Each frame corresponds to a different temperature as indicated.

states. Far away from a crossover the gap is large so C_v is small. Similarly, it is small exactly at a crossover because the gap is then zero. However, on either side of a crossover the gap is nonzero but not too large. Consequently, C_v is nonzero because neither the probability of a thermal excitation nor the heat absorbed in one are vanishingly small. This picture of an oscillatory heat capacity holds when other spin polarizations are taken into account. Indeed, for $B > 10$ T the ground states are expected to be fully polarized but at lower fields there is more structure in C_v when the ground-state spin depends on B.

In conclusion, the interaction of electrons in quantum dots leads to rich structure in their energy spectrum. However, FIR spectroscopy cannot probe it when the confining potential is quadratic because the optical excitations are then excitations of the cm and have exactly the same energies as single-electron excitations. The structure could be probed by deliberately engineering the dots so that the cm and relative motions are coupled or by measuring the thermodynamic properties of the electrons.

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