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Stability of the maximum-density droplet state in quantum dots: a quantum Monte Carlo study

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Abstract

We have applied the microscopic approach to study the stability of the maximum-density droplet (MDD) state in semiconductor quantum dots under external magnetic field. Explicit expressions for the trial wave functions of the post-MDD states with various spin and angular momentum values are constructed. Results are compared with those of the exact diagonalization approach. © 2000 Elsevier Science B.V. All rights reserved.

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Semiconductor quantum dots (QD) are small devices containing a tunable number of electrons in an external confinement potential [1]. There has been significant progress in the fabrication of QDs during the last few years, which has stimulated an increasing interest in investigating the properties of such systems. From the theoretical point of view, a QD is an ideal many-electron object for theoretical study of fundamental physical properties of correlated systems. One of the major theoretical goals is to understand the nature of the many-body ground states for various magnetic field strengths.

We use the usual model for a QD: electrons with an effective mass m^* are moving in two dimensions and are confined by a parabolic potential $\frac{1}{2}\omega_0^2 r^2$. The one-body problem is similar to the harmonic oscillator one (with frequency $\omega^2 = \omega_0^2 + \frac{1}{4}\omega_c^2$, where $\omega_c = eB/m^*c$) and is easily solved for an arbitrary magnetic field B [2]. The quantum Monte Carlo (QMC) method has shown to be an attractive approach to study the electronic structure of QDs for a wide range of magnetic field strengths [3–6].

Over a region in the magnetic field, the electrons are in the state called maximum-density droplet (MDD), which corresponds to the case of full spin polarization and occupation of the lowest possible angular momentum (L) values from the lowest Landau level (LLL). One interesting question is the nature of the ground states after MDD. In the previous QMC studies, only the fully spin-polarized states have been studied. In this paper, we study all the possible spin configurations for the post-MDD states. We concentrate on seven electrons and on the angular momentum range from $L_{\mathrm{MDD}} = 21$ to $L = 28$ which is the first possible spin-polarized lowest-energy state after MDD.

The LLL single-particle wave functions are polynomials of complex coordinate $z = x + \mathrm{i}y$ multiplied by a common exponential factor. This also simplifies the many-body wave functions. For example, the MDD wave function is in scaled units $\prod_{i<j}(z_i - z_j)$ $\exp(-\frac{1}{2}\sum_i |z_i|^2)$. The QMC many-body wave function used in this work is built in such a way that it has proper symmetry as the particles are interchanged. For fully spin-polarized cases, the wave function changes sign as a pair of electrons is interchanged. In the partially polarized cases, the wave function with proper symmetry can be build using a Young's tableau with two columns, first column for the indices of spin-up electrons and the second one for the rest of the indices. This can be done

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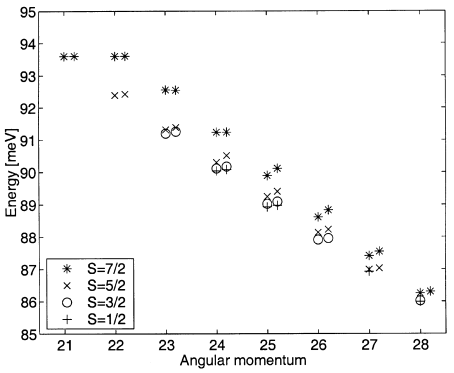

Fig. 1. Energy as a function of the angular momentum. The QMC energies are shifted to right for clarity. The statistical error in QMC results is smaller than the symbol used.

because the Hamiltonian used in this work does not operate directly on the spin. One should note that even if the electrons with different spins can be considered to be different species, they are coupled as we build the state to be an eigenstate of the center-of-mass motion. In addition, we assume that it is advantageous for each electron to place zeros at the position of the other spin-type electrons, also. Using this assumption, the wave function can be written as $\Psi = \mathrm{MDD} \times F$, where F is a polynomial of proper symmetry. Combining these results, the wave function can be written as

$$\Psi = \mathscr{Y}\,\mathrm{MDD} \prod_{i=1}^{N_\downarrow} \hat{z}_i \prod_{j=1}^{X} \hat{z}_{N-j+1}, \tag{1}$$

where $\mathscr{Y}$ is an operator corresponding to the Young's tableau for $N_\downarrow$ spin-down and $N_\uparrow$ spin-up electrons, $\hat{z} = z - z_{\mathrm{CM}}$ is a coordinate reducing center-of-mass motion to the lowest eigenstate, and $X = 0,1,\ldots,$ $N_\uparrow - N_\downarrow$ is an additional angular momentum (in total, $L = L_{\mathrm{MDD}} + N_\downarrow + X$).

In the actual calculations, we use GaAs material parameters, namely, $m^*/m_0 = 0.067$ and $\varepsilon = 13$. We omit the confinement $\hbar\omega_0 = 0$ and set $B = 5$ T. The Zeeman term $g^*\mu_B B S_z$ is not included, but can easily be added afterwards. For the parameters used, it shifts energies by roughly 0.064 meV for each spin.

In Fig. 1, the exact diagonalization and QMC energies are plotted as a function of the angular momentum. One can see that the agreement of the results is rather good. In the worst $S = \frac{7}{2}$ case, $L = 25$, the overlap of the QMC and diagonalization wave functions is around 0.93, which is still reasonable. There are only three diagonalization states (one for $L = 27$ and two for $L = 28$) that do not have simple interpretation in terms of the QMC wave function presented above. In order to describe them, one should allow higher orders of z in the trial wave function. It is interesting to note that if one includes the Zeeman term, the order of the $L = 28$ states is fully reversed.

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