Wave function for quantum-dot ground states beyond the maximum-density droplet

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We study the possible lowest energy states for spin-polarized electrons in a parabolic quantum dot in the strong magnetic field, for filling factors $1>\nu\geqslant 1/3$. We present a variational wave function that correctly predicts the possible angular momentum values obtained from numerical diagonalizations. The wave function is optimized using quantum Monte Carlo techniques. [S0163-1829(99)05927-5]

I. INTRODUCTION

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 QD's during the last few years,[2] 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 quantum dot: electrons with an effective mass m^* are moving in two dimensions and are confined by a parabolic potential $1/2\omega_0^2 r^2$. The one-body problem is similar to the harmonic oscillator one (with frequency $\omega^2=\omega_0^2+1/4\omega_c^2$, where $\omega_c=eB/m^*c$) and is easily solved for an arbitrary magnetic field B.[3] As we concentrate on the strong magnetic-field limit, the relevant one-particle states are on the lowest Landau level (LLL), and these states can be labeled by the angular momentum eigenvalue l. The interaction between electrons is included in the Hamiltonian by the terms $e^2/\epsilon r_{ij}$, where ϵ is the dielectric constant of the material.

The fully spin polarized N-electron state built from LLL states of angular momentum $l=0,\ldots,N-1$ is the maximum-density droplet (MDD) state. In the thermodynamic limit, the MDD corresponds to an integer quantum Hall state with filling factor $\nu=1$. The total angular momentum L is equal to $L_{MDD}=N(N-1)/2$. The many-body states for $\nu>1$, corresponding to lowest energy states in the weaker magnetic fields, can be easily obtained from a modified one-electron picture as presented in Ref. 4. In the stronger magnetic-field values, the angular momentum is larger than L_{MDD} and this region corresponds to the fractional quantum Hall regime in the thermodynamic limit, with filling factor defined as $\nu=L_{MDD}/L<1$. The L values of these possible lowest energy states, marked by L^* in this paper, do not contain all possible L values of the system, but only some of them. There is no theory to rigorously predict the L^* values.

There are a number of previous theoretical studies on this $\nu<1$ or post-MDD region.[7,8,10–14] Recently, high quality experiments with a symmetric QD have been done for this region.[5] The central theoretical question is mainly related to the angular momentum values of the possible lowest energy states and also to the topology of these many-body states.

The composite fermion (CF) wave function[7–9] is the only ''analytic'' construction the authors are aware of, in the ν range that we are currently interested in. The problem with the CF wave function is that the necessary LLL projection is difficult to calculate. It is possible to formulate the CF theory using only the LLL.[9] In the ''standard'' formulation of the CF theory, in which the composite fermions occupy several Landau levels of their own and the LLL projection of the wave function is needed, the possible L^* values are given by the noninteracting electrons in the reduced magnetic field. In the LLL formulation of the CF theory, as presented in Ref. 9, the L^* values are the same as in the standard formulation. The magnetoexciton states of Ref. 11 are presented mainly for $1>\nu\geqslant N-1/N+1$, and for smaller values of ν the magnetoexciton states have only a small overlap with the exact ground states.

II. WAVE FUNCTION

As a consequence of the parabolic potential, the model Hamiltonian discussed above can be separated into sum $H=H_{\rm cm}+H_{\rm rel}$ (Ref. 6) where the first term contains only center-of-mass coordinates and the second only relative coordinates. The Hamiltonian $H_{\rm cm}$ is exactly soluble. The Hamiltonian of the relative motion includes the Coulomb interaction and it cannot be exactly solved.

Next we will first discuss the LLL part of the wave function. The LLL one-particle states can be written as

$$\psi_l \propto z^l \exp\left(-\frac{r^2}{2}\right), \tag{1}$$

where $l=0,1,2,\ldots$ is the angular momentum and $z=x+iy$. The length is measured in units of $l_0=\sqrt{\hbar/m^*\omega}$. If one omits the electron-electron interaction, the many-body wave function can be written as a determinant of the one-body states above. In this case, the total energy is determined by the total angular momentum L, which is simply a sum over the l values of the single-particle states.

The determinant of the states $l=0,1,2,\ldots,N-1$ is MDD, and it can be written in a compact form as

$$\Psi_{MDD} = \prod_{i<j}^{N} z_{ij} \exp\left(-\sum_{i=1}^{N} \frac{r_i^2}{2} \right), \tag{2}$$

where $z_{ij} = z_i - z_j$. One should note that the phase part of the MDD wave function contains only relative coordinates, which means that the center-of-mass motion is in the lowest state. The total angular momentum of MDD is $L_{MDD} = N(N-1)/2$, and MDD is the only LLL state with this angular momentum value. The state with $L = L_{MDD}+1$ is also unique, as the only possibility to increase the angular momentum of the MDD by 1 is to move the electron from the $l = N-1$ state to the state with $l = N$. The state with $L = L_{MDD}+2$ has two configurations, namely $l = N-1 \rightarrow l = N+1$ or $l = N-2 \rightarrow l = N$.

If one now includes the Coulomb interaction, the energy of the N-electron configuration is not the same for all the configurations with the same L value. The interaction energy is smaller for the configurations that have less center-of-mass motion and more relative motion, because the relative motion keeps the electrons further away from each other. For this reason, one should restrict the center-of-mass motion to the lowest energy eigenstate. In practice, this requirement is most easily fulfilled by the following coordinate replacement:[10]

$$x + iy \rightarrow \hat{x} + i\hat{y} \equiv (x - x_{\text{cm}}) + i(y - y_{\text{cm}}), \tag{3}$$

where x_{cm} and y_{cm} are the coordinates of the center of mass. This replacement should be done only in the phase part of the single-particle states. The transformation can be understood by noting that the excitations of the center-of-mass motion involves the coordinate z_{cm} in the phase part of the wave function, and the rule of Eq. (3) removes these as

$$x_{\text{cm}} + iy_{\text{cm}} \rightarrow (x_{\text{cm}} - x_{\text{cm}}) + i(y_{\text{cm}} - y_{\text{cm}}) \equiv 0. \tag{4}$$

If this transformation is applied to a state without center-of-mass motion, the wave function does not change. This can easily be seen in the case of MDD, as

$$z_{ij} \rightarrow (z_i - z_{\text{cm}}) - (z_j - z_{\text{cm}}) = z_{ij}. \tag{5}$$

The exact LLL wave function for a certain value of L can be presented as a linear combination of all the possible configurations that have the correct angular momentum. The coefficients can be found, e.g., by the exact diagonalization method. The problem with this approach is that the number of configurations in the expansion increases rapidly as a function of the angular momentum. For this reason, the exact diagonalization method is limited both by the angular momentum and the number of electrons. This further motivates the search for approximative wave functions that could be used to study larger QD's also.

We have previously shown[15] that up to 98% of the Landau-level mixing can be captured in a three-electron QD by multiplying the LLL multiconfigurational many-body wave function by two-body correlation factors for each pair:

$$\prod_{i<j}^{N} J(r_{ij}), \tag{6}$$

where J is a correlation factor of the Jastrow form $J(r_{ij}) = \exp[ar_{ij}/(1+br_{ij})]$, with a and b as variational parameters. One should note that the function J contains only relative coordinates. This is satisfactory because of the separation of the Hamiltonian discussed above and because the Coulomb interaction changes only the H_{rel} part of the Hamiltonian. If the Landau-level mixing is properly captured by the Jastrow factors, the task remaining is to find an approximative LLL many-body wave function.

We start constructing the LLL approximative variational wave function from the single-particle states given in Eq. (1). A set of angular momentum values $\{l_i\}_{i=1}^{N}$ is selected, and a Slater determinant is constructed from these. The center-of-mass motion is restricted to the lowest energy state by using Eq. (3). This results, combined with the correlation factors J discussed above, a variational wave function given by

$$\Psi = \det[\{\psi_l\}] \times \prod_{i<j}^{N} J(r_{ij}), \tag{7}$$

which can be labeled by the set $\{l_i\}_{i=1}^{N}$. For a certain angular momentum value $L > L_{MDD}+2$, there are several different possibilities for the set $\{l_i\}$. As one moves to higher magnetic field, L increases and there are more and more unoccupied values of l in the set $\{l_i\}$. We have found that it is energetically favorable to have only one region of unoccupied values of l. In this way, the number of possible configurations is reduced. We have used the quantum Monte Carlo (QMC) method for finding the optimal parameters[16] and evaluating the energy.

The limitation of the wave function presented above is that as the magnetic field is made stronger, the difference in energy between different ''starting configurations'' discussed above is reduced. Due to this, the wave function should be presented as a sum over several configurations. For this reason, the wave function is less accurate for larger angular momentum values and for more accurate treatment one should expand the wave function as a sum over several configurations.

III. RESULTS

The best test for the variational wave function given above is to compare the results obtained with it with the ones from the exact numerical diagonalization. Due to the limitations of the exact diagonalization technique, the diagonalization can only be done in the LLL for the electron numbers studied in this work. For this reason, the direct comparison of the energies is not totally meaningful. A better test for the presented variational wave function is to compare the angular momentum values for the possible lowest energy states L^*. This comparison can be done also with the CF theory, without calculation of the CF wave function or its energy, as the possible L^* values are given by the simple mean-field rule.[7–9]

In Fig. 1, we compare the result obtained using this wave function with exact diagonalization for the seven-electron QD. The parameter values used are $m^*/m_0 = 0.067$, $\epsilon = 12.4$, and $B = 5$ T. The confinement and the Zeeman term are omitted. One can see that the QMC energy is lower for up to $L = 51$. After that the error in the LLL part of the QMC energy is larger than the gain in the energy obtained by including Landau-level mixing. The lines in the figure connect

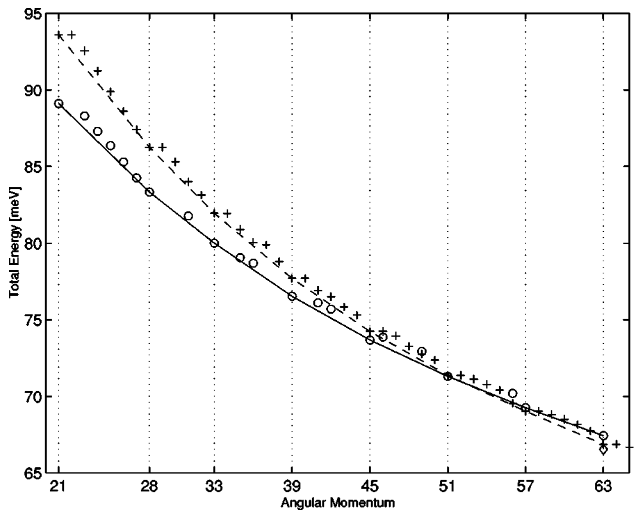

FIG. 1. Total energy as a function of the angular momentum for seven electrons. The numerical diagonalization energies are marked with ''+'' and the QMC energies are marked with ''○.'' The parameter values are $m^*/m_0=0.067$, $\epsilon=13.0$, $\hbar\omega_0=0$, and $B=5$ T. The vertical lines are drawn for the possible lowest energy L values L^*. The ''◇'' for $L=63$ is the energy of the Laughlin $\nu=1/3$ state with Jastrow correlation factor. The predicted L^* values are the same for diagonalization and QMC. For the states with more than one hole in the wave function, only the L^* and the neighboring states (with holes moved by one step towards center or edge) are plotted for clarity.

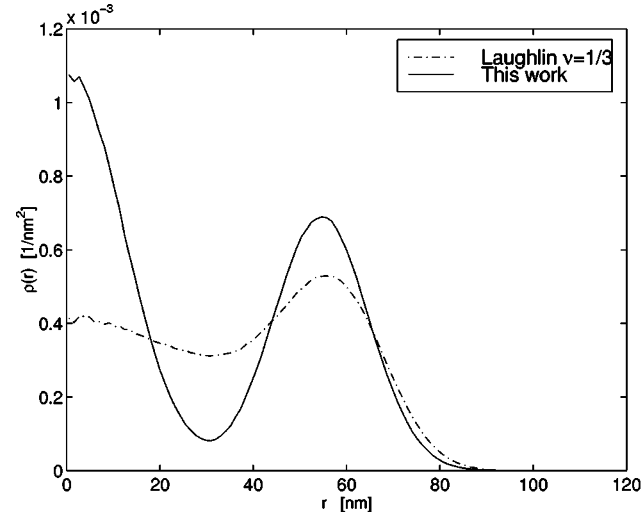

FIG. 2. The radial density $\rho(r)$ for the Laughlin $\nu=1/3$ state and for the variational wave function presented in this work. Normalization is such that $2\pi\int\rho(r)r\,dr=N$. The small r limit has the worst statistics, and the densities there are less accurate than in the large r limit.

the possible lowest energy states.[17] The important thing is that the predicted L^* values for the possible lowest energy states are exactly the same for the diagonalization and for the proposed variational wave function. One should note that $L=56$ is *not* a possible lowest energy state as claimed in Ref. 8 and falsely predicted by the CF mean-field rule.

In the QMC wave function, the state with $L^*=28$ has one hole in the center of the dot ($l=0$ unoccupied). The rest of the states have $l=0$ occupied and from 2 ($L^*=33$) to 7 ($L^*=63$) unoccupied states after that. One should also notice that the Laughlin $\nu=1/3$ state[18] combined with a Jastrow factor used above gives clearly the lowest energy. In Fig. 2 we have plotted the radial density $\rho(r)$ for the Laughlin $\nu=1/3$ state and for the variational wave function presented in this work. One can see that the density of the Laughlin's wave function is more smeared over the whole dot compared with the present wave function, which has a smaller density from $\sim$20 nm to $\sim$40 nm from the center of the dot. This can be seen as a consequence of having one starting configuration, unoccupied orbitals corresponding to this region. On the other hand, for the smaller angular momentum values, the number of unoccupied states is smaller and the error in ρ should also be smaller. In Ref. 14 the pair correlation functions for the $N=6$ case are plotted. The one for the $\nu=1/3$ state ($L^*=45$) differs significantly from the ones of smaller angular momentum values, especially from the $L^*=35$ state that has a clearer peak in the center of the dot.

In Fig. 3 similar results as in Fig. 1 are presented, but for ten electrons. Same parameters have been used as in the $N=7$ case. The diagonalizations are now limited to a smaller range of L. Again, one can see that the L^* values predicted are exactly the same. The mean-field rule of the CF theory is not able to predict the $L^*=61$ value.[8] The state with $L=73$ is not a possible lowest energy state as claimed in Ref. 8 and predicted by the CF mean-field rule. The first L^* state corresponding to $L^*=55$ has again a hole in the center. The state $L^*=61$ has $l=2$ and $l=3$ empty and $L^*=63$ has $l=1$ and $l=2$ empty, and both the states have thus two holes. The rest of the L^* states have $l=0$ and $l=1$ occupied and from 3 to 5 unoccupied states after that.

We have previously shown[4] that the transition points observed in the experiments of Ref. 5 for $N=6$, $\nu>1$ are very well predicted by the QMC simulations. It is interesting to compare the QMC prediction of the transition point from the MDD to the post-MDD region with the experimental findings. In the QMC simulations, we have used the same parameters as in Ref. 4. Using these, the transition occurs at $B\approx10.7$ T whereas the experimental value is rather close to 10.0 T. It is important to note that the assumption of constant, parabolic confinement is *not* valid in this experimental

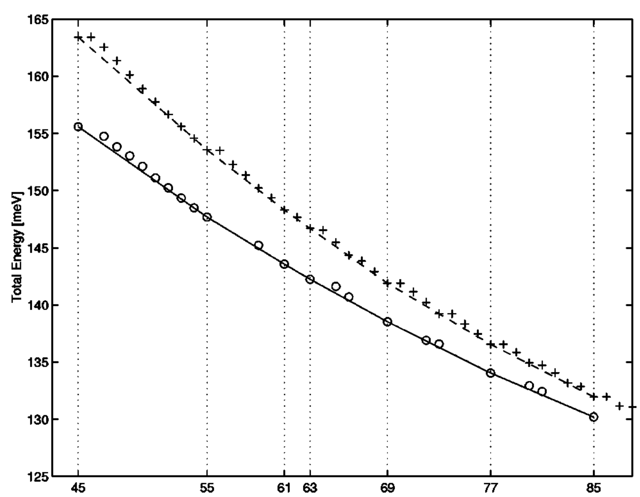

FIG. 3. Same as Fig. 1, but for ten electrons.

setup at B and is stronger than ~ 7 T (Ref. 19) and if the parabolic confinement is assumed, the strength of it $\hbar\omega_0$ should be smaller. We have found that having $\hbar\omega_0 = 4.25$ meV instead of $\hbar\omega_0 = 4.5$ meV predicts the transition at the correct B value.

IV. CONCLUSION

In summary, a simple variational many-body wave function for post-MDD states of a parabolic quantum dot is constructed. The proposed wave function correctly predicts the possible lowest energy angular momentum values, even in the cases where the mean-field rule of the CF theory fails. On the other hand, the very good agreement of the CF energies presented in Ref. 9 for the set of L values suggest that the few failures of the CF theory might not be used to judge the CF wave function itself, but that the mean-field rule used to obtain L^* values in the CF theory might be questionable. In addition, reasonable agreement with the experimental findings for the stability of the MDD is found in the $N = 6$ case.

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[19] See Ref. 2 for more details. It also gives a possible explanation in the Note 11: ''We believe that the smaller slopes in the experimental data of Fig. 5 for $B > \sim 7$ T are due to a changing confinement potential because screening from the leads is modified by the formation of Landau levels in the leads. This is also reflected in the changing stripe width at high B.''