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Ground state of two-dimensional electrons and the reversed spins in the fractional quantum Hall effect

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We have diagonalized numerically the Hamiltonian of a two-dimensional electron system of finite size, allowing some electron spins to be antiparallel to the magnetic field, in the lowest Landau level. We find that, in the case of the filling fraction $\nu = p/q$, with q odd and $p > 1$, the ground state with nonpolarized spins is energetically favored. The present results also indicate that filling factors $v = \frac{4}{9}$ and $v = \frac{4}{11}$ might be observable experimentally with partially polarized electron spins. At $\nu = \frac{1}{3}$ the spatial wave function for the ground state is found to be totally antisymmetric.

The discovery of the fractional quantum Hall effect,¹ where a two-dimensional electron gas in a strong perpendicular magnetic field exhibits special stable states, has received much attention theoretically.²⁻⁸ These stable states are found at certain values of v, where $v = 2\pi l^2 \rho$ is the filling factor of the Landau level, ρ the density of twodimensional electrons, and $l = (\hbar c/eB)^{1/2}$ the magnetic length. While the many-body calculations available so $far^{3,4}$ are successful in explaining some of the filling factors, in particular $v=1/m$, with m being an odd integer, the explanation of other fractions observed experimentally $(\nu = \frac{2}{5}, \frac{2}{7})$, etc.) has been a fairly complicated endeavor.³⁻⁵

In all these theoretical works, it has been assumed that the Zeeman splitting is larger than $e^2/\epsilon l$, the unit of potential energy, ϵ being the background dielectric constant, so that no spin degree of freedom need be considered. It was first pointed out by Halperin² that, because the Landé g factor and the effective mass of the electrons in GaAs are much smaller than the corresponding free-electron values, the ground state for some values of ν might have some electrons with reversed spins. In the limit of very weak magnetic field, the favored spin state for the twodimensional electron system is governed by. the exchange energy. In the presence of the strong magnetic field, however, the favored spin state is determined by the interplay between the Zeeman energy and the exchange energy. In fact, our earlier calculations⁸ at $v = \frac{2}{5}$ indicated that the two energies are quite comparable.

In this paper we have adopted the numerical diagonalization procedure for a finite electron system with periodic boundary conditions to investigate the eigenstates of the system with different spin polarization for various values of the filling factors. While we have restricted ourselves to only four electrons, the recent work of Yoshioka⁶ on polarized spins indicated that, inclusion of more particles into the system does not alter the result significantly. Our results indicate that the energies for nonpolarized electron spins are considerably lower for the filling factor $v = p/q$ with q odd
and $p > 1$.

The numerical diagonalization procedure for the finite system was first proposed by Yoshioka, Halperin, and Lee (YHL)⁶ to study the nature of the ground state at $v = \frac{1}{3}$. That study correctly indicated that the ground state is a liquidlike state and also exhibits downward cusps at $\nu = \frac{1}{3}$,

 $\frac{2}{5}$, and $\frac{2}{7}$. This method has been used later by Su⁷ to study the ground-state degeneracy. Following YHL, we consider the electrons in a rectangular cell in the $x-y$ plane, with the boundary of the cell $x=0$, $x=a$, $y=0$, $y=b$, and impose periodic boundary conditions in both x and y directions. We have used the Landau gauge, $\vec{A} = (0, xB)$ and $ab/2\pi l^2$ being equal to an integer m , according to the periodic boundary condition. There are, therefore, m different singleelectron states for each spin in the cell, with the wave functions,

$$
\psi_{j,\sigma}(\vec{\mathbf{r}}) = \phi_j(\vec{\mathbf{r}})\chi_{\sigma} \quad . \tag{1}
$$

Here, X_{σ} are the two spin functions for spin-up and spindown along the z axis,

$$
\chi_{\uparrow} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_{\downarrow} = \begin{pmatrix} 0 \\ 1 \end{pmatrix},
$$

\n
$$
\phi_{J}(\vec{r}) = \left(\frac{1}{b \pi^{1/2} l} \right)^{1/2} \sum_{k=-\infty}^{\infty} \exp[i(X_{j} + ka)y/l^{2} - (X_{j} + ka - x)^{2}/2l^{2}] ,
$$
\n(2)

where, $1 \le j \le m$ and $X_j = 2\pi l^2 j/b$ is the center coordinate of the cyclotron motion.

If we now specify the number of electrons n in the cell, the filling factor is given by $v=n/m$. We can, however, decompose ν in terms of the partial filling factors $\nu = \nu_1$ $+v_1$, according to the number of spin-up and spin-down electrons in the cell. The Coulomb interaction with the periodic boundary condition

$$
V(\mathbf{T}) = \sum_{s} \sum_{t} e^{2}/\epsilon |\mathbf{T} + s a \hat{x} + t b \hat{y}|
$$
 (3)

is spin independent. Hence, the Hamiltonian can be written in the form

$$
H = \sum_{j,\sigma} W a_{j\sigma}^{\dagger} a_{j\sigma} + \sum_{j_1, j_2, j_3, j_4} A_{j_1, j_2, j_3, j_4} a_{j_1, \sigma}^{\dagger} a_{j_2, \sigma'} a_{j_3, \sigma'} a_{j_4, \sigma} \qquad (4)
$$

where $a_{j\sigma}^{\dagger}(a_{j\sigma})$ is the creation (annihilation) operator for the jth state with spin σ and W the classical Coulomb energy of a Wigner crystal with rectangular unit cell.⁶

$$
732\\
$$

The two-electron part of the Hamiltonian is given by

$$
A_{j_1j_2j_3j_4} = \frac{1}{2ab} \sum_{q} \sum_{s} \sum_{t} \delta_{q_x,2\pi s/a} \delta_{q_y,2\pi t/b} \delta'_{j_1-j_4,t} \frac{2\pi e^2}{\epsilon q} \exp\left[-\frac{1}{2}l^2q^2 - 2\pi i s (j_1-j_3)/m\right] \delta'_{j_1+j_2,j_3+j_4}
$$
(5)

Here, the summation over q excludes $q_x = q_y = 0$ and the Kronecker delta with prime means that the equation is defined modulo m.

The Hamiltonian can be diagonalized exactly for a small number of electrons. In diagonalizing the Hamiltonian matrix several symmetries are utilized to reduce the amount of calculations. These symmetries are explained in detail in Ref. 6. The energy spectrum for the Hamiltonian can be classified in terms of the total spin S and its z-component S_z . For a given S, the spectrum is identical for different values of S_z . If we include the Zeeman energy, the ground state for a certain S corresponds to the maximum value of S_{z} .

For the four electron system, we have calculated the ground-state energy (per particle) for the polarized state $(S= 2)$, the partially polarized state $(S= 1)$, and the unpolarized state $(S=0)$. The results are given in Table I for various values of the filling factor ν . The energies for the spin-polarized state were calculated by YHL and presented here for comparison. As seen in Table I, except for $v = \frac{1}{3}$, the nonpolarized state has lower energy, as compared to the polarized state for all other ν considered in this work. For all the filling factors considered here, the lowest energy is found to correspond to the case where the filling factor for each spin state has odd denominators. The situation is also illustrated in Table I. It is interesting to note that $\nu = \frac{4}{9}$ has a partial filling factor of $\frac{1}{3}$ in the partially polarized state $(S = 1)$. Based on the fact that the filling factor $\nu = \frac{1}{3}$ is an experimentally observed stable state, it is tempting to predict that $v = \frac{4}{9}$ should be a stable state with partially polarized electron spins. As we shall see below, this fraction is indeed energetically favorable, even in the presence of the magnetic field.

We have not considered the Zeeman energy so far. This is given (per particle) as $E_z = (1-2p)g \mu_B B s$, where p is the ratio of the number of spins parallel to the field to the total number of spins, $\mu_B = e\hbar/2mc$ the Bohr magneton, and $s = \frac{1}{2}$. For GaAs with all spins parallel to the field,

 $E_z = -0.011e^2/\epsilon l$ for $B = 10$ T and $g \approx 0.52$, and $\epsilon \approx 13$. In this case, including the Zeeman energy, the energy for the polarized and the partially polarized states are similar in magnitude for $v=\frac{4}{11}$, while the unpolarized state has a higher energy than the above two states. While this filling fraction is a good candidate for experimental observations, the situation is much more interesting for the filling factor $v = \frac{4}{9}$. Here, the partially polarized state has somewhat *lower* energy than those of the polarized and the unpolarized states. Therefore, an experimental observation of the quantized Hall effect at $v=\frac{4}{9}$ would probably raise the following interesting possibility: the $\frac{4}{9}$ state partially polarized, as our finite system results, indeed, would indicate. There are, however, other effects, e.g., mixing of higher Landau levels, which might reduce the difference in potential energy between the states of different spin polarization.⁹ In that case, the $\frac{4}{9}$ state would be spin polarized. Finally, in the face of a small energy difference for the four-electron system, one should also consider the possibility that the ground state of the infinite system would be fully polarized even, for the ideal case of no Landau-level mixing.

One obvious way to improve our finite system results would be to include more electrons in the cell. However, as stated earlier, for the polarized state at $v = \frac{4}{9}$, Yoshioka⁶ has calculated the energy for eight electrons which is only $\sim 0.002e^2/\epsilon l$ higher than the energy for four electrons. For the different spin polarization with eight particles, the Hamiltonian has a formidable size. Therefore, we have to content ourselves with the hope that the situation here is perhaps similar to that of the spin-polarized case, and a system of larger size will not change our present results significantly, leaving our predictions about the filling -fractions $\nu = \frac{4}{9}$ and $\frac{4}{11}$ probably unchanged.

The ground state at $\nu = \frac{1}{3}$ is found to be a spin-polarized state even in the limit of weak magnetic field. In other words, the spin state $S = 2$ is energetically favored compared with other spin states. As a result, the spatial part of the

TABLE I. Potenial energy (per particle) for the four-electron system for $\nu \leq \frac{4}{9}$ in the case of polarized $(S=2)$, partially polarized $(S=1)$, and unpolarized $(S=0)$ electron spins, and the partial filling factor v_1 and v_1 of the ground states. The Zeeman energy is not included.

$\boldsymbol{\nu}$	$S = 2$	Potential energy $S=1$	$S=0$	Ground state	v_{\uparrow}	\mathbf{v}_1
$\frac{1}{3}$	-0.4152	-0.4120	-0.4135	Polarized		$\bf{0}$
$rac{2}{7}$	-0.3870	-0.3868	-0.3884	Unpolarized		寺
$\frac{2}{5}$	-0.4403	-0.4410	-0.4464	Unpolarized		$\frac{1}{5}$
$\frac{4}{13}$	-0.3975	-0.3997	-0.3970	Partially polarized	$\frac{3}{13}$	$rac{1}{13}$
$\frac{4}{11}$	-0.4219	-0.4278	-0.4241	Partially polarized	$\frac{1}{11}$	$\frac{1}{11}$
$rac{4}{9}$	-0.4528	-0.4600	-0.4554	Partially polarized		$\frac{1}{9}$

wave function is fully antisymmetric. As discussed above, the favored spin polarization in exchange energy' is found to depend on the filling factor. We speculate that this qualitative result obtained for the finite system would hold for an infinite system. At $v = \frac{1}{3}$, Laughlin's wave function⁴ tends to keep. electrons very well separated and requires a fully polarized spin state. Any change in the symmetry property of the wave function will deviate from Laughlin's choice. At other filling fractions, however, Laughlin's wave function with fractional values of m does not satisfy the Fermi statistics of the system, and the actual ground-state energy for the polarized state is higher than the energy calculated with the use of Laughlin's wave function in the onecomponent plasma. 3 In that case, the energy could be lowered by introducing the spin degree of freedom. Our previous calculation⁸ for the two-spin state at $v = \frac{2}{5}$ supports this speculation,

In summary, we have found new possibilities for the ground state for some filling factors $v = \frac{4}{9}$ and $\frac{4}{11}$, in which

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the electron spins are partially polarized. Recent experiments have found evidence¹⁰ for a quantized Hall effect at $\nu = \frac{4}{9}$. However, at the present state of the experiment, it is not possible to study the electron spin polarization at $v = \frac{4}{9}$. Further experimental work at this fillng factor should be very interesting. Since the Zeeman energy depends on the magnetic field, and the properties of the materials of the system, the instabilities of the nonpolarized spin states might also be interesting for future experiments on the fractional quantum Hall effect.

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