Ground State of Two-Dimensional Electrons in Strong Magnetic Fields and $\frac{1}{3}$ Quantized Hall Effect

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The authors have diagonalized numerically the Hamiltonian of a two-dimensional system of up to six interacting electrons, in the lowest Landau level, in a rectangular box with "periodic" boundary conditions. They find that the ground state has a pair correlation function quite different from that of a Wigner crystal, and its energy is significantly lower. They also find some indications of a downward cusp in the energy at $\frac{1}{3}$ filling.

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The origin of the quantized Hall effect of a two-dimensional electron system in a strong magnetic field[1] is now well understood.[2-5] However, there has been no satisfactory explanation for the anomalous quantized Hall effect, which is observed in AlGaAs-GaAs heterojunctions.[6,7] In this experiment the Hall conductivity σ_{xy} shows plateaus at $\sigma_{xy}=\frac{1}{3}e^2/h$ and $\frac{2}{3}e^2/h$. Since the AlGaAs-GaAs heterojunction has a very high electron mobility, it is natural to suspect that the effect comes from the Coulomb interaction between electrons. However, an attempt to explain the effect by the formation of a Wigner-crystal-like charge-density-wave (CDW) state was not successful.[8] It was found that $\frac{1}{3}$ or $\frac{2}{3}$ filling of the lowest Landau level did not lead to any observable singularity in the energy, and it was also shown that in the crystalline state, σ_{xy} takes as values only *integer* multiples of the quantum e^2/h, if the crystal is pinned by impurities.[9,10] We need a new state which has lower energy than the crystal to explain the anomalous quantized Hall effect.

In the present paper, we investigate numerically the eigenstates of an electron system, in the first Landau level, in a rectangular cell with "periodic" boundary conditions, and up to six particles. We find that the ground state has significantly lower energy than that of a Hartree-Fock Wigner crystal, and that the pair correlation function $g(\vec{r})$ looks quite different from that of a crystal. States resembling the Wigner crystal with regards to energy and $g(\vec{r})$ appear at higher energy.

We take the coordinate system such that the boundary of the cell is given by $x=0$, $x=a$, $y=0$, $y=b$, with the vector potential $\vec{A}=(0, xB)$. Our boundary condition requires that $ab/2\pi l^2$ *be an integer* m, where $2\pi l^2=hc/eB$. Then there are m different single-electron states in the cell, whose wave functions are given by

$$\varphi_j(\vec{r})=\left(\frac{1}{b\pi^{1/2}l}\right)^{1/2}\sum_{k=-\infty}^{\infty}\exp\left[i\frac{(X_j+ka)y}{l^2}-\frac{(X_j+ka-x)^2}{2l^2}\right]. \quad (1)$$

Here integer j, $1\leq j\leq m$, specifies the state, and $X_j=2\pi l^2 j/b$ is the center coordinate of the cyclotron motion.

The electrons in the cell interact with each other and with the uniform positive background charge by the Coulomb interaction. Because of the boundary condition, the Coulomb potential in real space is given by

$$V(\vec{r})=\sum_s\sum_t e^2/\epsilon|\vec{r}+sa\hat{x}+tb\hat{y}|, \quad (2)$$

where ϵ is the dielectric constant, and $\hat{x}$ and $\hat{y}$ are the unit vectors along the x and y axes, respectively. Since we consider only the lowest Landau level, the Hamiltonian consists entirely of the Coulomb

interaction term:

$$H=\sum_j S a_j^\dagger a_j+\sum_{j_1}\sum_{j_2}\sum_{j_3}\sum_{j_4} A_{j_1 j_2 j_3 j_4} a_{j_1}^\dagger a_{j_2}^\dagger a_{j_3} a_{j_4}, \tag{3}$$

where a_j is the destruction operator for the jth state. The single-electron part comes from the interaction between an electron and its image, so that S is a known constant related to the Coulomb energy of the classical rectangular Wigner crystal.[11]

The two-electron part is given by

$$A_{j_1 j_2 j_3 j_4}=\tfrac{1}{2}\int d^2r_1 \int d^2r_2\, \varphi_{j_1}^*(\vec{r}_1)\varphi_{j_2}^*(\vec{r}_2)V(\vec{r}_1-\vec{r}_2)\varphi_{j_3}(\vec{r}_2)\varphi_{j_4}(\vec{r}_1)$$
$$=\frac{1}{2ab}\sum_q{}'\sum_s\sum_t \delta_{q_x,2\pi s/a}\,\delta_{q_y,2\pi t/b}\,\delta'_{j_1-j_4,t}\,\frac{2\pi e^2}{\epsilon q}\exp\left[-\frac{l^2q^2}{2}-2\pi i s\frac{j_1-j_3}{m}\right]\delta'_{j_1+j_2,j_3+j_4}. \tag{4}$$

The Kronecker δ with prime means that the equation is defined modulo m, and the summation over q excludes $q=0$.

We specify the number n of electrons in our cell, so the filling factor ν is given by n/m. The Hamiltonian of the system has particle-hole symmetry, after a constant term, which equals $-(\pi/8)^{1/2}\nu^2(e^2/\epsilon l)$ in the infinite-n limit, has been removed. Our calculations are done for $\nu\leq 0.5$ and extended to $\nu>0.5$ using this symmetry.

The basis n-electron wave function is specified by the occupation of the single-electron state: $(j_1, j_2, \ldots, j_n)$. The total number of the basis is given by $\binom{m}{n}$. However, the Hamiltonian H conserves the total momentum in the y direction, $J=j_1+j_2+\ldots j_n \pmod m$. So the number of the basis for fixed m, n, and J is approximately $m^{-1}\binom{m}{n}$, which gives the dimension of the Hamiltonian matrix.

Two values of J which differ by a multiple of n are equivalent, since $(j_1, j_2, \ldots, j_n)$ and $(j_1+1, j_2+1, \ldots, j_n+1)$ differ only by translation in the x direction. Hence when m and n have no common factor, the energy spectrum of the Hamiltonian is independent of J and every eigenenergy is at least m-fold degenerate. On the other hand, when m and n have a common factor, the states are less degenerate and the ground state is realized only at certain choices of J. For example, at $\nu=\frac{1}{3}$ and $n=4$, the threefold-degenerate ground state is found at $J=2$, 6, 10.

Since we are interested in the ground states near $\nu=\frac{1}{3}$, the diagonalization was done numerically for $n=4$, 5, and 6, and $0.25\leq n/m=\nu\leq 0.5$ except for $n=6$ where we calculate only up to $m=20$ or $\nu=0.3$. Figure 1 shows the ground-state energy of n-electron systems as a function of the filling factor $\nu=n/m$ for the choice of aspect ratio $a/b=n/4$. (This choice of a/b seems to give an approximate local minimum in the energy.) To investigate the nature of the eigenstates of the Hamiltonian we also calculated the pair correlation function $g(\vec{r})$, which is the same for all states in a degenerate multiplet. For $n=4$ the $g(\vec{r})$ for the ground state has fourfold rotational symmetry and has peaks at $\vec{r}=(\pm a/2, 0)$ and $(0, \pm b/2)$, but *not* at $\vec{r}=(\pm a/2, \pm b/2)$, where we would expect to have peaks if the state were a square crystal. States which correspond to a square crystal and a triangular crystal are found at higher energy for even m. The energy of the triangular crystal is lower than that of the square crystal and it has a minimum at $a/b=2/\sqrt{3}$. Here $g(\vec{r})$ has the form

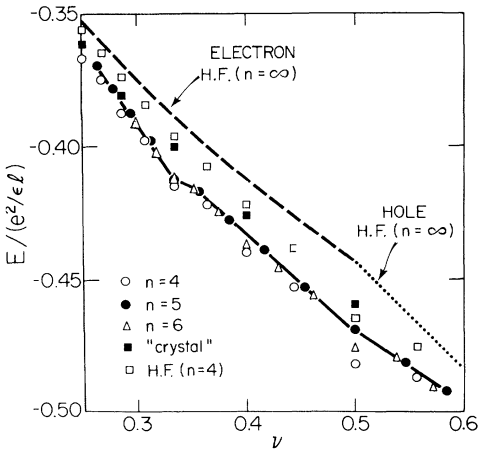

FIG. 1. The energies per particle of two-dimensional electron systems vs the fractional filling of the first Landau level. The dashed and dotted lines show energy of the electron and hole crystals resulting from the Hartree-Fock approximation for the infinite system. Open circles, closed circles, and triangles show the ground-state energies for n = 4, 5, and 6 electrons for $\nu\leq\frac{1}{2}$ and n = 4, 5, and 6 holes for $\nu>\frac{1}{2}$. Closed squares show the crystal state for the n = 4 system. Open squares show the energy of the crystal state for the n = 4 system obtained by the Hartree-Fock approximation. The solid line drawn through the n = 5 ground-state energies is a guide to the eye only.

similar to that of the triangular crystal obtained by the Hartree-Fock (HF) approximation in the infinite system. The energy of this crystalline state is also shown in Fig. 1.

In order to clarify further the nature of the ground state and to clarify the boundary effect, we also apply the Hartree-Fock approximation to the Hamiltonian of the four-electron system. We assume order parameters $\Delta_{j_1 j_2} \equiv \langle a_{j_1}{}^{\dagger} a_{j_2} \rangle$, to be finite, decouple the Hamiltonian, and obtain self-consistent solutions for $\Delta_{j_1 j_2}$.[12] The state we obtain is always a triangular CDW state except for $\nu = \frac{1}{2}$, where we get a unidirectional CDW state. The energy becomes minimum at $a/b = 2/\sqrt{3}$. This energy is also shown in Fig. 1.

The HF energy of the four-electron system is slightly lower than the HF energy of the infinite crystal, shown in Fig. 1 by the dashed and dotted curves for the electron and hole crystals, respectively. This difference comes from the boundary condition. In the finite system the Coulomb potential between an electron and its image separated by $R = (ma, nb)$ is always $e^2/\epsilon R$, whereas an average over the Gaussian charge distribution is required in the infinite crystal. The energy difference between the finite and infinite systems is completely explained by this effect.

Next, we note that the $n = 4$ HF energies are slightly higher than the energies of the "crystal states" obtained in the exact diagonalization. The difference, which we would like to attribute to the correlation between nearest electrons, is about 2 times larger than the correlation energy estimated by Yoshioka and Lee[8] by second-order perturbation theory, which seems reasonable. However, as mentioned above, the crystal states are not the lowest states of our systems.

As seen in Fig. 1, the *ground-state energies* of our small systems tend to have downward cusps at simple rational values of ν. Clearly it is not possible to extrapolate our data to $n = \infty$. Nevertheless, it is interesting that the downward cusp at $\nu = \frac{1}{3}$ remains roughly constant for the three systems calculated ($n = 4, 5, 6$). A cusp is also visible at $\nu = \frac{2}{5}$, but unfortunately we have data points only for two values of n. By contrast, the ground-state energy at $\nu = \frac{1}{2}$ shows a large, nonmonotonic variation with n. As a guide to the eye we have connected the points in Fig. 1 for $n = 5$, for which there are no low-order rationals except for $\nu = \frac{1}{3}$ and $\frac{1}{2}$. It is interesting that this curve shows almost no cusp at $\nu = \frac{1}{2}$.

At this point, we can make a number of speculations regarding the infinite system and the relation to the experiment. We regard our data as supportive of the idea that the ground state is not crystalline, but a translationally invariant "liquid." We speculate that this liquid has commensurate energy at $\nu = \frac{1}{3}$ (and possibly other simple rational values), and that for a large but finite system, the ground state at $\nu = \frac{1}{3}$ is threefold degenerate and separated by an energy gap from a variety of excited states. By going to a moving frame, it is then clear that at $\nu = \frac{1}{3}$ a Hall current will flow without dissipation, even in the presence of impurities. At ν *close* to $\frac{1}{3}$, we further suppose that the ground state, which is now highly degenerate, can be described as the $\nu = \frac{1}{3}$ ground state plus an additional small density of quasi "particles" or "holes." This leads naturally to a downward cusp in the energy as function of ν. The Hall plateau at $\sigma_{xy} = \frac{1}{3} e^2/h$ can then be explained if the quasiparticles are localized by impurities and thus do not contribute to the Hall current, which is simply carried by the underlying $\nu = \frac{1}{3}$ state. Very recently, we have learned of a very original proposal by Laughlin of a wave function for a liquid state at $\nu = 1/p$, for p odd, which appears to have the requisite commensurate energy.[13]

An alternative explanation of the Hall conductance plateau is also possible, assuming the existence of a commensurate energy E_c at $\nu = \frac{1}{3}$, if one believes that the electron system in the GaAs accumulation layer is in equilibrium with the donor states in GaAlAs by tunnelling.[14] For ν near $\frac{1}{3}$, it is energetically favorable to pin the density at $\frac{1}{3}$, provided that the energy gain $|\Delta n| E_c$ exceeds the charging energy $2\pi L_d (e\Delta n)^2/\epsilon$ to transfer $\Delta n \equiv (\nu - \frac{1}{3})/2\pi l^2$ electrons across a depletion layer of thickness L_d. If we extract a rough estimate of $E_c \approx 0.008 (e^2/\epsilon l)$ from the depth of the cusp in Fig. 1 near $\nu = \frac{1}{3}$, and we use $L_d = 240$ Å and $l = 66$ Å ($B = 15$ T), this would lead to a full width of the Hall step at $\nu = \frac{1}{3}$ of $\delta\nu/\nu \approx 20\%$, which is consistent with current experiments. Clearly, this alternative explanation depends on the details of the layer structure and we find it less appealing than the first explanation we offered.

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[1]K. V. Klitzing, G. Dorda, and M. Pepper, Phys. Rev. Lett. 45, 494 (1980).

[2]R. B. Laughlin, Phys. Rev. B 23, 5632 (1981).

[3]D. J. Thouless, J. Phys. C 14, 3475 (1981).

[4]H. Aoki and T. Ando, Solid State Commun. 38, 1079 (1981).

[5]B. I. Halperin, Phys. Rev. B 25, 2185 (1982).

[6]D. C. Tsui, H. L. Stormer, and A. C. Gossard, Phys. Rev. Lett. 48, 1559 (1982).

[7]H. L. Stormer, D. C. Tsui, A. C. Gossard, and J. C. M. Hwang, in Proceedings of the Sixteenth International Conference on the Physics of Semiconductors (to be published).

[8]D. Yoshioka and P. A. Lee, Phys. Rev. B 27, 4986 (1983).

[9]H. Fukuyama and P. M. Platzman, Phys. Rev. B 25, 2934 (1982).

[10]D. Yoshioka, Phys. Rev. B 27, 3637 (1983).

[11]L. Bonsall and A. Maradudin, Phys. Rev. B 15, 1959 (1977).

[12]H. Aoki, J. Phys. C 12, 633 (1979).

[13]R. B. Laughlin, private communications.

[14]G. A. Baraff and D. C. Tsui, Phys. Rev. B 24, 2274 (1981).