Correlation effects in a quantum dot at high magnetic fields

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Abstract

We investigate the effects of electron correlations on the ground state energy and the chemical potential of a droplet confined by a parabolic potential at high magnetic fields. We demonstrate the importance of correlations in estimating the transition field at which the first edge reconstruction of the maximum density droplet occurs in the spin polarized regime.
The electronic structure of a quantum dot has been of great interest both theoretically and experimentally. The chemical potential $\mu_N$, the energy required to add one electron to a dot, of a droplet of $N$ electrons can be directly measured from the conductance peaks resulted from resonant tunneling of an electron through a quantum dot. The magnetic field induces spin and orbital angular momentum changes of the ground state, thus, the resulting $B - N$ phase diagram has been a subject of many theoretical studies. The rich dependence of $\mu_N$ on the applied magnetic field provides information on electron-electron interactions, especially, in the spin polarized regime, because any transition in this regime results from many-body phenomena which cannot be explained by a single electron picture. In recent experiments, Klein and his coworkers reported a divergent spin susceptibility, which was explained successfully by Hartree-Fock (HF) theory. However, the HF theory failed to predict the size of the magnetic field window in which the maximum density droplet (MDD) state is the ground state.

In this paper, we examine the correlation effects in a droplet containing a small number of electrons and calculate the ground state energy and the chemical potential via an exact treatment of electron-electron interactions which includes Landau level mixings. Our calculations show that the region of magnetic fields in which the ground state of the spin polarized droplet is the MDD state is much reduced, compared with the HF calculations, demonstrating the importance of correlations. With the Landau level mixing, we also find that magnetizations are reduced and susceptibility peaks are shifted to higher magnetic fields. We find bumps in the chemical potentials with varying the magnetic field, which gives rise to a ripple in the $\mu - B$ diagram which was observed by single electron capacitance spectroscopy.

For simplicity, we first consider the Hamiltonian ($H$) for a spin polarized droplet of $N$ electrons confined by a parabolic potential $\frac{1}{2}m^*\omega_0^2 r^2$. The generalization to an arbitrary spin case is straightforward. In the strong magnetic limit where all electrons are in the lowest Landau level, many-electron states in symmetric gauge with total angular momentum $L$ can be written as...
\[ \Psi_{L,N} = \prod_{i<j}(z_i - z_j)P_M(z_1, z_2, \ldots, z_N)e^{-\frac{1}{2l^2} \sum |z_k|^2}, \]  

where \( z_k = x_k - iy_k \) gives the coordinate of the \( k \)th electron and the effective magnetic length \( l \) is given by \( l^2 = \frac{\hbar}{2m^*\omega_0(B)} \), where \( \omega_0(B) = \sqrt{\omega_0^2 + \omega_c^2/4} \) and \( \omega_c \) is the cyclotron frequency. \( P_M(z_1, z_2, \ldots, z_N) \) is an \( M \)th order symmetric polynomial of \( N \) variables, where \( M = L - N(N-1)/2 \) is the excess angular momentum. For each angular momentum \( L \), the energy can be obtained by diagonalizing the Hamiltonian matrix for all possible \( N \)-particle basis functions \( \Psi_{L,N} \). Once the ground state \( | L, N \rangle \) is obtained, the contribution from the Coulomb interaction to the ground state energy can be expressed,

\[ \langle L, N | \sum_{i<j} e^2/\epsilon r_{ij} | L, N \rangle = \frac{e^2}{el} C(L, N), \]

where \( \epsilon \) is the dielectric constant and \( C(L, N) \) is a dimensionless quantity which only depends on \( L \) and \( N \).

To study the electronic structure of the droplet, previous theoretical attempts were mostly relied on Hartree-Fock theory \(^7\) or exact calculations which use a basis set in the Hilbert space restricted to the lowest one or two Landau levels. \(^3\), \(^5\) In our calculations, instead of extending the basis states to those belonging to higher Landau level indices, which are computationally too expensive, we employ a symmetric Jastrow correlation factor which will be multiplied to \( \Psi_{L,N} \) so that electron correlations are effectively included through the mixing of higher Landau levels. We test various kinds of the Jastrow factor using a variational Monte Carlo method and find that a simple form of \( \exp[-\sum_{i<j}u(r_{ij})] \), where \( u(r) = ar + br^2 \), gives the lowest energy as shown in Table I. Throughout this work, however, we set \( a = 0 \) to reduce computational demands and to perform computations in an analytical fashion.

With information on \( C(L, N) \) in Eq. (2), the ground state energy in the variational many-body state, \( \Phi_{L,N}(b) = e^{-b\sum_{i<j}r_{ij}^2} \Psi_{L,N} \), can be evaluated in an analytical fashion. First, let us decompose the Hamiltonian into two parts, \( H_\Omega \) and \( V_\Omega \), where

\[ H_\Omega = \sum_i \left[ \frac{\vec{p}_i^2 - \frac{\hat{A}_i^2}{m^*}}{2m^*} + \frac{1}{2} m^*\omega_0^2 r_i^2 \right] - \frac{1}{2} g^* \frac{m^*}{m_0} h\omega_c S_z - \sum_{i<j} \frac{1}{2} m^*\Omega^2 r_{ij}^2, \]
\[
V_\Omega = \sum_{i<j} \left( \frac{1}{2} m^* \Omega^2 r_{ij}^2 + \frac{e^2}{\epsilon |\vec{r}_i - \vec{r}_j|} \right),
\]

where the total spin angular momentum \( S_z \) is \( N/2 \) for a spin polarized droplet. If the parameter \( b \) in \( \Phi_{L,N}(b) \) is replaced by \( m^* \frac{\Omega_0 - \omega_0(B)}{2N} \), where \( \Omega_0 = \sqrt{\omega_0^2(B) - N\Omega_0^2} \), \( \Phi_{L,N}(\Omega) \) will be the eigenstates of \( H_\Omega \). Then, the eigenvalues of \( H_\Omega \) for the states of zero center-of-mass angular momentum (a general case will be discussed later) are

\[
H_\Omega \Phi_{L,N}(\Omega) = [E_\Omega(N) + L\hbar(\Omega_0 - \omega_c/2)] \Phi_{L,N}(\Omega),
\]

where

\[
E_\Omega(N) = \hbar\omega_0(B) + (N - 1)\hbar\Omega_0 - \frac{1}{2} g^* \frac{m^*}{m_0} \hbar \omega_c S_z.
\]

The expectation value of the first term (an \textit{ad hoc} harmonic potential) in Eq. (4) can be evaluated analytically by using the raising (\( a_{ij}^+ \) and \( b_{ij}^+ \)) and lowering (\( a_{ij}^- \) and \( b_{ij}^- \)) operators defined as

\[
a_{ij}^+ = \left[ \frac{1}{4 m^* \hbar \Omega_0} \right]^{\frac{1}{2}} \left[ m^* \Omega_0 z_{ij} - i(p_{ij,x} - i p_{ij,y}) \right],
\]

\[
b_{ij}^+ = \left[ \frac{1}{4 m^* \hbar \Omega_0} \right]^{\frac{1}{2}} \left[ m^* \Omega_0 z_{ij}^* - i(p_{ij,x} + i p_{ij,y}) \right],
\]

where \( a_{ij}^- (b_{ij}^-) \) is the hermitian conjugate of \( a_{ij}^+ (b_{ij}^+) \), \( \bar{p}_{ij} = \bar{p}_i - \bar{p}_j = (p_{ij,x}, p_{ij,y}) \), and \( z_{ij} = z_i - z_j \). Then, it follows that

\[
\frac{m^* \Omega_0}{\hbar} r_{ij}^2 = a_{ij}^+ a_{ij}^- + b_{ij}^+ b_{ij}^- + a_{ij}^+ b_{ij}^- + a_{ij}^- b_{ij}^+ + 2.
\]

Considering the states of zero center-of-mass angular momentum, the polynomial \( P_M \) in Eq. (4) can be expressed only in terms of relative coordinates, and the variational many-body state is rewritten with the use of \( z_{ij} = (\frac{\hbar}{m^* \Omega_0})^{1/2} (a_{ij}^+ + b_{ij}^-) \),

\[
\Phi_{L,N}(\Omega) = \prod_{i<j} z_{ij} P_M \left( \sum_{i \neq 1} z_{1i}, \sum_{i \neq 2} z_{2i}, \ldots, \sum_{i \neq N} z_{Ni} \right) \Psi_v
\]

\[
= \left( \frac{\hbar}{m^* \Omega_0} \right)^{L/2} \prod_{i<j} a_{ij}^+ P_M \left( \sum_{i \neq 1} a_{1i}^+, \sum_{i \neq 2} a_{2i}^+, \ldots, \sum_{i \neq N} a_{Ni}^+ \right) \Psi_v.
\]
where $\Psi_v$ denotes the vacuum state, i.e., $a_{ij}^{-}\Psi_v = b_{ij}^{-}\Psi_v = 0$, and is given by

$$\Psi_v = \exp\left[-\frac{N^*m_r\omega_0(B)}{2\hbar}\tilde{R}^2 - \frac{m_r\Omega_0}{2N\hbar} \sum_{i<j} r_{ij}^2\right]$$

where $\tilde{R}$ is the center-of-mass coordinate. Using the commutation relations of $a_{ij}^\pm$ and $b_{ij}^\pm$, the expectation value of the ad hoc harmonic potential is

$$\langle \Phi_{L,N}(\Omega) \bigg| \frac{1}{2} m^*\Omega^2 \sum_{i<j} r_{ij}^2 \bigg| \Phi_{L,N}(\Omega) \rangle = \frac{\hbar\Omega^2}{2\Omega_0} \langle \Phi_{L,N}(\Omega) \bigg| \sum_{i<j} (a_{ij}^+a_{ij}^- + 2) \bigg| \Phi_{L,N}(\Omega) \rangle = \frac{\hbar\Omega^2}{2\Omega_0} [NL + N(N-1)].$$

For the Coulomb interaction energy in the variational state $\Phi_{L,N}(\Omega)$, replacing $l$ by $\Gamma_\Omega(=\sqrt{\frac{\hbar}{2m^*\Omega_0}})$ in Eq. (2) leads to the expectation value,

$$\langle \Phi_{L,N}(\Omega) \bigg| \sum_{i<j} e^2 \epsilon_{r_{ij}} \bigg| \Phi_{L,N}(\Omega) \rangle = \frac{e^2}{\epsilon\Gamma_\Omega} C(L, N).$$

From Eqs. (3), (12), and (13), we finally get the total energy $E_{L,N}$ for total angular momentum $L$ and zero center-of-mass angular momentum by minimizing $\langle \Phi_{L,N}(\Omega) \big| H \big| \Phi_{L,N}(\Omega) \rangle$ over the variable $\Omega$;

$$E_{L,N} = \text{min}_\Omega \{ E_\Omega(N) + L\hbar(\Omega_0 - \omega_c/2) + \frac{\hbar\Omega^2}{2\Omega_0} [NL + N(N-1)] + \frac{e^2}{\epsilon\Gamma_\Omega} C(L, N) \}. \quad (14)$$

In general, the total angular momentum is given by $L = M_r + M_c$, where $M_r$ and $M_c$ represent the angular momentums of the relative and center-of-mass motions, respectively. If $M_c \neq 0$, the total energy should include an additional energy, $M_c\hbar[\omega_0(B) - \omega_c/2]$, with $L$ replaced by $M_r$ in Eq. (14). However, one can see that the states with $M_c \neq 0$ give higher energies for given $N$ and $B$. Thus, the ground state energy of the $N$-electron droplet at magnetic field $B$ is a minimum value of $E_{L,N}$ calculated for $L \geq \frac{N(N-1)}{2}$ and $M_c = 0$.

For a droplet with arbitrary spin states, we can generalize the total energy $E_{L,N}$ to $E_{L,S_z,N}$ by replacing $C(L, N)$ with $C(L, S_z, N)$, which is defined analogously to Eq. (2). In this case, instead of $\Psi_{L,N}$ in Eq. (1), we use $\Psi_{L,S_z,N}$ defined as,

$$\Psi_{L,S_z,N} = e^{-\frac{\hbar^2}{2\hbar^2} \sum_k |z_k|^2} \sum_n Q_L^{(n)}(z_1, z_2, \ldots, z_N) \chi_n, \quad (15)$$
where $Q_L^{(n)}$ is an $L$th order polynomial of $N$ variables, $\chi_n$ is a $N$-product of single particle spinors, and $n$ denotes possible spinor configurations. Although $\Psi_{L,S_z,N}$ is totally antisymmetric, each of $Q_L^{(n)}$ and $\chi_n$ does not necessarily satisfy the antisymmetric property.

The ground state energies in the variational many-body state $\Phi_{L,S_z,N}$ for a six-electron quantum dot are plotted as a function of magnetic field in Fig. 1. Throughout this work, we use the confinement strength of $\hbar \omega_0 = 2.5$ meV and the usual values for $\epsilon$ and $m^*$ in GaAs. Compared with the results of conventional exact calculations using $\Psi_{L,S_z,N}$ in Eq. (15), our calculated energies are generally lower with significant reductions at lower magnetic fields. This is because the Jastrow factor introduces more effectively the Landau level mixing and the correlation effect in the region of low magnetic fields, which are absent in the conventional scheme. From Fig. 1, one can notice that with the Jastrow factor magnetizations ($-dE/dB$) are relatively decreased whereas susceptibility peaks are shifted to higher magnetic fields. We also note that the variational ground states exhibit different orbital and spin angular momentum quantum numbers, compared with the conventional exact calculations.

At low magnetic fields, $0 < B < B_c = 1.1$ T, the quantum dot is found to favor the equal occupations of the up- and down-spin states, i.e., $L = 6$ and $S_z = 0$, while the minimum total spin state only appears in a very narrow range near zero field in the conventional calculations without the Jastrow factor. At $B_c$, the transfer of electrons between the up- and down-spin states begins and continues due to the Zeeman splitting energy up to the value of $B_I = 1.25$ T, where a spin polarized state appears. With varying the magnetic field, the bumps in the chemical potentials ($\mu_N = E_N - E_{N-1}$), which are associated with the ground state transitions, are clearly seen in Fig. 2 exhibiting a ripple in the $\mu_N - B$ diagram. In fact, such a feature in the $\mu_N - B$ graph was observed in single electron capacitance spectroscopy measurements.

Our calculations show a spin polarized droplet ($S_z = N/2$) above $B_I$, and a magnetic field window in which the ground state of the spin polarized droplet is the maximum density droplet [$L = N(N-1)/2$] where electrons occupy one-electron eigenstates of angular
momentum indices, \( m = 0, 1, \ldots, \) and \((N - 1)\). As the magnetic field increases, since the Coulomb interaction energy grows due to the reduction of the radius of the MDD, the MDD must undergo a transition to a higher angular momentum state \((L = 20 \text{ and } S_z = 2)\) to lower the ground state energy. In the \( N = 6 \) droplet, the edge of the MDD is reconstructed at \( B_r = 3.7 \) T, and at this field an abrupt upward shift of the chemical potential appears, as shown in Fig. 2. Such a step at \( B_r \) is the reminiscent of the chemical potential jump in the fractional quantum Hall effect, which is caused by quasi-hole creation. Indeed, experimentally, an upward step in \( \mu_N \) at \( B_r \) was observed for a droplet in the spin polarized regime.

Recently, Klein and his coworkers observed many transition fields in a droplet of \( N \sim 30 \) electrons, and showed that the HF theory describes successfully their experimental data with a fitting parameter \( \hbar \omega_0 \) for \( B \leq B_I \). However, the transition field \( B_r \) was overestimated severely. Because of the computational difficulties for higher values of \( N \), our calculations are restricted to droplets of \( N \leq 7 \). Nevertheless, we are able to see the effect of electron correlations on the transition fields. By varying the confinement strength from 1 to 5 meV for the \( N = 7 \) droplet, we plot the size of the magnetic field window, \((B_r - B_I)\), in which the MDD is the ground state of the spin polarized droplet, as a function of \( B_I \) in Fig. 3. With the Jastrow correlation factor, we find that the size of \((B_r - B_I)\) is significantly reduced by about 1 T, compared with the HF calculations, while in the conventional exact calculations with only the lowest Landau level the reduction is about 0.5 T. Thus, it is important to include the correlation effect in predicting the transition fields for the MDD state.

In conclusion, we have made a detailed study of the correlation effect on the ground state, the chemical potential, and the transition fields in strong magnetic fields. Using an exact treatment of electron-electron interactions through the Landau level mixing, we find that magnetizations are reduced while the transition fields are shifted to higher magnetic fields by the correlation effect. We present a ripple in the \( \mu_N - B \) diagram, which has not been explained by previous calculations. In estimating the size of the magnetic field window in which the MDD appears, we attribute the failure of the HF theory to the neglect of electron
correlations.

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FIGURES

FIG. 1. The ground state energies vs magnetic field for a six-electron quantum dot with the confinement strength of $\hbar \omega_0 = 2.5$ meV. The arrows indicate the transition fields at which the ground state crossings occur. Some chosen ground states are labeled by the quantum numbers $(L, 2S_z)$.

FIG. 2. (a) The chemical potential $\mu_N$ vs magnetic field for $\hbar \omega_0 = 2.5$ meV. (b) The details of $\mu_N$ for $N = 7$. Curve segments between two downward arrows are labeled by the ground state quantum numbers $(L, 2S_z)$ of the $N = 7$ droplet, while those between two upward arrows correspond to the ground states of the $N = 6$ droplet.

FIG. 3. For the spin polarized droplet of $N = 7$ electrons, $(B_r - B_I)$ is plotted as a function of $B_I$ which is determined by varying the confinement strength from 1 to 5 meV. The present results with the Jastrow correlation factor are compared with the Hartree-Fock and conventional exact calculations without the Jastrow factor.
TABLE I. The variational ground state energies calculated by a Monte Carlo method are compared for various forms of the Jastrow factor, \( \exp[-\sum_{i<j} u(r_{ij})] \). We use \( N = 3, B = 3 \) T, and \( \hbar \omega_0 = 5.4 \) meV.

| \( u(r) \)          | Ground state energy (meV) |
|----------------------|--------------------------|
| \( br^2 \)           | 41.041                   |
| \( ar + br^2 \)      | 40.866 ± 0.005           |
| \( a \log(r) \)      | 41.248 ± 0.010           |
| \( br/(1 + ar) \)    | 41.230 ± 0.010           |
| \( \frac{a}{\sqrt{r}}[1 - \exp(-\sqrt{r/b} - r/2b)] \) | 41.194 ± 0.005          |
| \( a[1 - \exp(-br)]/r \) | 41.750 ± 0.100          |
