

Charge-Density-Wave Ordering in Half-Filled High Landau Levels

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We report on numerical studies of two-dimensional electron systems in the presence of a perpendicular magnetic field, with a high Landau level (index $N \geq 2$) half filled by electrons. Strong and sharp peaks are found in the wave-vector dependence of both the static density susceptibility and the equal-time density-density correlation function, in finite-size systems with up to twelve electrons. Qualitatively different from the partially filled lowest ($N = 0$) Landau level, these results are suggestive of a tendency toward charge-density-wave ordering in these systems. The ordering wave vector is found to decrease with increasing N .

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Two-dimensional (2D) electron gas systems subject to a perpendicular magnetic field display remarkable phenomena, reflecting the importance of electronic correlations. The most important among them is the fractional quantum Hall effect (FQHE), which was found in the strong field limit, where the electrons are confined to the lowest ($N = 0$) or the second ($N = 1$) Landau levels. The physics of FQHE is reasonably well understood [1]: the kinetic energy of the electrons is quenched by the strong perpendicular magnetic field and the Coulomb interaction dominates the physics of the partially filled Landau level; at certain Landau level filling factors (ν , defined to be the ratio of the number of electrons to the number of Landau orbitals in each Landau level) the electrons condense into a highly correlated, incompressible quantum fluid, giving rise to quantized Hall resistivity (ρ_{xy}) and thermally activated longitudinal resistivity (ρ_{xx}).

Experimentally, the FQHE has never been found at filling factors $\nu > 4$, when the partially filled Landau level has Landau level index $N \geq 2$ (taking into account the two spin species of the electrons). Nevertheless, recent experiments [2,3] on high quality samples have revealed remarkable transport anomalies for $\nu > 4$, especially when ν is near a half integer, which means the partially filled Landau level is nearly half filled. Such anomalies include a strong anisotropy and nonlinearity in ρ_{xx} . They reflect intriguing correlation physics at work in these systems that is qualitatively different from the FQHE and yet to be completely understood.

It was argued [4], before the discovery of the FQHE, that the ground state of a 2D electron gas in a strong magnetic field may possess charge density wave (CDW) order. Recent Hartree-Fock (HF) calculations [5–7] find that single-Slater determinant states with CDW order have energies lower than the Laughlin-type liquid states for $N \geq 2$. The CDW state with 1D stripe order, or stripe phase [5–7], which is predicted to be stable near half filling for the partially filled Landau level, can in principle give rise to transport anisotropy as the orientation of the

stripe picks out a special direction in space. Questions remain, however, with regard to the stability of the HF states against quantum fluctuations as well as disorder, especially when N is not too large.

In this paper we report on results of numerical studies of partially filled Landau levels with $N \geq 2$, in finite size systems with up to $N_e = 12$ electrons and torus geometry. The torus is ideal for this study, because, while it maintains translational and rotational invariance in the plane for the infinite system, it does break them for finite sizes and therefore produces a preferred direction that allows for the CDW state to be aligned in one direction. The spherical geometry (which is another popular geometry for finite size studies), on the other hand, will rotationally average the state and necessarily introduce defects. We assume the magnetic field is sufficiently strong so that the filled Landau levels are completely inert and mixing between different Landau levels can be neglected. We calculate numerically the energy spectra, the wave vector dependence of the static density susceptibility [$\chi(q)$], and the density-density correlation in the ground state [$S_0(q)$]. We find strong and sharp peaks in both $\chi(q)$ and $S_0(q)$. These results are strongly suggestive of a tendency toward charge density wave ordering in the ground state. In accordance with this, we find nearly degenerate low-energy states that are separated by the ordering wave vector.

The methods used in the present study are identical to those used in numerical studies of the partially filled lowest Landau level [8]. Since the kinetic energy is quenched by the magnetic field, the Hamiltonian contains the Coulomb interaction alone, which, after projecting onto the N th Landau level [8], takes the form

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

where \mathbf{R}_i is the guiding center [8] coordinate of the i th electron, $L_N(x)$ 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 for convenience. In this work we impose periodic boundary conditions in both x and y directions in the finite-size system under study, and the \mathbf{q} 's are wave vectors that are compatible with the size and geometry of the system. We diagonalize the above Hamiltonian exactly and calculate various correlation functions.

In Fig. 1 we present the energy spectrum of a half-filled $N = 2$ Landau level with ten electrons, rectangular geometry, and aspect ratio 0.75. The spectrum is qualitatively different from the known incompressible FQHE states in the following aspects: (i) the ground state is not separated from the excited states by a gap; instead, there are several nearly degenerate low-energy states, separated by a characteristic wave vector \mathbf{q}^* (the physical importance of \mathbf{q}^* will be discussed later). This almost exact degeneracy is not specific to this particular geometry; in Fig. 2 we have plotted the energy levels (for all momenta) versus aspect ratio a , in which it is clear that the near degeneracy is present for $0.7 < a < 1.0$. A gap in the spectrum, on the other hand, is the most important property of a FQHE state that gives rise to incompressibility. (ii) The momentum of the ground state is, in general, not related to any reciprocal lattice vectors and is sensitive to the geometry of the system; such sensitivity to boundary conditions is characteristic of compressible states. The known FQHE states, however, all have ground state momentum equal to one half of a reciprocal lattice vector and are independent of system geometry, reflecting intrinsic topological properties of the state. The spectra and quantum numbers of these ground states are also very different from the Fermi-liquid-like compressible state at half filling in the lowest Landau level [9]. In that case clusterlike ansatz variational wave functions [10,11] have remarkably

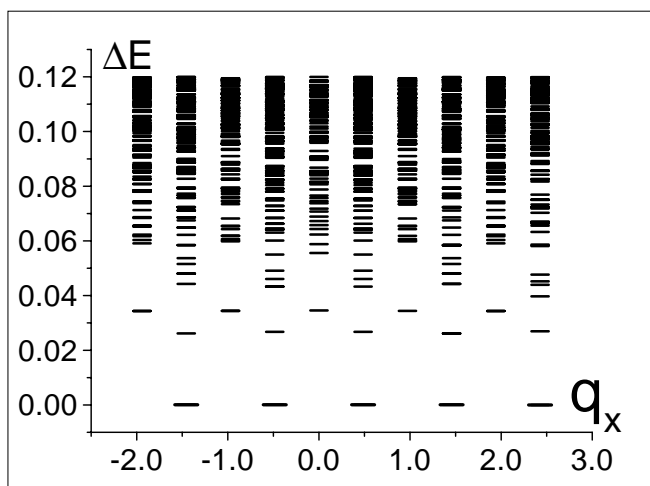


FIG. 1. Energy (in unit of $e^2/\epsilon\ell$) versus the x component of the momentum for the half-filled $N = 2$ Landau level with ten electrons, rectangular geometry, and aspect ratio 0.75. The momenta of the five nearly degenerate low-energy states are $(\pm 0.485, 0)$, $(\pm 1.456, 0)$, and $(2.427, 0)$.

large overlaps with the exact ground state and, from the shape of the optimal cluster for a given geometry, *predict* the momentum of the ground state with remarkable accuracy [11]. The momenta of the ground states here, however, do not match those of the optimal cluster states. Important differences are also seen in the response functions studied below. We thus conclude that these states are compressible and have properties that are qualitatively different from the Fermi-liquid-like compressible state at half filling in the lowest Landau level.

We now turn to the discussion of response functions. Here the fundamental quantity of interest is the dynamical structure factor, defined to be

$$S_0(\mathbf{q}, \omega) = \frac{1}{N_e} \sum_n |\langle 0 | \sum_i e^{i\mathbf{q}\cdot\mathbf{R}_i} | n \rangle|^2 \delta(E_n - E_0 - \omega). \quad (2)$$

The summation is over states in the given Landau level that is being studied. Various physically important quantities may be calculated from $S_0(\mathbf{q}, \omega)$ [8]; in particular, the projected static density response function is the inverse moment of $S_0(\mathbf{q}, \omega)$:

$$\chi(\mathbf{q}) = \int_0^\infty d\omega S_0(\mathbf{q}, \omega) / \omega, \quad (3)$$

and the projected equal time density-density correlation function is the 0th moment of $S_0(\mathbf{q}, \omega)$:

$$S_0(\mathbf{q}) = \int_0^\infty d\omega S_0(\mathbf{q}, \omega). \quad (4)$$

In Figs. 3 and 4 we present the \mathbf{q} dependence of $\chi(\mathbf{q})$ and $S_0(\mathbf{q})$ for half filled $N = 2$ and $N = 3$ Landau levels, respectively. The data were taken from systems with 10 electrons and rectangular geometry, for several different aspect ratios. We see sharp and strong peaks in $\chi(\mathbf{q})$ at $\mathbf{q}^* = (0.97, 0)$ and $\mathbf{q}^* = (0.84, 0)$ for $N = 2$ and $N = 3$

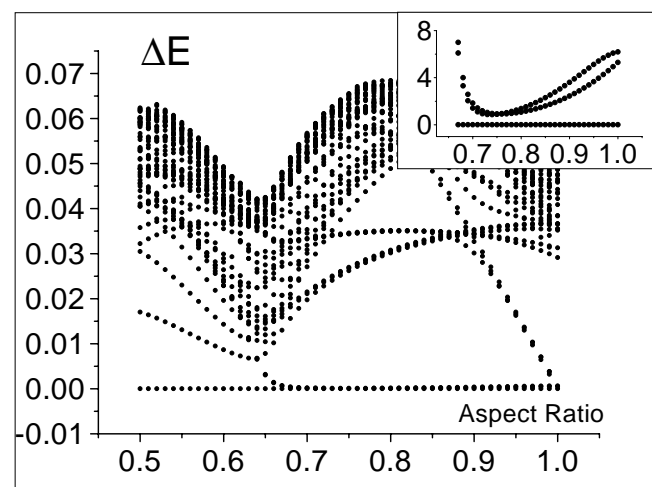


FIG. 2. Energy levels versus aspect ratio for half-filled $N = 2$ Landau level with ten electrons and rectangular geometry. The inset is a blowup of the low-energy spectra for aspect ratio between 0.7 and 1.0; the energies have been multiplied by 10^4 .

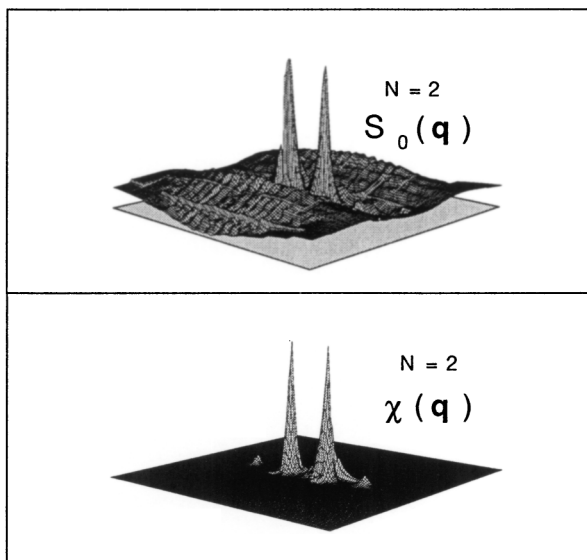


FIG. 3. $S_0(\mathbf{q})$ and $\chi(\mathbf{q})$ (in unit of $\epsilon\ell/e^2$) for half-filled $N = 2$ Landau level with ten electrons. The data were taken from systems with rectangular geometry, and a number of different aspect ratios. The highest peak value for $S_0(\mathbf{q})$ and $\chi(\mathbf{q})$ are 3.7 and 39726.3, respectively, which occur at aspect ratio 0.75.

Landau levels, respectively. At the scale of the peak value of χ , the response at different \mathbf{q} 's is indistinguishable from zero, except for a secondary peak positioned at *exactly* $3\mathbf{q}^*$, the height of which is much smaller but quite noticeable.

This is strongly suggestive of a tendency toward CDW ordering, as an (unpinned) CDW responds strongly to an external potential modulation with a wave vector that matches one of its reciprocal lattice vectors. The fact that secondary peaks appear only at integer multiples of the primary wave vector (\mathbf{q}^*) suggests that the CDW has 1D (stripe) structure. The absence of response at $2\mathbf{q}^*$ (and any other even multiples) is consistent with the presence of particle-hole (PH) symmetry in the underlying Hamiltonian at half filling: the PH transformation of the CDW state is equivalent to translation by half a period. Consistent with the stripe CDW picture, sharp peaks are also observed in $S_0(\mathbf{q})$ at $\mathbf{q} = \mathbf{q}^*$, indicating strong density-density correlation in the ground state at the ordering wave vector. Similar behavior is also seen at higher Landau levels and other filling factors. Again, these results are in sharp contrast with FQHE states (like $\nu = 1/3$ in the lowest Landau level), or the Fermi liquid-like state of the half-filled lowest Landau level. In the former case, χ is small (below 20) for all q 's due to the large gap in the spectrum [8]; while in the latter case although there are peaks in both $\chi(q)$ and $S_0(q)$, the peak position is tied to $q = 2k_F = 2$ and the height of the peak in $\chi(q)$ is in general much smaller than those seen here and the peaks are broader [11].

The origin of the strong peaks in χ at \mathbf{q}^* may be traced to the almost exact degeneracy of the low-energy

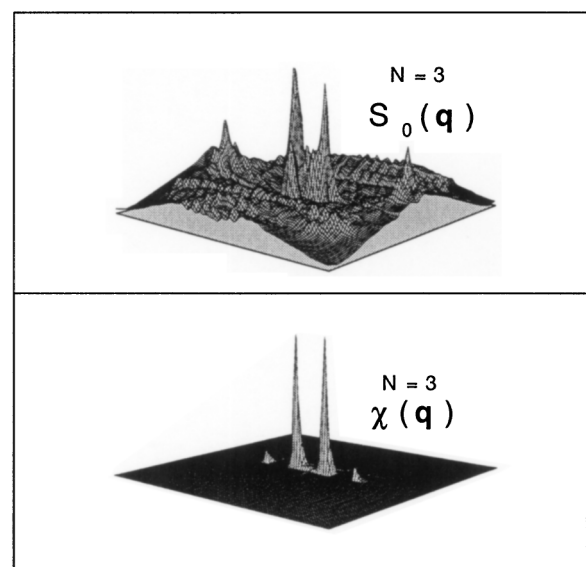


FIG. 4. Same as in Fig. 3, for $N = 3$ Landau level. The highest peak values are 4.17 and 2953432.4, respectively, which occur at aspect ratio 0.56.

states in the spectra that are separated by \mathbf{q}^* . Since these states are connected by a potential modulation with wave vector \mathbf{q}^* , an extremely small energy denominator ensures huge response from the system. We emphasize that such near degeneracy is a generic property of the system and not specific to a particular system size or geometry [12]. This can be seen clearly in Fig. 1b, where we plot energy levels from different geometries together. If the system develops long-range CDW order in the thermodynamic limit, we would expect the number of nearly degenerate states to increase with system size; in the thermodynamic limit, there will be infinitely many of them, spaced in momentum by \mathbf{q}^* , that become *exactly* degenerate. In this case a ground state that *spontaneously* breaks the translational symmetry may be constructed by taking linear combinations of these degenerate states, even though this is not possible (unless degeneracy is exact) in any finite system where all eigenstates must have a definite momentum.

In Fig. 5 we plot the Landau level dependence of q^* for half filled Landau levels. For systems with a given number of electrons in a given Landau level, we define q^* to be the modulus of the wave vector that gives the largest $\chi(\mathbf{q})$ for all geometries (aspect ratios). Despite the small and nonsystematic dependence on the number of electrons, it is clear that q^* decreases with increasing N . We are unable to accurately determine q^* beyond $N = 4$, as in this case $1/q^*$ becomes comparable to (and eventually exceeds) the linear size of the largest size system that we are able to study. This result is qualitatively consistent with Hartree-Fock theory [5–7], which predicts that the period of the CDW is set by the scale of the cyclotron radius in a given Landau level.

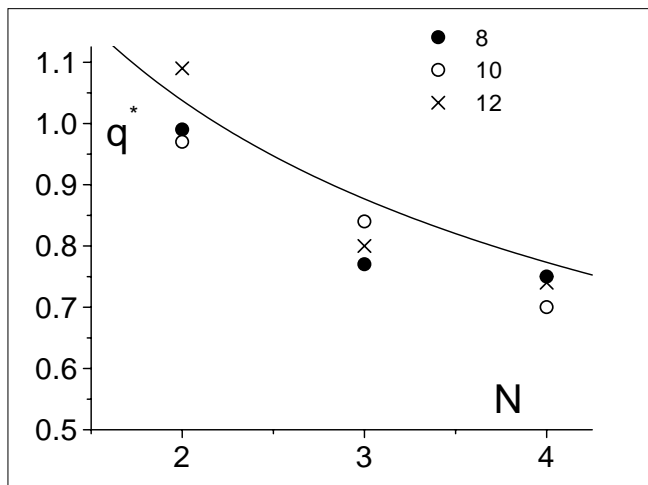


FIG. 5. Estimated ordering wave vector q^* versus Landau level index N . The solid curve is the prediction of Hartree-Fock theory.

In units of inverse magnetic length, this implies $q^* \propto 1/\sqrt{2N+1}$.

We have also performed numerical studies away from half filling, at filling factors $\nu = 1/4, 1/3, 2/5$, etc., for Landau levels $2 \leq N \leq 6$. At all these filling factors, we have seen qualitatively similar behavior in χ and S_0 , which are suggestive of a tendency toward CDW ordering. No evidence of incompressible FQHE states is found. This is consistent with Hartree-Fock theory, which predicts [13] no FQHE for $N \geq 2$. Hartree-Fock theory also predicts that when sufficiently far away from half filling, the stripe phase becomes unstable against a different type of CDW ordering, the “bubble phase” [6], which has a two-dimensional lattice structure. In our calculations we have seen some indication that this may be the case; however, more work is needed to make a clear distinction between these two types of structures. We leave this to future investigation.

As stated above, the physical properties of the systems that we have studied here are qualitatively consistent with predictions of Hartree-Fock theory. We also find that in the single Slater determinant basis for the wave functions, the Hartree-Fock single Slater determinant (with simple stripe structure) has the highest weight in the exact ground state. For example, in $N = 2$ and $N = 3$ Landau levels with ten electrons and rectangular aspect ratios of 0.75 and 0.56, respectively, the highest weight single Slater determinant has the occupation pattern (in Landau gauge) 11111000001111100000 (and ones that may be obtained by translating this pattern), where 1 stands for an occupied orbital and 0 stands for an empty orbital. The maximum weights are 0.1463 and 0.1986 for $N = 2$ and $N = 3$ Landau levels; the next highest weight single Slater determinant has a weight that is approximately fifteen times smaller for $N = 2$ and 1400 times smaller for $N = 3$. However, by making a linear

combination of the five nearly degenerate states we can single out the above occupation pattern and construct an approximate eigenstate that breaks translational symmetry. The overlaps (squared) with HF wave function then become 0.7338 for $N = 2$ and 0.9930 for $N = 3$. While there are still some fluctuations on top of HF states for $N = 2$, these fluctuations are completely gone for $N = 3$. Fradkin and Kivelson [14] recently considered the effects of thermal and quantum fluctuations on the Hartree-Fock stripe phase, and predicted a number of novel phases. Because of the limited system sizes in numerical studies, we are unable to distinguish among these phases (whose distinctions show up at large distances only).

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