Thermodynamic properties of quantum dots in a magnetic field

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The magnetization, magnetic susceptibility, and specific heat of heliumlike confined quantum dots are calculated. The Schrödinger equation for the relative motion of the two electrons is solved numerically and the solutions are used to calculate the partition function. We found a sharp peak in the susceptibility and an additional structure in the specific heat. The correlation energy and spin contribution are shown to be important.

Quantum dots are composed of a small number of electrons ($N \leq 200$) laterally confined in two dimensions. Due to the development of semiconductor techniques, the experimental investigation of this zero-dimensional nanostructure has become possible.[1-3] Self-consistent calculations[7,8] of the confinement potential in quantum dots have shown that, to a good approximation, they can be described by a simple one-parameter adjustable parabolic potential.[4-15] Most of the experimental work on quantum dots in GaAs and InSb are in agreement with this result. As a consequence of the parabolicity, the infrared absorption of these systems occurs only via center of mass and is, therefore, insensitive to the electronic correlations. The application of a magnetic field perpendicular to the dot plane will introduce an interesting structure on the energy levels, but will not effect significantly far-infrared absorption patterns. This is a consequence of the fact that the magnetic field only introduces a parabolic term in the Hamiltonian.

A second important contribution is the electronic spin. The simplest heliumlike dot will show a low magnetic-field behavior in which the ground state is spinless. The same behavior is observed in more complicated multielectron systems with an even number of electrons. At high magnetic field the resulting pattern shows the spins to be aligned. In most of the early theoretical calculations,[6,7,13] the electron-electron interactions were neglected. Maksym and Chakraborty[14] and Merkt, Huser and Wagner[15] have included the electron-electron interactions. In Ref. 14 the specific heat was calculated diagonalizing the Hamiltonian numerically within a truncated basis of Fock states. Merkt, Huser, and Wagner have obtained the energy spectra for the two-electron system neglecting the spin interactions. Recently, the same authors have reported[16,17] the inclusion of spin effect and the calculation of the magnetization for GaAs.

The purpose of this paper is to present the results of a calculation of the energy levels, partition function, and related thermodynamic properties for quantum dots consisting of two electrons by solving the full Hamiltonian, including spin interaction, with methods that allow us to obtain the energy spectrum and eigenstates with an arbitrary accuracy.

We are interested in the thermodynamic quantities such as the magnetization, the susceptibility, and the specific heat of a gas of noninteracting quantum dots. These should be a good approximation because dot spacings are usually larger than the dot size (about 100 nm).

Within the effective-mass approximation, the Hamiltonian for an interacting pair of electrons moving in perpendicular magnetic field in a medium characterized by a dielectric constant ε is

$$\mathcal{H}=\frac{\hbar^2}{2m^*}(\Delta_1^2+\Delta_2^2)+\frac{e^2}{\varepsilon|\mathbf{r}_1-\mathbf{r}_2|}+\frac{m^*\omega^2}{2}(\mathbf{r}_1^2+\mathbf{r}_2^2) -\frac{eB\hbar}{2m^*c}(L_{z_1}+L_{z_2}+gm^*/mS_z)\,, \tag{1}$$

where m^* is the effective mass and g is the effective gyromagnetic factor. The frequency ω depends on both the magnetic field and the confinement frequency parameter ω_0, and is given by

$$\omega=(\omega_0^2+e^2B^2/4m^{*2}c^2)^{1/2}\,. \tag{2}$$

The Hamiltonian is rotationally invariant without coupling between the spin and the orbital angular momentum. Therefore, we search for eigensolutions that are common to both operations. The crucial property of the parabolic potential is that it is separable by the introduction of the center-of-mass coordinate $\mathbf{r}_{cm}=(\mathbf{r}_1+\mathbf{r}_2)/\sqrt{2}$, and the relative coordinate $\mathbf{r}=(\mathbf{r}_1-\mathbf{r}_2)/\sqrt{2}$, obtaining

$$\left[-\frac{\hbar^2}{2m^*}\Delta_{cm}^2+\frac{m^*\omega^2}{2}r_{cm}^2-\frac{eB\hbar}{2m^*c}L_z^{cm}-\varepsilon_{cm}\right]\Phi_{cm}=0\,, \tag{3}$$

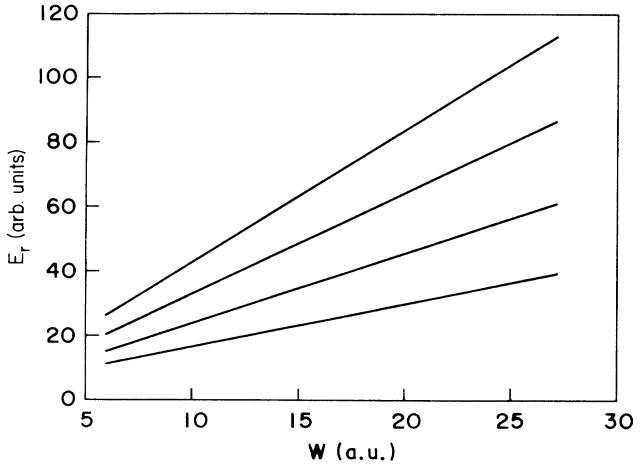

FIG. 1. First low-energy levels as a function of magnetic field calculated with the parameter for InSb. Only low-field behavior is shown.

$$\left[-\frac{\hbar^2}{2m^*}\Delta_r^2+\frac{m^*\omega^2}{2}r^2-\frac{eB\hbar}{2m^*c}L_z^r+\frac{\sqrt{2}e^2}{\varepsilon r}-\varepsilon_r\right]\Phi_r=0\ , \tag{4}$$

$$\left[\frac{|e|B\hbar}{2mc}gS_z\right]\Phi_{\text{spin}}=\varepsilon_{\text{spin}}\Phi_{\text{spin}}\ , \tag{5}$$

where

$$\varepsilon_{\text{spin}}=\frac{|e|B\hbar g}{2mc}M_{\text{spin}}\ . \tag{6}$$

The center-of-mass and spin equations, Eqs. (3) and (5), respectively, can be solved analytically by traditional methods, giving[18]

$$\varepsilon_{\text{cm}}=\frac{eB\hbar M_{\text{cm}}}{2m^*c}+\hbar\omega(2N_{\text{cm}}+|M_{\text{cm}}|+1)\ . \tag{7}$$

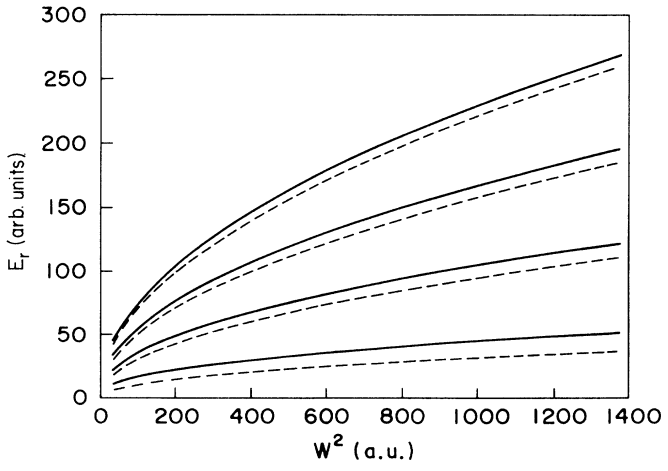

FIG. 2. Comparison between the energy level calculated with the full Hamiltonian and the pure harmonic approximation.

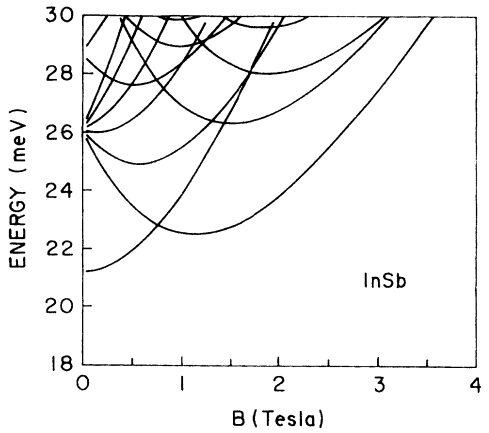

FIG. 3. Energy levels as a function of B. The crossing of the $M_r=0$ and $M_r=1$ states is seen for $B=0.75$ T; other crossing occurs for $B=5.5$ T.

The radial equation [Eq. (4)] cannot be solved in a closed form and a numerical solution is required. This equation was solved by the Frobenius recursion expansion, where the coefficients of a series are exactly calculated until the desired convergence limit is achieved.

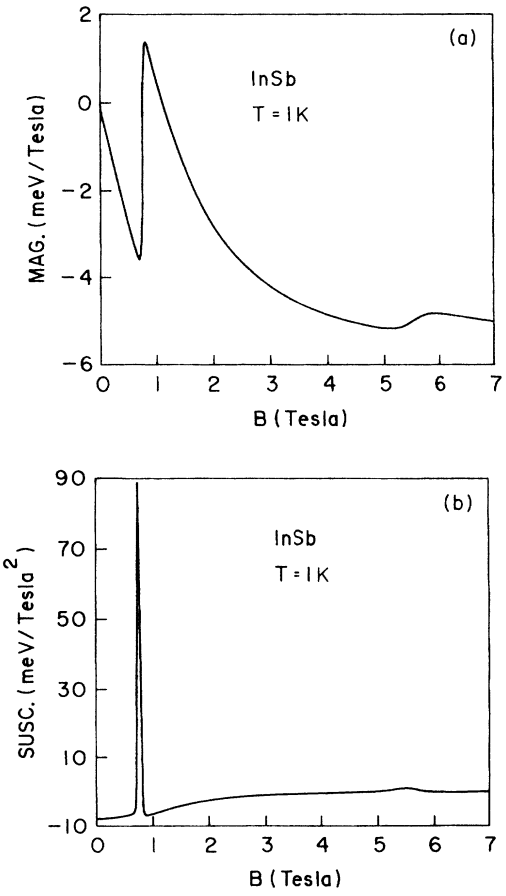

FIG. 4. (a) Magnetization as a function of magnetic field. (b) Magnetic susceptibility as a function of B. In M and χ we observe the structure at $B=0.75$ T that corresponds to the transition from the $M_r=0$ to the $M_r=1$ state.

A surprisingly simple behavior is found for the energy levels as a function of the effective squared frequency ω^2. For low field, the electron-electron interaction gives the dominant contribution in Eq. (4), and in this region an almost linear behavior for the energy levels is found. In Fig. 1, the first low-energy levels are presented as a function of B, using parameters appropriate to InSb, where $\varepsilon=17.88$, $m^*/m=0.014$, $\hbar\omega_0=7.5$ meV, and $g=-50$. The value of g, for InSb, varies from this low-field value until $g=-40$ for $B=10$ T.[19] The variation, however, only causes small modifications on the energy spectrum. In order to see the effect of electron-electron correlations, we compare, in Fig. 2, our results (full curves) with previous calculations where these interactions were neglected (dashed curves) and only the parabolic confinement potential and the magnetic field were taken into account. It is clear that the harmonic-oscillator-type solution is a good approximation only in the very high-field limit. For low field there is not even a qualitative agreement between the two model systems; these differences also will be clear in the thermodynamic properties.

In Fig. 3 we show the first few levels as a function of the magnetic field. Due to the linear Zeeman and spin terms, the low-field ground state will cross the $m=1$ excited state at $B=0.75$ T. This crossing separates the low-field simplest phase and a ferromagnetic-oriented one. At higher fields other level crossings occur.

Due to the effectiveness of the recursion-series technique, a sufficiently large number of energy levels is available to obtain convergence in the partition function. For $T=1$ K we need about two levels; for higher temperatures more levels are needed for the same convergence.

Having the partition function for $T=1$ K, the magnetization M and susceptibility χ have been calculated; in Fig. 4 we show m and χ as a function of B. For $B=0.75$ T, a sharp peak is observed, and other structures are also observed at higher fields, e.g., 5.5 T; however, their intensities are much smaller than the one at 0.75 T. Previous work[14] neglected the spin interaction and did not observe these transitions. The specific heat at constant volume C_v was also computed and shown in Fig. 5; again, the transition at $B=0.75$ T is seen and here the double-peak structure due to the crossover at the $M_r=0$ and $M_r=1$ states has the same intensity as the one at $B=5.5$ T. These structures are linked to the crossing of the lowest with a higher level, at which point the nature of the ground state changes.

The relative importance of the electron-electron and spin-interaction terms can be seen when the C_v is calculated without the electron-electron interaction term; the first double-peak structure at 0.75 T moves to higher field with an intensity decrease very small, and also the structures at higher fields are not observed for low temperatures. If the spin interaction is neglected the structure at $B=0.75$ T is absent.

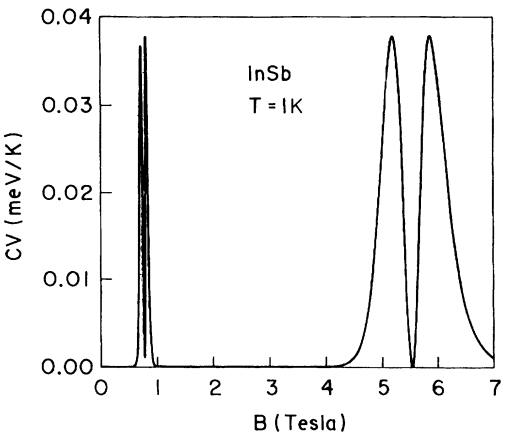

FIG. 5. Specific heat C_v as a function of B.

Before we conclude, we would like to compare the results presented here for InSb with the results for GaAs obtained in Refs. 16 and 17. The crossings in the energy levels as a function of the magnetic field are sharper in the case of InSb when compared to GaAs. The Landé factor in the former case is two orders of magnitude larger, which causes an enhancing of one order of magnitude in the susceptibility.

In conclusion, we showed that if the full Hamiltonian for a gas of quantum dots is solved, a sharp transition between a ferromagnetic and a spinless phase will be observed. A specific quantum-dot system can be engineered to probe this transition. The electron-electron and spin interactions are crucial in such experiments. Generalization for $N\geq 3$ quantum dots is now possible thanks to the quasianalytical nature of the one-particle range of B.

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