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## LETTER TO THE EDITOR

# Finite-size scaling studies of 2D electrons at half-filling

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**Abstract.** Finite-size exact diagonalization of the Hamiltonian for four, eight and 16 electrons in a half-filled Landau level under periodic boundary conditions in a rectangular geometry was carried out. The magnitude of the peak value of the structure factor is found to increase with the system size to the power 0.36, consistent with a picture of a quasi-solid discussed by Chui. The energy difference of the lowest-energy state of the two different particle-hole symmetry manifolds decreases as the system size is increased, suggestive of broken particle-hole symmetry.

The discovery of the integer and fractional quantized Hall effect (FQHE) has generated much excitement recently. The FQHE is believed to come at odd-denominator filling factors so that the ground state does not possess long-range positional order and a gap exists in its excitation spectrum. As yet the study of the physics of the ground state at other filling factors, such as those with even denominators or at low densities, is still in its infancy.

The first violation of the odd-denominator rule occurs at  $\nu = \frac{5}{2}$  and is interpreted as being due to a spin effect [1]. Violations of the odd-denominator rule because of different physics at half-filling for narrow channels was predicted by Chui [2,3]. This phenomenon was subsequently observed by Timp *et al* [4]. For 2D samples at even denominator filling factors such as one-half, Jiang *et al* [5] found a dip in the longitudinal resistivity but no Hall plateau, very different from that of the conventional FQHE. This was interpreted [6] in terms of a quasi-solid wave function with algebraic long-range positional order previously considered by Chui *et al* [7]. This coherent state of intermediate long-range order presents new interesting features in its excitation spectrum. The phonon excitations, which were the Goldstone modes when the long-range order was completely broken, are no longer gapless because the long-range order is only algebraic. Gapless excitations corresponding to the Goldstone mode that consist of density fluctuation can still be constructed from this wave function, however. The possibility of a 'quasi-solid' phase at half-filling is also suggested by variational [7] and renormalization group [9] calculations. The energy of the trial wave function is found to be close to that from extrapolations from finite-cluster diagonalization studies [8].

Wigner [10] was the first to suggest that for an electron gas at a low enough density, the potential energy dominates the kinetic energy and the system becomes a solid. In the presence of an extremely strong magnetic field, all the electrons would be coerced into having the same kinetic energy of zero-point motion, and only the Coulomb energy would remain effective in governing their distribution in space. The electrons would then assume a configuration that would minimize the mutual repulsion, presumably a regular lattice. A

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strong magnetic field could, therefore, be expected to facilitate the formation of a crystal from an electron fluid. From this simplistic argument, one might conclude that electrons *always* form a solid when only the lowest Landau level is occupied.

Solids and charge-density waves (CDWs) [11] were amongst the first ideas examined for electrons in strong magnetic fields, but were found wanting in the absence of a sizable ground state energy in the Hartree-Fock approximation [12]. The next improvement is to introduce correlations. In the harmonic approximation, this yields the magnetophonon solid wavefunction which has been discussed by Chaplik [13] and recently simplified by us [7]. One can improve upon this by going to self-consistent magnetophonons [14], but a glaring defect remains in that exchange effects have not yet been included. For electrons in a strong field, because of the  $v \times B$  force, if we try to increase the correlation between the motion of the electrons and keep them apart in one direction, the electrons would come closer together on average due to decreased correlation in the other direction. However they would be able to lower their energy because exchange effects keep the electrons apart. The direct Coulomb energy would suffer only a relatively small increase, since the correlations were first optimized with respect to this aspect. This effect, we think, is the reason why fluctuations are so large. At odd denominators, multiparticle exchanges become possible with the help of the Bohm-Aharonov (BA) phase factor [15]. At even denominators, the BA phase factors act instead to suppress large-scale fluctuations. This is the physical reason why we believe the state is a quasi-solid.

Other possible ground states at half-filling have also been proposed. Kuramoto *et al* [16] have studied a CDW state with long-range order at half-filling in a mean field and found that the square lattice is more stable than the triangular (hexagonal) lattice. Fano *et al* [8] and Tosatti *et al* [17] have considered a triangular lattice with long-range order and its coexistence with hexagonal lattices, and the question of particle-hole symmetry. Recently Halperin *et al* [18] conjectured that the half-filled state is a fluid, also with gapless excitations. To clarify the nature of the ground state in a more quantitative fashion, we carried out finite-size scaling studies of the half-filled system, and present the results in this paper.

Numerical exact diagonalization studies on finite clusters at half-filling were performed by Fano *et al* [8] for spherical geometry up to 12 electrons and Chui [3] and Chakraborty *et al* [19] for the rectangular geometry. Chen and Tosatti [20] studied *short-range* three-particle correlations in small systems and found triangular (hexagonal)-type behaviour for  $\nu$  smaller (larger) than  $\frac{1}{2}$ ; the short-range order is reduced at  $\nu = \frac{1}{2}$ . Because of the possibilities of solid formation of different crystal symmetries, it is important that the boundary conditions be commensurate with the possible lattice symmetries. For this reason, the rectangular geometry seems more appropriate, as it can be made to be commensurate with both the triangular (hexagonal) and the rectangular lattices.

Rectangular boundary conditions may enhance the formation of a solid. As the system size is increased the influence of the boundary will be decreased. Thus if the system was a liquid but stabilized by the boundary condition, its structure factor should not increase as the system size is increased. The structure factor that we found increases as the system size is increased, indicating that the tendency to form a solid is even stronger. Incidentally, numerical calculations with rectangular boundary conditions produced correctly the fluid state at  $\frac{1}{3}$  filled with a gap. To ascertain the nature of the ground state it is important to study the size dependence in samples that are similar in shape to each other. These kinds of systematic study have not been carried out.

In this paper we studied samples of four, eight and 16 electrons because of the constraint of shape similarity. To understand the nature of the ground state, we focus on its structure

factor  $S(Q) = \sum_{i,j} \exp(iQ \cdot r_{ij})/N = 1 + \sum_{i \neq j} \exp(iQ \cdot r_{ij})/N$ . The first term in the sum is not a function of the system size but can easily mask the size dependence of the second term which can be numerically smaller than the first for small systems. For this reason we focus on the quantity  $S(Q) - 1$ . Our results are summarized in figures 1 and 2:

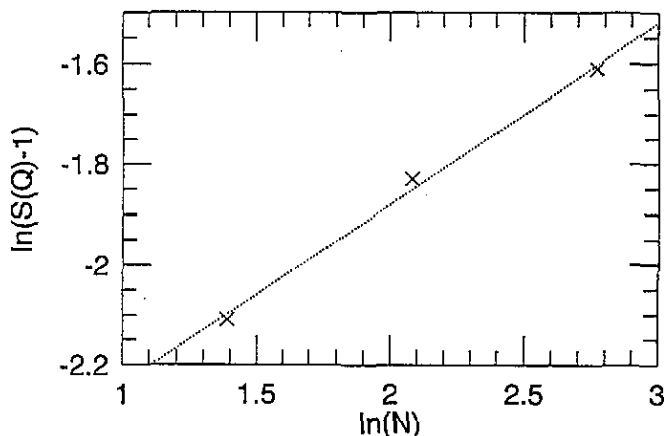


Figure 1. The peak value of the structure factor as a function of the system size.

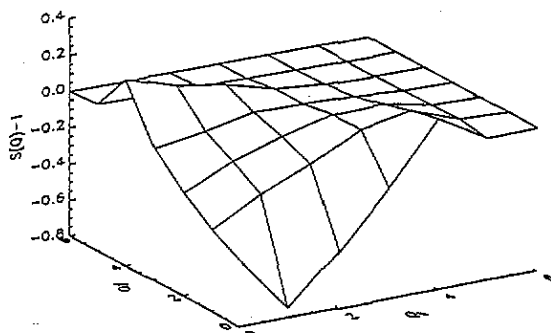


Figure 2. The structure factor as a function of the momentum transfer in units of  $2\pi(1/L_x, 1/L_y)$ .

In figure 1 we show the log-log plot of the peak value of  $S(Q) - 1$  as a function of system sizes. Also shown is a least-squares straight line fit through the data points. This peak value increases in a power law manner as a function of system size with an exponent of 0.36. This behaviour, if true in the limit of infinite size, is only consistent with that of a quasi-solid. For a fluid, we expect the peak value to remain unchanged or decrease slightly whereas for a solid with true long-range order we expect the peak value to increase linearly with the system size (the power will then be unity).

In figure 2 we show the two-dimensional dependence of the structure factor on the momentum transfer ( $Q_x, Q_y$ ) for the 16-particle system. The aspect ratio  $L_x/L_y$  for this case was chosen to be  $\sqrt{3}/2$  so that the box size is commensurate with both the triangular

and the rectangular symmetries. The peak occurs at either  $Q_x = 0$  or  $Q_y = 0$ . The positions of the peaks are the same for all the sample sizes that we looked at. The structure factor quickly approaches one as the momentum is increased because  $S(Q) - 1$  is proportional to  $\exp(-Q^{2/4})$ . We now describe our calculation in detail.

The formalism for the diagonalization calculation is by now straightforward. The basis set can be written as product wavefunctions of Landau orbitals given by [21]

$$\begin{aligned}\phi_j(\mathbf{r}) &= \exp(ix_j y - (x - x_j)^2/2)/(\pi^{1/2} L_y)^{1/2} \\ x_j &= (2\pi/L_y)j.\end{aligned}$$

$L_y$  is the width in the  $y$  direction. We set the magnetic length  $l = (\hbar c/eB)^{1/2} = 1$ . The Hamiltonian in the second quantized form can be written as

$$H = \sum_{|j|} A(j_1, j_2, j_3, j_4) C_{j_1}^+ C_{j_2}^+ C_{j_3} C_{j_4} + \sum_i \epsilon_M C_i^+ C_i$$

Where the values of  $A$  are integrals of the Coulomb potential and the Landau orbitals  $\phi_j$

$$A(j_a, j'_b, j_b, j'_a) = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \phi_{j_a}(\mathbf{r})^* \phi_{j'_b}(\mathbf{r}')^* \phi_{j_b}(\mathbf{r}) \phi_{j'_a}(\mathbf{r}') / |\mathbf{r} - \mathbf{r}'|$$

and  $\epsilon_M$  is the Madelung energy [22]. We have assumed the particles are confined in a rectangle under periodic boundary conditions. An aspect ratio of 0.866 (1.7321) was used in most of our calculations for four, 16 (eight) particles so as to be commensurate with triangular and rectangular lattices.

Haldane has emphasized that there is an additional translation symmetry along the  $x$  axis by an amount proportional to  $2\pi/\nu L_y$ . We have incorporated this symmetry in our calculation. For the 16-particle system, the total number of states is about a million after this symmetry is incorporated.

The Hamiltonian at half-filling possesses particle-hole symmetry. A state of total  $y$  momentum  $J = \sum j_i$  is transformed to one with total  $y$  momentum  $(N_s(N_s + 1)/2 - J \bmod N_s)$ . Only at special momenta is the total  $y$  momentum unchanged under a particle-hole transformation. We found that the lowest-energy state occurs at these special momenta (for example,  $J = N_s/2$ ). At these momenta for an even number of sites the total  $y$  momenta also remain unchanged under a parity transformation. When these symmetries are incorporated the total number of states for 16 particles is of the order of 300 000. We have verified our program by comparing the outputs for small systems with and without incorporating these symmetries. We now describe some details of our 16-particle calculation.

We represent a configuration by a bit configuration of a 32-bit integer (corresponding to 32 sites); the occupancy of a site is represented by setting a bit. A hashing technique is used to speed up the identification of the  $3 \times 10^5$  allowable site-occupation configurations among the possible  $2^{32}$  bit configurations with the label of that allowable configuration. The Hamiltonian connects those configurations that differ from each other by four and only four bits. The program is checked for the eight-particle case with short integers (16 bits) against previous calculations without these improvements.

The Hamiltonian matrix is sparse. The number of non-zero matrix elements for each column is of the order of 200. We use the Lanczos algorithm with partial reorthogonalization for its diagonalization [23]. On an IBM workstation, it takes a day to generate the Hamiltonian and half a day for the diagonalization, which takes about 20 iterations. The

lowest-energy state occurs at  $J_x = L_y/4l^2$ ; and positive particle-hole and parity eigenvalues. Just as in the eight-particle case, 90% of the spectral density of the ground state wave function is concentrated in 0.3% of the basis states.

We tested for broken particle-hole symmetry by examining the energy separation between the two particle-hole symmetric manifolds at the same total momenta containing the lowest-energy manifold. For the four-particle case, all states possess positive eigenvalues under the particle-hole transformation. For the eight- and the sixteen-particle cases, the energy separations between the manifolds are 0.22 and 0.08, respectively. The energy difference decreases as the system size is increased, consistent with the interpretation of a broken particle-hole symmetry. The ground state energy is equal to  $-0.4813$ ,  $-0.4731$ ,  $-0.4676$  for four, eight and sixteen particles, quite close to Fano's estimate of  $-0.469 \pm 0.05$ . In contrast the energy difference between the first excited states within the same symmetry manifold is equal to 0.28, 0.19 and 0.18 for four, eight and sixteen particles.

The structure factor is calculated from its second quantized form

$$\left\langle \sum \exp[-q^2/2 + iq_x(k_1 - k_2 + qy)] C_{k_1+q}^\dagger C_{k_2-q}^\dagger C_{k_2} C_{k_1} \right\rangle.$$

The two peaks of the structure factor occur at wave vectors  $Q = (4\pi/a3^{1/2}, 0)$  and  $Q = (0, 2\pi/a)$  where  $a$  is the 'lattice constant' given by  $a^2 = 2\pi l^2/3^{1/2}$ . The magnitude of the peak of the structure factor along the  $x$  and the  $y$  directions differs in magnitude for the four- and sixteen-particle cases with the same aspect ratio. We think this is a result of the asymmetry of the  $x$  translation ( $1/\nu$ ) and  $y$  translation (continuous) symmetries. The asymmetry decreases as the system size is increased. It is 50% and 38% for four and sixteen particles. When the magnitude of the peak is smaller, the width becomes correspondingly larger. The peak value in figure 1 is the average of these two peaks. One can also look at the rate of growth of the two peaks separately, obtaining exponents of 0.28 and 0.41. We next compare our results with those at  $\frac{1}{3}$  filling.

At  $\frac{1}{3}$  filling, the peak structure factor minus one for four and eight particles at aspect ratios of 0.866 and 1.7321, respectively are 0.066 and 0.069, a change of 5%. In contrast, at  $\frac{1}{2}$  filling, the corresponding  $S(Q)-1$  is 0.119 and 0.179, a bigger value and a significant increase. (We cannot easily look at the sixteen-particle case at  $\frac{1}{3}$  filling because it is too large and the additional particle-hole symmetry cannot be incorporated. For eight particles, the number of basis states with only translation symmetry incorporated is 103 at  $\frac{1}{2}$  filling and 3840 at  $\frac{1}{3}$  filling.)

The systematics of the structure factor is more complicated for the higher-lying manifold with a negative charge conjugation eigenvalue. For the sixteen-particle case, the structure factor peaks at positions expected of a triangular (hexagonal) lattice but also with unequal peak values. For the eight-particle case, the structure factor peaks along the  $x$  or the  $y$  axis.

We have also examined the higher-lying manifold with  $J_x = 0$ . The behaviour of the structure factor is identical to the above except that the lower-lying manifold now possesses negative particle-hole symmetry.

In summary, we have performed size dependence studies of the structure of the ground state of 2D electrons in a half-filled Landau level. Our results indicate quasi-solid behaviour so that the positional order increases, but not as fast as the system size. Even though the order is similar to that of a finite-temperature solid, the state is *coherent* whereas the finite-temperature solid is not. Because of this partially broken symmetry, there are excitations with and without gaps. Our calculation also indicates that only a small fraction of the basis states is important. This suggests that the problem is a weak-coupling problem and may be amenable to analytic calculations.

We thank E Tosatti, who suggested that we look for the size dependence of the energies of the two particle-hole symmetric manifolds as an indication of a possible degeneracy.

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