Ground-State Phase Diagram of 2D Electrons in a High Landau Level: A Density-Matrix Renormalization Group Study

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The ground-state phase diagram of 2D electrons in a high Landau level (index $N = 2$) is studied by the density-matrix renormalization group method. Pair correlation functions are systematically calculated for various filling factors from $\nu = 1/8$ to $1/2$. It is shown that the ground-state phase diagram consists of three different charge density wave states called stripe phase, bubble phase, and Wigner crystal. The boundary between the stripe and the bubble phases is determined to be $\nu_c^{\text{s-b}} \sim 0.38$, and that for the bubble phase and Wigner crystal is $\nu_c^{\text{b-W}} \sim 0.24$. Each transition is of first order.

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The electrons in two-dimensional systems are confined to the lowest Landau level under a high perpendicular magnetic field. In this limit, Laughlin proposed the ground state many body wave function at filling factors $\nu = 1/q$ (q is an odd integer) written by the Jastrow-type wave functions [1], which are exact zero-energy eigenstates of short-ranged repulsive interactions. This Laughlin state is an incompressible liquid with an excitation gap, and the experimental results of fractional quantization are explained.

In weak magnetic fields electrons occupy higher Landau levels. Since the filled Landau levels are inert, it will be a good approximation to consider only the partially occupied Landau level. Then naively we may think that the electrons in the partially filled level behave similarly to those in the partially filled lowest Landau level. However, this is not correct. The wave function in the higher Landau levels extends over a space with oscillations, and the interaction between them is more long ranged. Therefore, the Laughlin state, which is the ground state for short-range interaction, ceases to be the good candidate for the ground state in the higher Landau levels, and the fractional quantum Hall state becomes unstable.

For high Landau levels with its index $N > 1$, Koulakov *et al.* proposed that the electrons form charge density waves (CDW's) called stripes and bubbles [2–4]. The evidence of the CDW's has been experimentally observed as anisotropic resistivity and reentrant integer quantum Hall state on ultrahigh mobility samples [5–7]. The formation of the CDW's was recently supported by the exact diagonalization studies, and the results of the exact diagonalizations are in good agreement with the Hartree-Fock (HF) theory [8,9].

In spite of such recent development of the theoretical studies, the detailed properties of the CDW's and the ground-state phase diagram for high Landau levels are still in question because Koulakov *et al.* used HF approximations, which neglect the effect of quantum fluctuations, and the exact diagonalization studies are restricted to some special filling and size of systems due to the limitation of available memory space. Reliable, detailed study is imperative to understand the nature of the reentrant phase and to understand the way the anisotropy disappears as the filling factor is changed away from half-filling.

In this paper we present the numerical results for large size systems obtained by the density-matrix renormalization group (DMRG) method [10] which is applied to the 2D electron systems in a high Landau level of $N = 2$. The calculated pair correlation functions show that the ground state phase diagram consists of three CDW states, the stripe phase, bubble phase with only two-electron bubbles, and Wigner crystal. The obtained phase diagram is similar to that of the HF calculations except that there are no bubbles with more than two electrons per bubble [11]. The boundary between the stripe phase and the bubble phase is shown to be $\nu_c^{\text{s-b}} \sim 0.38$, and that for the bubble phase and Wigner crystal is $\nu_c^{\text{b-W}} \sim 0.24$. It is also clarified that each transition is of first order.

To deal with large size systems, we use the DMRG algorithm [10], which was originally developed for 1D quantum systems. In this method we can calculate the ground-state wave function and the energy with high accuracy. The outline of the algorithm is summarized as follows: We start from small finite systems, i.e., four-site system, and divide the system into two blocks. Then add new sites at the end of two blocks and expand the blocks with restricting the number of basis states. The restriction of the basis states is carried out by keeping only eigenstates of large eigenvalues of the density matrix which is calculated from the ground-state wave function. Thus the numerical error due to the truncation of basis states is estimated from the eigenvalues of the density matrix which are truncated off, and the accuracy of the wave function is systematically improved by increasing the number of states kept in the blocks. We repeat the expansion of the blocks, and finally get the desired size of the system within a controlled accuracy.

Since the above algorithm is designed for 1D systems, we have to find appropriate mapping to a 1D model. In this study we use the eigenstate of free electrons as the local basis, and represent the wave function in the Landau gauge.

Since each wave function in the Landau gauge is uniquely identified by the x component of the center coordinates $X_j = 2\pi\ell^2 j/L_y$ (j : integer), we can map the present 2D system onto a 1D lattice model.

The important difference between the present model and the usual 1D quantum systems is that the present model has additional conserved quantity, the center of mass of electrons, $\sum_{i=1}^{N_e} X_i$. This is due to the conservation of y-momentum $\sum_{i=1}^{N_e} p_i^y$ in the original two-dimensional system, where p_i^y is related with X_i as $p_i^y = X_i/\ell^2$ under the Landau gauge. This conservation law causes some technical problems in the infinite system algorithm of the DMRG. To avoid this problem we have to keep additional basis states which are not included in the density matrix of the ground state. However, after we switch to the finite system algorithm, we need not care about such problems.

The Hamiltonian for electrons in Landau levels contains only the Coulomb interactions. After the projection onto the Nth Landau level, the Coulomb interaction is written as

$$H = \sum_{i<j} \sum_{\mathbf{q}} e^{-q^2/2} [L_N(q^2/2)]^2 V(q) e^{i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)}, \quad (1)$$

where $\mathbf{R}_i$ is the guiding center coordinate of the ith electron, which satisfies the commutation relation, $[R_j^x, R_k^y] = i\ell^2\delta_{jk}$, $L_N(x)$ are the Laguerre polynomials, and $V(q) = 2\pi e^2/q$ is the Fourier transform of the Coulomb interaction. The magnetic length ℓ is set to be 1. We consider the uniform positive background charge to cancel the component at $q = 0$ in Eq. (1), and neglect the electrons in fully occupied lower Landau levels. In the following we calculate the ground-state wave function of the Hamiltonian for the high Landau level of $N = 2$ using both the infinite system and finite system algorithms of the DMRG. We study various sizes of systems with up to 18 electrons in the unit cell of $L_x \times L_y$ with periodic boundary conditions in both x and y directions. The truncation error in the DMRG calculation is typically 10^{-5} for 18 electrons with 200 states in each blocks. The existing results of exact diagonalizations are completely reproduced within the truncation error. Since the present Hamiltonian has the particle-hole symmetry, we consider only the case of $\nu \leq 1/2$ [12].

In Fig. 1 we show the ground-state pair correlation functions $g(\mathbf{r})$ in guiding center coordinates,

$$g(\mathbf{r}) \equiv \frac{L_x L_y}{N_e(N_e - 1)} \left\langle \Psi \left| \sum_{i \neq j} \delta(\mathbf{r} + \mathbf{R}_i - \mathbf{R}_j) \right| \Psi \right\rangle, \quad (2)$$

where $|\Psi\rangle$ is the ground state and N_e is the number of the electrons in the unit cell. This is essentially the correlation function of the center of the cyclotron motion. We find clear discontinuity in the shape of the correlation function between $\nu = 2/5$ and $4/11$, and between $\nu = 1/4$ and $2/9$. Since we have set the x and y axes to give continuous change as much as possible, the discontinuity in Fig. 1 means drastic change in the pattern of the correlation function. Thus the transition is first order. As shown below, the pattern of the correlation function is characterized by stripes between $\nu = 1/2$ and $2/5$, bubbles between $\nu = 4/11$ and $1/4$, and Wigner crystal below $\nu = 2/9$. Hence, we obtain the phase diagram shown in Fig. 2(a). In the following we show the detailed structure of the correlation functions in each phase.

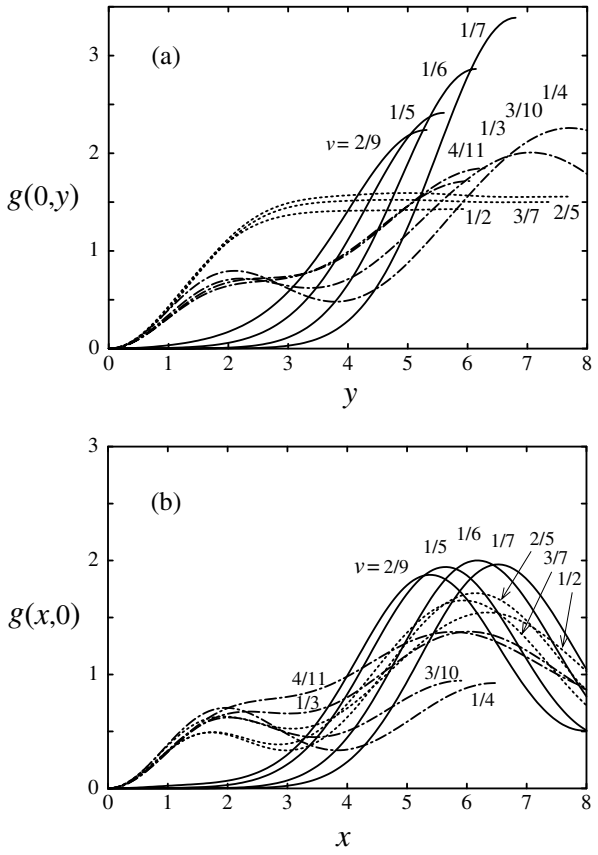

FIG. 1. Ground-state pair correlation functions in the guiding center coordinates for electrons in the high Landau level of $N = 2$. The magnetic length ℓ is set to be unity. The number of electrons in the unit cell is 18 for $\nu = 1/2$ and 8 for $\nu = 1/7$. The aspect ratio L_x/L_y is chosen to obtain maximum energy gain around $L_x/L_y = 1$.

We start from the stripe phase which appears around the half filling. In Fig. 3 we show the pair correlation functions at $\nu = 3/7$ in the guiding center coordinates. In this figure, we clearly observe the stripe structure. The similar stripe structure is obtained in the HF calculations, but we find no clear modulation that is predicted in the HF theory [13]. The clear stripe structure similar to the present result is obtained also for $\nu = 1/2, 6/13, 5/11, 4/9$, and $2/5$ with a different number of electrons and size of systems as expected from Fig. 1.

The detailed structure of the stripes such as the mean separation depends on the aspect ratio L_x/L_y. To determine the optimal stripe structure, we next compare the ground-state energy. In Fig. 3(d) we show the ground-state

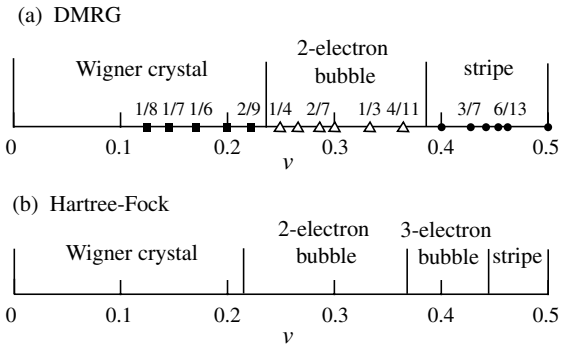

FIG. 2. Ground-state phase diagram of 2D electrons in high Landau level of $N = 2$ obtained by (a) the DMRG and (b) the Hartree-Fock theory [11].

energy for various aspect ratios. In this figure we find a minimum at $L_x/L_y = 1.3$. At this ratio the mean separation of the stripes is 6.2, which is close to the results 6.0 obtained by the HF theory. With increasing L_x/L_y, both the mean separation and the ground-state energy increases. At $L_x/L_y = 1.6$, the orientation and the number of the stripes in the unit cell are changed due to the level crossing of the ground state. Then both the mean separation and ground-state energy decrease. The energy takes the minimum again around $L_x/L_y = 1.9$, where the mean separation is 5.9. Further increasing L_x/L_y, level crossing occurs again and the number of stripes increases to four in the unit cell. Then the ground-state energy takes the minimum at $L_x/L_y = 2.3$, where the mean separation is 6.2. Thus the optimal structure where the energy takes the minimum does not depend so much on L_x/L_y. Since the interval between the minima that appears on the L_x/L_y axis becomes shorter with increasing the size of the unit cell, the optimal structure at the energy minimum will be realized in the bulk limit for any L_x/L_y.

Now we switch to the bubble phase. The correlation function in the guiding center coordinates at $\nu = 8/27$ for 16 electrons is shown in Fig. 4(a). The aspect ratio is chosen to be 1.9 where the minimum energy is obtained. In this figure we find 8 bubbles in the unit cell on the triangular lattice. Since the number of electrons is 16 in the unit cell, two electrons are clustering together in the guiding center coordinates. This pairing of the two electrons makes a ring structure in the correlation functions around the origin. As expected from Fig. 1, the same pattern of the two-electron bubbles is obtained also for $\nu = 4/11, 1/3, 4/13, 3/10, 2/7, 4/15,$ and $1/4$, and the lattice spacing increases with decreasing ν. The similar two-electron bubbles are obtained in the HF calculations. However, as shown in Fig. 2(b), the HF theory predicts also the three-electron bubbles, each of which contains three electrons. Since we cannot find three-electron bubbles in the present study, we think the energy gain due to the quantum fluctuations is relatively small for three-electron bubbles.

In the usual electron coordinates the pair correlation functions are almost circularly symmetric around the origin as shown in Figs. 5(a) and 6. This symmetric correlation contrasts to the anisotropic correlation in the stripe phase. In Fig. 6, we also plot the result at $\nu = 2/9$ where the ground state is the Wigner crystal. We find that the results

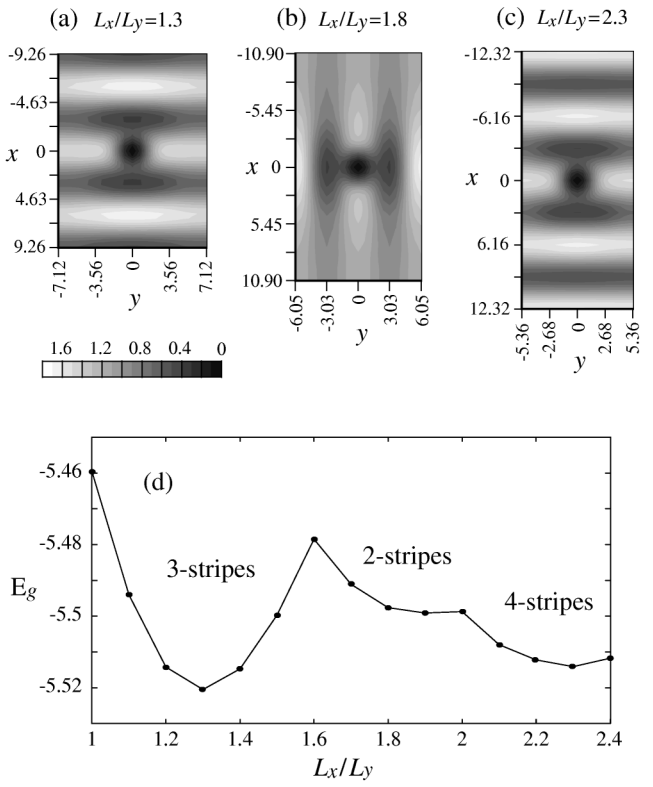

FIG. 3. Ground-state pair correlation functions in the guiding center coordinates and the energy at $\nu = 3/7$. The number of electrons is 18. (a) Pair correlation functions for $L_x/L_y = 1.3$, (b) $L_x/L_y = 1.8$, (c) $L_x/L_y = 2.3$. (d) The ground-state energy in units of $e^2/\epsilon\ell$.

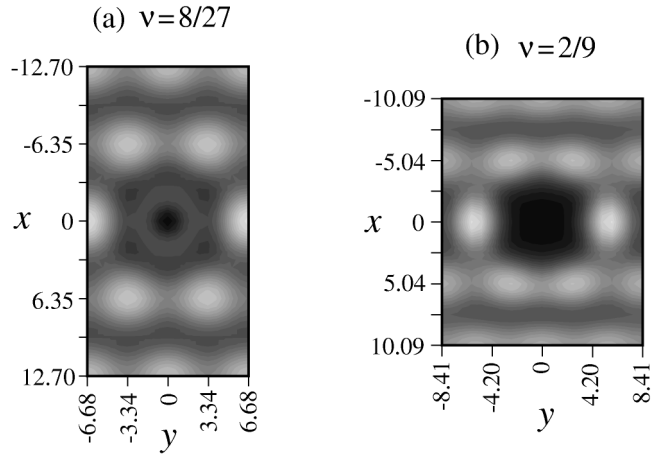

FIG. 4. Pair correlation functions in the guiding center coordinates at (a) $\nu = 8/27$ with 16 electrons, (b) $\nu = 2/9$ with 12 electrons.

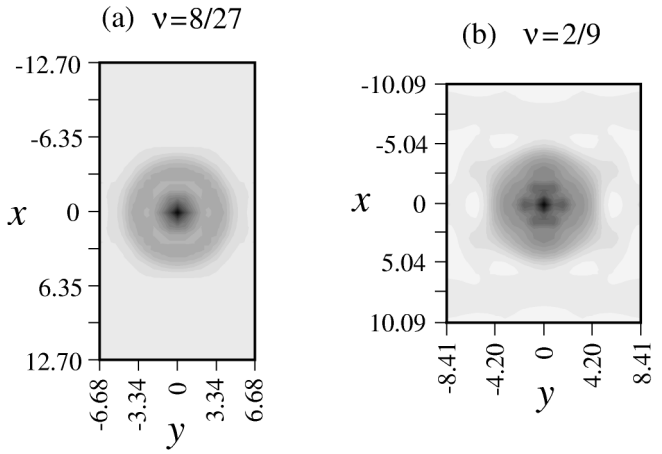

FIG. 5. Pair correlation functions in the electron coordinates. (a) $\nu = 8/27$, 16 electrons. (b) $\nu = 2/9$, 12 electrons.

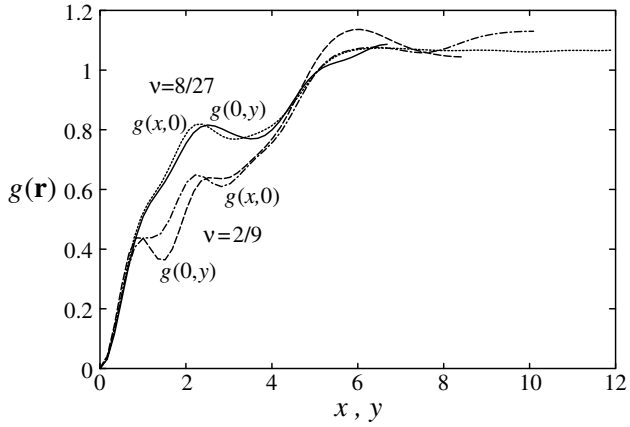

FIG. 6. Pair correlation functions in the electron coordinates for $\nu = 8/27$ with 16 electrons, and $\nu = 2/9$ with 12 electrons.

of $\nu = 8/27$ show the enhancement over the case of $\nu = 2/9$ around $r \sim 2.5$. This is caused by the clustering of the electrons in the bubble phase. Similar to the guiding center correlation, this enhancement makes a ring structure around the origin as shown in Fig. 5(a).

Finally, we consider the ground state at low density $\nu \lesssim 2/9$. In the limit of $\nu \to 0$ the electrons are separated from each other. When the distance to the other electrons exceeds the typical length of the single electron wave function, we expect the difference of the Landau levels becomes almost negligible. Thus we expect the formation of Wigner crystal as in the lowest Landau level. The result for $\nu = 2/9$ with 12 electrons shown in Fig. 4(b) actually shows that the center of the cyclotron motion forms a triangular lattice with 12 lattice points in the unit cell. This shows the tendency to form Wigner crystal. Thus we expect the ground state is the Wigner crystal for $\nu \lesssim 2/9$. Even in the electron coordinates shown in Figs. 5(b) and 6, the correlation function has peaks at the triangular lattice points and the hexagonal symmetry is clearly seen. We expect clear crystallization for smaller ν.

Thus we have obtained a reliable phase diagram for a system in the third lowest Landau level ($N = 2$) in the strong magnetic field. Since we have neglected the spread of the wave function in the third dimension, and screening effect by electrons in the lower Landau levels, the phase boundary may have a slightly different value in the actual system. The absence of the three-electron bubble phase is consistent with the experiment. This phase is predicted by the HF theory [11], and has not been denied by the exact diagonalization study [9]. From the phase diagram we can speculate that the reentrant phase is the two-electron bubble phase. The coexistence of the Wigner crystal and the bubbles at the phase boundary around $\nu = 1/4$ brings finite dissipation into the system separating the two integer quantum Hall states. This idea would be jeopardized if the three-electron bubble were realized, since then there would be another reentrant phase.

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[12] The filling factor in this paper is that of the relevant Landau level.
[13] The lack of the modulation is related to the fact that the transition to the bubble phase is of first order.