

## Computer renormalization-group calculation for the fractionally quantized Hall effect

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Results of a computer renormalization-group calculation for electrons in a magnetic field are presented for clusters with up to 16 electrons for the  $\frac{1}{3}$ -filled case for the first time. The structure factor is computed. We found a "Bragg-like" peak at a finite wave vector. The height of this peak increases as the system size is increased. This behavior is different from that of the Laughlin fluid but is much closer to that of a quasisolid.

Wigner first pointed out that electrons may form a crystal if the density  $n$  of electrons is low enough. A magnetic field will quench out the kinetic energy and hence make the Wigner solid experimentally more accessible. Recent experiments<sup>1</sup> discovered two new phenomena, the integral-quantized and the fractionally quantized Hall effects (FQHE). In the FQHE, the system is particularly stable when the Landau levels are filled to a specific ratio  $\nu$ , where  $\nu$  is a rational number with an odd integer as denominator.

To explain this, Laughlin<sup>2</sup> proposed that the electrons form a fluid. He wrote a trial wave function which provided a good estimate of both the ground-state energy as well as the magnitude of the gap. The small-distance behavior of this wave function agrees with recent work based on the direct diagonalization of the Hamiltonian of small clusters.<sup>3</sup> Recently Chui, Ma, and Hakim<sup>4</sup> (CMH) proposed a trial quasisolid wave function which has a lower energy than that of Laughlin. The probability density of this wave function looks like the partition function of a two-dimensional (2D) solid at a *finite* temperature. It only possesses "algebraic" long-range translational order. The phonons of this wave function exhibit a gap of the same magnitude<sup>5</sup> (0.076) as that of Laughlin. Because the ground state does not have true translational long-range order, Goldstone's theorem is not violated. Whereas the small-distance behavior of these two wave functions is very similar, the large-distance behavior is not. Limited by the large number of basis states, the cluster calculations have been carried out on relatively small samples (less than six and eight particles for periodic and spherical boundary conditions, respectively) and they cannot distinguish between the above two possibilities unambiguously.

In this Rapid Communication we report a computer renormalization-group (CRG) calculation for clusters with up to 16 electrons in a square with periodic boundary conditions for the  $\frac{1}{3}$ -filled case for the first time. We find that the static structure factor  $S(\mathbf{q})$  possesses a peak; the magnitude of this peak increases as the size of the sample is increased. In Fig. 1 we plot  $S(q_x, q_y=0)$  as a function of  $q_x$  for samples with 4 and 16 particles. The magnitude of the peak changes from around 1.17 for 4 particles to 1.9 for 16 particles. Furthermore, the peak sharpens considerably. For the Laughlin fluid, the pair correlation function  $g(r)$  rises from 0 to 1 at the first neighbor and

exhibits very little oscillation afterwards. If this picture is correct,  $S(\mathbf{q})$  should not exhibit a peak (Fig. 1). Our calculation is not exact but the approximations are controlled and very good. This comes about because there is a hidden small parameter in the problem which we exploited.

A hint of the structure in  $S(\mathbf{q})$  had been previously seen in the 2D pair correlation function calculated by Yoshioka<sup>6</sup> for the six-particle sample. He found that  $g(r)$  exhibited an oscillation after the first neighbor. However, it is difficult to rule that oscillation out as a size effect for that case.

The CRG technique was first applied by Wilson<sup>7</sup> to the Kondo problem. Its applications to one-dimensional problems have been discussed by several authors.<sup>8</sup> The only detailed calculations with this technique in 1D have been carried out by us. This technique was first applied to the 1D Hubbard model. Recently we have applied it to 1D spin chains in a magnetic field.<sup>9</sup> For the present problem, in the Landau gauge the basis set can be written as

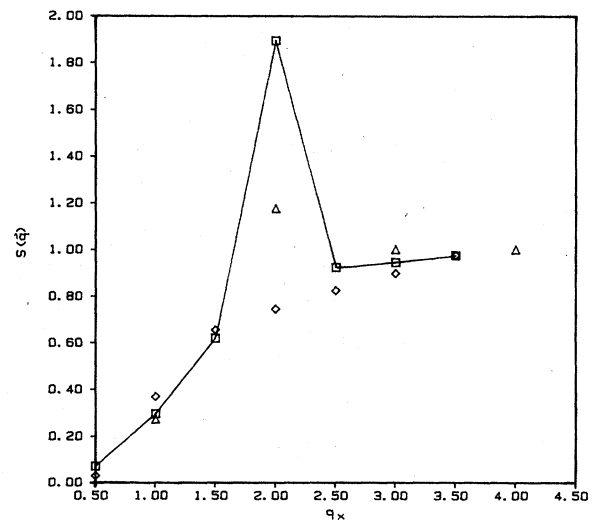


FIG. 1. The structure factor  $S(\mathbf{q})$  for  $q_y=0$  as a function of  $q_x$  for 16 ( $\square$ ) and 4 ( $\triangle$ ) particles. The unit of  $q_x$  is  $\sqrt{\pi}/6/l$ . Straight lines are drawn through the points to guide the eye.  $S(\mathbf{q})$  for the Laughlin fluid is also shown ( $\diamond$ ). Here  $S(\mathbf{q})$  is defined to be  $\langle \rho_{\mathbf{q}} \rho_{-\mathbf{q}} \rangle$ , where  $\rho_{\mathbf{q}} = \sum_j e^{i\mathbf{q} \cdot \mathbf{r}_j} / \sqrt{N}$ .

product wave functions of Landau orbitals in the lowest Landau level. These orbitals are given by

$$\phi_j(\mathbf{r}) = \exp[ix_j y/l^2 - (x - x_j)^2/2l^2]/(\pi^{1/2}lL)^{1/2}, \quad (1)$$

$$x_j = (L/N_s)j,$$

where  $L$  is the width in the  $y$  direction and  $N_s$  is the total number of possible states. The Hamiltonian in second-quantized form can be written, except for trivial constants, as

$$H = \sum_{\{j\}} A(j_1, j_2, j_3, j_4) C_{j_1}^\dagger C_{j_2}^\dagger C_{j_3} C_{j_4}. \quad (2)$$

The  $A$ 's are integrals of the Coulomb potential and the Landau orbitals  $\phi_j$ . Since the label  $j$  is "one dimensional," the present problem also becomes a 1D problem except that we now have much longer range interactions.

In the CRG technique, one focuses on the low-lying eigenstates of larger systems by building it from those of smaller clusters iteratively. The Hamiltonian  $H_{2n}$  of a system with  $2n$  particles is broken down as that of clusters on the left and right and an interaction between these clusters, viz.,  $H_{2n} = H_{nl} + H_{nr} + H_I$ . In any given step, the eigenfunctions of  $H_{2n}$  are those of  $H_n$  perturbed by  $H_I$ . The eigenfunctions of  $H_n$  have  $n^{-1/2}$  of their weight at the ends of the chain, and so if we renormalize  $H_{2n}$  in terms of the eigenfunctions of  $H_n$  ( $H_{nr}$  and  $H_{nl}$ ), the off-diagonal matrix elements will be of the order of  $1/n$ . Since the number of eigenstates of  $H_n$  goes as  $8^n$ , only a limited number may be retained at each iteration after  $H_4$ . High-lying states of the smaller clusters are systematically discarded, because they are not as strongly coupled to the low-lying states, thereby making the calculation possible. To obtain reliable results, a large number of states needs to be kept. To retain this large number of states requires careful programming for memory management and efficiency. There have been other calculations that retain a much smaller number (about ten) of states per iteration. These are much easier to program but it is much more difficult to predict the reliability of the results of these calculations.

A dimensionless measure of the coupling between the states discarded and the low-lying states is the ratio of the off-diagonal matrix elements between the clusters to the separation between the energy levels. In the Kondo problem and the Hubbard model in the non-half-filled-band case, the separation between the energy levels also goes down as the system size is increased. This is not so in the present problem because of the existence of the energy gap. In this sense the present problem is easier.<sup>10</sup> The complication in the present problem comes from the large number of intercluster interactions that need to be calculated. To simplify matters on the first try, we have approximated the Hamiltonian by truncating the long-distance interaction. In our calculation for 16 particles only 106 kinds of intercluster coupling are kept. We shall come back to this point later.

We now discuss the details of our calculation. The eigenstates of the system are characterized by two quantum numbers, the total  $y$  momentum  $j$  and the total charge  $n$ . By trial and error, we have found that adequate

maximum fluctuations for  $j$  and  $n$  to be 14 and 4, respectively. At each stage of the iteration, a maximum of 51 combinations of  $j, n$  can be kept. For each such  $j, n$  manifold, a maximum of 300 basis states can be kept. Our calculation is performed for periodic boundary conditions. It is basically done for a strip, whose width in the  $y$  direction is decided at the beginning. This fixes the allowed values of  $x_j$  [ Eq. (1) ] and the form of the Hamiltonian in the Landau gauge. The ends of this strip are allowed to interact at the final stage of the iteration. We have performed two checks to ensure that our program is correct. For the 12-site four-electron problem, no states are discarded and our calculation is "exact." First we have verified the threefold degeneracy of the ground state. Second, we have compared our result with that from the straightforward diagonalization of the Hamiltonian; identical results are found. Our calculation takes 20 minutes of central processing unit time on an IBM 3081D computer at the University of Delaware. In our calculation, we found that for a cluster with  $2^k$  electrons, a lot of the intercluster coupling matrix elements are zero. Of those matrix elements that are larger than  $0.001/2^k$ , in absolute magnitude, their average magnitude is  $0.007/2^k$ . The energy difference between the ground state and the lowest state that we discarded is larger than  $1.4/2^k$ . *The dimensionless coupling parameter between states that we discarded and the ground state is thus of the order of 0.005, a small number indeed.* Hence our approximation of discarding the high-lying states is good.

Our second approximation consists of truncating part of the Hamiltonian. We rewrite Eq. (1) in a different form to bring out the similarity to the Hubbard model as

$$H = \sum_{m,j} V(m) n_j n_{j+m} + \left[ \sum_{l=1} \sum_{m=1} t_l(m) \sum_i C_{i-l}^\dagger C_i C_{i+m} C_{i+m+l}^\dagger + \text{c.c.} \right]. \quad (3)$$

The  $t$ 's are the hopping integrals. We found that  $t_2(m)$  is of the order of  $t_1(m)/3$  because of the smaller overlap of the Landau orbitals in the former case. In our calculation we have only kept  $t_1(m)$  and  $t_2(1)$ . The  $n_i$  is the number operator at site  $i$ . We have shifted the values of  $V(m)$  so that they approach zero at large  $m$ . We have discarded the large-distance  $V(m)$  and  $t_1(m)$  when their magnitude is less than 0.1 of that at the maximum. The  $V(m)$  and the  $t_1(m)$  that we retained are shown in Fig. 2. Note that  $V(m)$  attains a maximum and then comes down as one approaches the origin. This comes from the exchange. More precisely,

$$V(m) = 2[A(j_{23}=0, j_{13}=m) - A(j_{23}=m, j_{13}=0)],$$

where  $j_{ab} = j_a - j_b$ ; the first (second) term is the direct (exchange) contribution. At small distances  $m$ , these two terms are comparable in magnitude; the net value of  $V$  is reduced. As  $m$  increases, the exchange contribution dies off exponentially fast and only the first term remains. It is this behavior of  $V$  that accounts for the "accidental degeneracies"<sup>2</sup> of the ground state for the  $\frac{1}{2}$ -filled case in

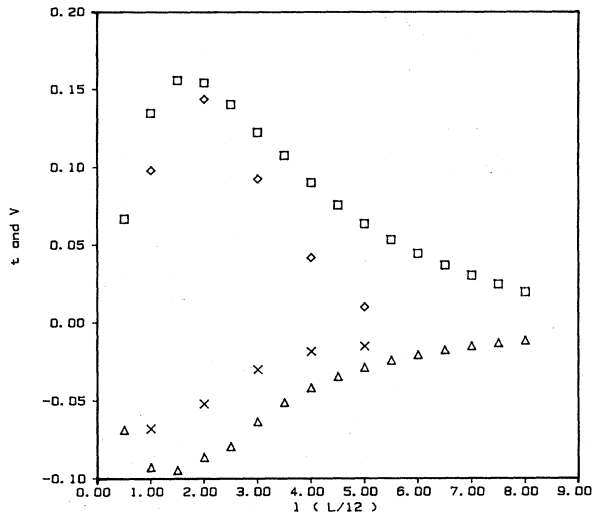


FIG. 2. The Hamiltonian parameters  $V(l)$ ,  $t(l)$  that we have retained as a function of  $l$  for 16 ( $\square$  and  $\triangle$ ), and 4 ( $\times$  and  $\diamond$ ) particles.

the four-electron calculation. At a density of  $\frac{1}{2}$ , a uniform electron spacing would have placed the electrons at a separation  $l=2$  where  $V(l)$  is maximum, an unstable point. The particles can move either left or right to lower its energy and a lot of low-lying states of comparable energies developed. These energies then spread into a band when the hopping integral  $t$  is taken into consideration.

We do not, however, have a proof that it causes the degeneracy for the half-filled case in general.

An idea of the approximation of truncating  $V(l)$ ,  $t(l)$  at large  $l$  can be obtained by looking at the magnitude of the gap  $\Delta$  and the ground state energy  $E_0$  that we found. We found that  $\Delta=0.046, 0.04$ ,  $E_0=-0.41, -0.395$  for the 4,16 particle samples. Calculations with the full Hamiltonian for periodic boundary conditions for electrons in a square performed by Su for four, five, and six particles gave  $\Delta=0.06$ ,  $E_0=-0.4$ . We found that the ground-state properties are not a sensitive function of this truncation whereas the magnitude of the gap is, which may be because  $\Delta$  is the difference of two large numbers. For example, if  $t_2(l)$  and  $t_1(l)$  with  $l$  greater than 12 are set equal to 0,  $S(q)$  and  $E_0$  change by less than 10% whereas  $\Delta$  changes from 0.04 to 0.1. We have also experimented with changing the range of  $V(l)$  and have come to the same conclusion. Similar results on the range of the potential have been noted previously by Haldane.

To summarize, a controlled approximation for the FQHE was exploited to calculate the physical properties of clusters with up to 16 electrons. The gap energy agrees with previous calculations; the static structure factor develops a peak as the system size is increased. These results are more similar to those of the quasisolid proposed by CMH.

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<sup>1</sup>K. V. Klitzing, G. Dorda, and M. Pepper, Phys. Rev. Lett. **45**, 494 (1980); D. C. Tsui, H. L. Stormer, and A. C. Gossard, *ibid.* **48**, 1559 (1982); H. L. Stormer *et al.*, *ibid.* **50**, 1953 (1983).

<sup>2</sup>R. B. Laughlin, Phys. Rev. Lett. **50**, 1395 (1983); see R. S. Markiewicz, A. Widom, and J. Sokoloff, Phys. Rev. B **28**, 3654 (1983), for an alternative explanation.

<sup>3</sup>D. Yoshioka, B. I. Halperin, and P. A. Lee, Phys. Rev. Lett. **50**, 1219 (1983); R. B. Laughlin, Phys. Rev. B **27**, 3383 (1983); W. P. Su, *ibid.* **30**, 1069 (1984); F. D. M. Haldane and E. H. Rezayi, Phys. Rev. Lett. **54**, 237 (1985).

<sup>4</sup>S. T. Chui, K. B. Ma, and T. M. Hakim (unpublished).

<sup>5</sup>The unit of energy is  $e^2/(\text{Larmor radius})$  in this paper and will

not be explicitly specified from now on.

<sup>6</sup>D. Yoshioka (unpublished).

<sup>7</sup>K. Wilson, Rev. Mod. Phys. **47**, 773 (1975).

<sup>8</sup>S. D. Drell, M. Weinstein, and S. Yankielowicz, Phys. Rev. D **14**, 487 (1976); **16**, 1769 (1977); S. T. Chui and J. W. Bray, Phys. Rev. B **18**, 2426 (1978); **19**, 4876 (1978); **21**, 1380 (1980).

<sup>9</sup>S. T. Chui and K. B. Ma, Phys. Rev. B **27**, 4515 (1983); **29**, 1287 (1984).

<sup>10</sup>In the terms used in the study of critical phenomena, one is far from the critical point and the weak-coupling regime is quickly reached.