Spin-Singlet Wave Function for the Half-Integral Quantum Hall Effect

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We present an analytic wave function describing a spin-singlet incompressible fluid of electrons confined to a single Landau level, which exhibits a *half-integral* quantum Hall effect. Our numerical studies suggest that this state may be responsible for the recently observed effect with $\nu=\frac{5}{2}$.

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The observation by Willett *et al.*[1] of a quantum Hall effect (QHE) with even-denominator fractional quantization $\nu=\frac{5}{2}$ has seemed to cast doubt on the current theoretical picture[2-5] which has so far predicted only odd-denominator fractional quantizations of the QHE in two-dimensional electron systems occurring in a single-well heterostructure device.[6] In this Letter, we report our discovery of a new incompressible quantum liquid state of electrons in a nonpolarized spin-singlet state which has a *half-integral* QHE quantization, and we present its explicit wave function. Two new conditions present in the experiments of Ref. 1 favor our state: (i) reduced Zeeman energy for spin reversal, and (ii) lower correlation energy of electrons in the same cyclotron orbit, due to the node in the second Landau-level orbital wave function.

We consider a two-dimensional (2D) electron gas in a uniform magnetic flux density B. The effective mass and interparticle interaction $V(r)$ are isotropic in the 2D plane, and substrate disorder is absent. When the ground state is incompressible,[2] a small amount of substrate disorder leads to a QHE plateau with[7] $\sigma^{xy}=[\partial\sigma/\partial B]_{\mu}=\nu e/\Phi_0$, where σ is the electronic charge density and $\Phi_0=h/e$ is the London flux quantum. In the absence of a substrate potential, ν reduces to the Landau-level "filling fraction" $|\sigma\Phi_0/eB|$.

In the "extreme quantum limit," where the cyclotron energy $\hbar\omega_c$ dominates the Zeeman and interaction energies, filled Landau levels are inert, closed-shell structures, and a partially filled level has particle-hole symmetry. Systems with filling fractions $2n+\nu$ or $2n+2-\nu$ are then *formally* equivalent to lowest Landau-level systems with filling fraction $\nu\leq 1$. The interaction is then completely parametrized by the *pseudopotentials*[3,8] $\{V_m\}$, which are the correlation energies of two-particle states with relative angular momentum $m\geq 0$. Essential differences between fractionally filled Landau levels with different quantum numbers n can only result from differences in the pseudopotentials, which depend[8] on n as well as the effective interaction $V(r)$.

The mapping of a higher Landau-level system to the equivalent $\nu\leq 1$ system allows a unified treatment[8] of fractional QHE phenomena in the extreme quantum limit. Correlation functions calculated for the equivalent $\nu\leq 1$ problem are easily transformed[8,9] back to the original ν. However, we will not do this, as we feel that it obscures physical similarities between related fractional QHE states.

The first eight pseudopotentials for a pure Coulomb interaction $V(r)\propto 1/r$ and Landau quantum numbers $n=0$ and $n=1$ are shown in Fig. 1. The most prominent difference between the $n=0$ and $n=1$ cases is the reduction in the "contact" term V_0, the correlation energy of particles in the same cyclotron orbit, which couples only opposite-spin electrons.

Numerical exact diagonalization of finite-size systems[8,10,11] has proved to be a powerful tool for the study of fractional QHE states. Motivated by Ref. 1, we extended an investigation[12] of the effect of varying V_0 in systems with spin reversal to filling fractions near $\frac{1}{2}$.

We used the spherical geometry[3] where N particles are confined to the surface of a sphere with N_Φ Dirac monopoles at its center. In this formalism, the number

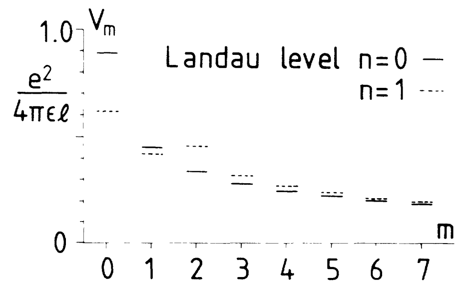

FIG. 1. Coulomb-interaction pseudopotentials for Landau levels $n=0$ and $n=1$. Units are $e^2/4\pi\epsilon l$, $l=|\hbar/eB|^{1/2}$. Note the reduction of V_0 for $n=1$.

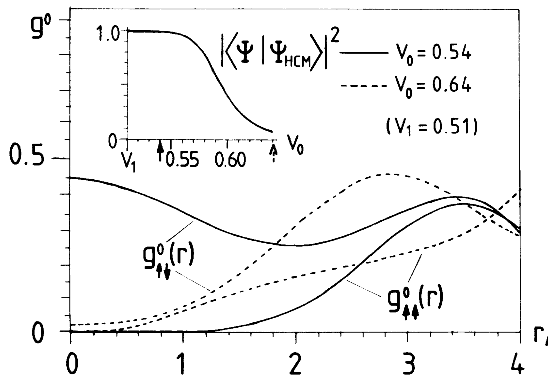

FIG. 2. Effect of varying V_0 in the six-particle $N_\Phi = 8$ system. The $m > 0$ pseudopotentials were kept at the $n = 0$ Coulomb values, for which $V_0 = 0.987$ (for finite N_Φ, they differ from values shown in Fig. 1). Equivalent $n = 0$ pair correlation functions g^0 (in units representing local "filling fractions") are shown for two values of V_0. Here r is the geometric (chord) separation on the sphere; for $N_\Phi = 8$, the sphere diameter is $4.0l$. Note the disappearance of the correlation hole in $g^0_{\uparrow\downarrow}$ for $V_0 < 0.55$, and the change from r^2 to r^6 short-distance behavior of $g^0_{\uparrow\uparrow}$ (the r^2 component becomes very small). Inset: Projection of the ground state onto the HCM ground state as a function of V_0.

of orbitals in a Landau level is not N_Φ but $N_\Phi + (2n+1)$, and the QHE quantization ν is not directly given by a "filling fraction"; instead the more fundamental relation of Ref. 7 must be used. An incompressible state occurs at a *sequence* of sizes where $N_\Phi = \nu^{-1}N + \delta$. Identification of two successive members of the sequence determines $\nu = \Delta N/\Delta N_\Phi$. For example, the $\nu = 1/m$ Laughlin states[2] occur when[3] $2l = N_\Phi = m(N-1)$, where $l = \frac{1}{2}N_\Phi$ is the orbital angular momentum of a lowest Landau-level particle on the sphere.

To model a possible sequence of spin-unpolarized states with $\nu = \frac{1}{2}$, we used a simple construction in which pairs of opposite-spin electrons are placed in the same cyclotron orbit and treated as charge-$2e$ spinless bosons in a symmetric Laughlin state. To correspond to $\sigma^{xy} = \frac{1}{2}e^2/h = \frac{1}{8}(2e)^2/h$, this must be a "$\nu = \frac{1}{8}$" boson state. On the sphere, the pair has orbital angular momentum $l = N_\Phi$, and the sequence is $2N_\Phi = 8(\frac{1}{2}N - 1)$, i.e., $N_\Phi = 2(N-2)$, N even.

Though the pairing idea (suggested earlier[13] in the context of *spin-polarized* electrons) gives a heuristic picture of our state, we emphasize that there are no attractive forces leading to bound-state formation. Rather, "pairing" is a description of the collapse of a correlation hole between opposite-spin electrons.

We studied the six-particle system ($N_\Phi = 8$) which reduces to the diagonalization of matrices with dimensions 152, 140, 106, and 102. We chose the $n = 0$ Coulomb interaction, modified by variation of V_0. For V_0 at its Coulomb value, the pair correlation function

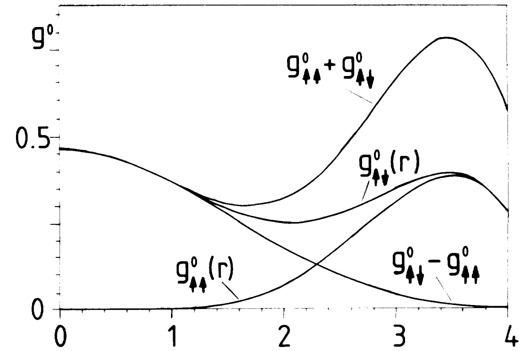

FIG. 3. Pair correlations of the six-electron HCM ground state. Note that the spin density $g^0_{\uparrow\downarrow} - g^0_{\uparrow\uparrow}$ vanishes identically for r at the sphere diameter, implying the existence of a sum rule special to this state (this is only an approximate feature of the $V_0 = 0.54$ state in Fig. 2). $g^0_{\uparrow\uparrow}$ has exact r^6 short-distance behavior.

$g^0_{\uparrow\uparrow}(r)$ vanishes like r^2 as $r \to 0$, and there is a deep correlation hole in $g^0_{\uparrow\downarrow}(r)$. The system shows none of the signs of incompressibility seen in earlier studies[10] at $\nu = \frac{1}{3}$.

As V_0 is reduced, a qualitative change in the correlations occurs over a narrow range of couplings (Fig. 2). The correlation hole in $g^0_{\uparrow\downarrow}$ is replaced by a *peak* at the origin, and the r^2 term in $g^0_{\uparrow\uparrow}$ becomes very small: r^6 behavior is seen.

Motivated by the observation that the Laughlin state of the fully spin-polarized Landau level with $\nu = \frac{1}{3}$ is the *exact*[3] ground state of a model interaction potential with $V_1 > 0$, but $V_3, V_5, \ldots = 0$, we then studied a model interaction with $\{V_m\} = \{0,1,0,0,\ldots\}$. *In complete analogy with the Laughlin ground state, we find that this "hollow core" model (HCM) has a unique zero-energy ground state when $N_\Phi = 2(N-2)$.* The pair correlations of this state are given in Fig. 3, and show that it is very similar to the ground state of the modified Coulomb interaction model at $V_0 = 0.54$. This is confirmed by the overlap of these two states, shown as an inset in Fig. 2.

In Fig. 4 we show the ground-state correlation energy of the six-particle HCM as a function of the magnetic flux N_Φ. For $N_\Phi > 15$, the zero-energy states are highly degenerate, and all values of the total spin quantum number S occur. $N_\Phi = 15$ is the lowest flux at which a fully spin-polarized ($S = 3$) zero-energy state occurs. This state is the $\nu = \frac{1}{3}$ Laughlin state. *At smaller values of N_Φ, the maximum spin of the zero-energy states decreases, with one spin reversal for every two flux quanta removed from the system.* A nondegenerate nonpolarized ground state is finally reached at $N_\Phi = 8$, which is the $\nu = \frac{1}{2}$ state reported here. This is the lowest flux at which a zero-energy state is found. A clear picture emerges of gradual spin depolarization for $\nu > \frac{1}{3}$, ending with a nonpolarized incompressible QHE state at $\nu = \frac{1}{2}$.

We now construct the analytic wave function Ψ_{HCM}

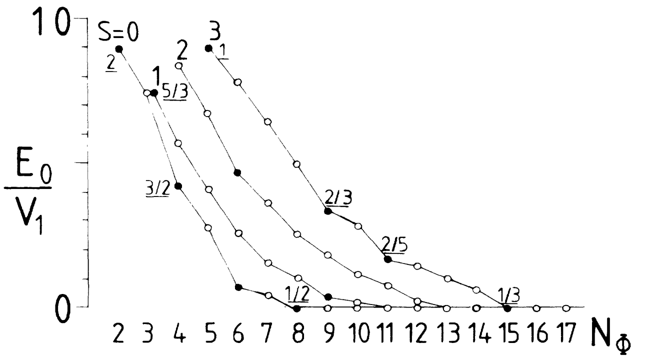

FIG. 4. Six-electron HCM ground-state correlation energy as a function of the magnetic flux N_Φ and the total electronic spin S. Full circles represent states where (for a given S) the ground state is nondegenerate; cusps in the ground-state energy at these points indicate a QHE state. A Zeeman energy hS must be subtracted to give the total energy; for $\nu \leq \frac{1}{3}$ (large N_Φ) this gives full spin polarization in the ground state. For $\frac{1}{3} < \nu < \frac{1}{2}$, and weak Zeeman energy ($h \lesssim V_1$), the ground state continuously depolarizes. In this model there will be a cusp in energy at $\nu = \frac{1}{3}$ entirely due to the Zeeman term. Currently identified QHE states are indicated; the singlet state at $N_\Phi = 4$ is the $\nu = \frac{3}{2}$ state (sequence $N_\Phi = \frac{2}{3} N$), which is obtained from the $\nu = \frac{1}{2}$ state by particle-hole conjugation. We tentatively identify the singlet state at $N_\Phi = 6$ as a $\nu = \frac{2}{3}$ unpolarized state with sequence $N_\Phi = \frac{3}{2} N - 3$.

for the zero-energy spin-singlet HCM ground state at $N_\Phi = 2(N-2)$. In the absence of spin-orbit coupling, the many-particle wave function for spin-$\frac{1}{2}$ electrons factorizes into a spatial part and a spin part. If the total spin quantum number is S, the spatial wave function must belong to the permutation group representation $(2^{(N/2)-S} 1^{2S})$. The Fock conditions[14] require that it must be separately antisymmetric in a set of $N_\uparrow = \frac{1}{2} N + S$ coordinates and the remaining set of $N_\downarrow = \frac{1}{2} N - S$ coordinates, and that *it is not possible to further antisymmetrize the function between the* $\uparrow$*-spin coordinates and one of the* $\downarrow$*-spin coordinates.* If $\sigma_i = \uparrow, \downarrow$ indicates to which group a coordinate belongs, then the second condition is

$$\delta_{\sigma_i,\downarrow} \left[1 - \sum_j \delta_{\sigma_j,\uparrow} e(i,j) \right] \Psi = 0, \tag{1}$$

where $e(i,j)$ is the permutation operator that exchanges the values of coordinates i and j.

In the spherical geometry,[3] wave functions must be polynomials of equal degree N_Φ in each pair of variables

$$(u_i, v_i) = (\cos \tfrac{1}{2} \theta_i \exp(i \tfrac{1}{2} \phi_i), \sin \tfrac{1}{2} \theta_i \exp(-i \tfrac{1}{2} \phi_i))$$

which are complex spinor coordinates on the spherical surface. The Laughlin wave functions with $\nu = 1/m$ are given by[3]

$$\Psi_m(\{u_i, v_i\}) = \prod_{i<j} (u_i v_j - v_i u_j)^m.$$

Homogeneous states are rotationally invariant on the sphere. These states are built from rotationally invariant factors $Z_{ij} \equiv u_i v_j - v_i u_j$ and are either totally symmetric (N) states or totally antisymmetric (1^N) states, depending on whether m is even or odd.

To model systems without full spin polarization, Halperin[13] has considered the natural generalization of Ψ_m to a family of wave functions

$$\Psi^{\{\sigma_i\}}_{m_\uparrow, m_\downarrow, m} = \prod_{i<j} (Z_{ij})^{m(\sigma_i, \sigma_j)}, \tag{2}$$

where $m(\sigma, \sigma) = m_\sigma$, $m(\sigma, -\sigma) = m$. For $m_\uparrow = m_\downarrow = m$, (2) reduces to the Laughlin state Ψ_m. Otherwise, the states (2) have $N_\Phi - m = (\nu_\sigma)^{-1} (N_\sigma - 1)$, with partial filling factors $\nu_\sigma = (m_\sigma - m)/(m_\uparrow m_\downarrow - m^2)$. The wave function $\Psi^{\{\sigma_i\}}_{1,1,0}$ describes a filled Landau level ($\nu = 2$) and has symmetry type $(2^{N/2})$.

For $m_\uparrow, m_\downarrow$ odd, the wave functions (2) are antisymmetric in same-spin coordinates. In general, however, they do *not* satisfy (1), and are *not* acceptable wave functions for a system with spin-independent forces.[8] Only the subset with $m_\sigma = m + 1$, m even (which includes Halperin's $\nu = \frac{2}{5}$ state[13]) are valid spin-$\frac{1}{2}$ electron states.[8] These are the product of a symmetric Laughlin-Jastrow factor Ψ_m with the filled Landau-level wave function, and have odd-denominator $\nu = 2/(2m+1)$.

Other wave functions in the set (2) may describe electronic systems with two *physically distinct* components: for example, spin-polarized electrons in *two coupled* 2D layers, where interlayer interactions are weaker than intralayer interactions. [We have previously found that the state $\Psi^{\{\sigma_i\}}_{3,3,1}$ corresponding to $\nu = \frac{1}{2}$ ($\nu = \frac{1}{4}$ per layer) can be stable in such circumstances.[6]]

To construct the unique HCM ground state seen in the numerical study, we need a wave function with $N_\Phi = 2(N-2)$ which is a spin-singlet [i.e., its symmetry type is $(2^{N/2})$], and which has no $m = 1$ pair correlations (spin-rotation invariance guarantees this provided $\Psi_{\rm HCM}$ vanishes like Z_{ij}^3 as parallel-spin electrons approach).

While $\Psi^{\{\sigma_i\}}_{3,3,1}$ has $\nu = \frac{1}{2}$, it has $N_\Phi = 2(N-2) + 1$, does not have a definite symmetry type, and vanishes if opposite-spin electrons coincide. We multiply it by a factor that corrects these problems: $\Psi^{\{\sigma_i\}}_{\rm HCM} = \Psi^{\{\sigma_i\}}_{3,3,1} \operatorname{per} | M^{\{\sigma_i\}} |$, where $M^{\{\sigma_i\}}_{ij}$ is a $\frac{1}{2} N \times \frac{1}{2} N$ matrix of the inverse complex distances Z_{ij}^{-1} between the ith spin-$\uparrow$ particle and the jth spin-$\downarrow$ particle. (The *permanent* per$|M|$ is the symmetric analog of det$|M|$.)

The permanent reduces the polynomial degree in each coordinate by 1, and so $\Psi^{\{\sigma_i\}}_{\rm HCM}$ has the correct N_Φ. The function $\Psi^{\{\sigma_i\}}_{3,3,1}$ contains a factor Z_{ij} for *each* pair of opposite-spin particles; each term in the expansion of the permanent corresponds to one of the $(\frac{1}{2} N)!$ ways of grouping opposite-spin particles into pairs, and removes the corresponding factors of Z_{ij} from the wave function, allowing it to remain finite when coordinates i and j coincide.

We note that $\det|M^{\{\sigma_i\}}|$ is a Cauchy determinant equal to $\Psi_{1,1,-1}^{\{\sigma_i\}}$, and so $\Psi_{\rm HCM}^{\{\sigma_i\}}$ can also be written

$$\Psi_{\rm HCM}^{\{\sigma_i\}}=\Psi_2 \det|M^{\{\sigma_i\}}| \,\mathrm{per}\, |M^{\{\sigma_i\}}|. \tag{3}$$

To prove that (3) does indeed have symmetry type $(2^{N/2})$, and hence establish that it *is* the required wave function, we need a mathematical result that the product of the Cauchy determinant [i.e., that of an $N \times N$ matrix of the form $(x_i-y_j)^{-1}$] with the corresponding permanent is a function of symmetry type (2^N) satisfying the Fock conditions. Though we have not found a simple algebraic proof, numerical evaluation of the left-hand side of (1) for small N (≤ 6) and arbitrary values $\{x_i, y_i\}$ confirms that it vanishes identically, empirically proving the required result.

A simple physical picture emerges from our study. The two spin components of an unpolarized electron gas at $\nu=\frac{1}{2}$ have partial filling fractions $\nu_\sigma=\frac{1}{4}$. This is in the range $\nu \leq \frac{1}{3}$ in which a single-spin-component electron gas can have r^6 behavior of its pair correlations at short distances. However, the interactions between opposite-spin particles force a correlation hole in $g^0_{\uparrow\downarrow}$ when V_0 is large. This excluded area effectively increases the density of each spin component above $\frac{1}{3}$ filling, forcing r^2 behavior on $g^0_{\sigma\sigma}$. Collapse of the correlation hole as V_0 is decreased allows an effective expansion of each of the two components of the unpolarized electron gas and the restoration of r^6 correlations.

The new features of the experimental regime explored by Willett *et al.*[1] include lower magnetic fields (hence lower Zeeman energy) and electrons with higher Landau index ($n=1$), which have a lowered V_0. These are features favoring our new spin-singlet half-integral fractional QHE state $\Psi_{\rm HCM}$, the existence of which was previously unsuspected. We believe that $\Psi_{\rm HCM}$ is a very promising candidate state for the observed $\nu=\frac{5}{2}$ fractional QHE, though definitive conclusions cannot be reached without quantitative studies using reliable values of the $\{V_m\}$ and the Zeeman energy appropriate to the experimental conditions.

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Note added.—Numerical studies[15] carried out since the submission of this Letter appear to show that projection of a "realistic" $V(r)$ (including layer-thickness effects) into the second Landau level does not, on its own, lower V_0 sufficiently to produce a $\nu=\frac{1}{2}$ QHE. Landau-level-mixing effects become more important at the lower magnetic fields of Ref. 1, and we are investigating a possible mechanism[16] for selective additional reduction of V_0 involving virtual admixture of states with different Landau index.

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