Possibility of p-wave pairing of composite fermions at $\nu = \frac{1}{2}$

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(Received 22 June 1998)

We find that the composite Fermi sea at $\nu = 1/2$ is on the verge of an instability to triplet pairing of composite fermions. It is argued that a transition into the paired state, described by a Pfaffian wave function, may be induced if the short-range part of the interaction is softened by increasing the thickness of the two-dimensional electron system. [S0163-1829(98)52440-X]

It has been over 10 years since the discovery of an even-denominator fractional quantum Hall effect (FQHE) at Landau level (LL) filling fraction $\nu = 5/2$.[1] In this state the lowest ($n=0$) LL is filled for both up spins and down spins and the effective filling factor of the first-excited ($n=1$) LL is 1/2. In an attempt to explain how this state was able to escape the usual ''odd denominator rule'' of the FQHE, Haldane and Rezayi[2] proposed a trial wave function which described an incompressible singlet state for a half-filled LL and argued that this state might be stable at $\nu = 5/2$. Despite some initial experimental support for the not fully polarized nature of the state in tilted field experiments,[3] questions persisted from the very beginning about whether this was in fact the correct description of the $\nu = 5/2$ state.[4] Exact diagonalization calculations[5,6] also indicate that the true *Coulomb* ground state at $\nu = 5/2$ is not spin singlet even in the limit of zero Zeeman coupling. Greiter *et al.*[7] raised an alternative possibility in which the 5/2 FQHE state is *fully polarized* and described by the Pfaffian wave function proposed by Moore and Read.[8] This scenario was recently further explored by Morf.[6]

In contrast, there has been significant progress in our understanding of the physics of the compressible state at $\nu = 1/2$ in terms of the composite fermion (CF) theory, where composite fermions are electrons bound to an even number of vortices in the many-body wave function.[9] According to this theory, interacting electrons in the lowest LL are described in terms of composite fermions at an effective magnetic field. In particular, the FQHE for electrons can be viewed as an effective *integer* quantum Hall effect for composite fermions[9] and the *compressible* state at a half-filled LL as a ''metal'' of composite fermions with a sharp Fermi surface.[10] A growing number of experiments have confirmed the existence of such a ''CF sea'' at $\nu = 1/2$.[11] Recently, Haldane and Rezayi[12] have suggested that the true ground state at $\nu = 1/2$ may actually be a ''weakly coupled'' paired CF state for the Coulomb interaction, going smoothly into the ''strongly coupled'' Pfaffian state as the pseudopotential V_3 is increased relative to its Coulomb value; the CF sea

appears as the $T > T_c$ normal state in this scenario. A pairing instability of a more complex nature has been discussed by Baskaran.[13]

Motivated by these issues, we have carried out a systematic study of five different trial wave functions. Specifically we have considered wave functions which describe the compressible spin singlet and spin polarized CF sea states,[9] the incompressible spin singlet Haldane-Rezayi[2] and Belkhir-Jain[14] states, and finally the incompressible spin polarized Pfaffian state.[8] Our principal finding is that at $\nu = 1/2$ the Pfaffian state has an energy that is surprisingly close to that of the fully polarized CF sea, and in fact, there is numerical evidence that a transition to the former may take place as a function of increasing thickness of the electron wave function perpendicular to the plane of the two-dimensional electron system.

We have performed our simulations using Haldane's spherical geometry[15] in which N electrons are confined to the surface of a sphere of radius R. A monopole at the center of the sphere produces a radial field corresponding to $2Q$ flux quanta ($\phi_0 = h/e$) piercing the surface of the sphere. The one-body eigenstates are the monopole harmonics[16] $Y_{Q,l,m}(\theta_i, \phi_i)$ where l and m are the angular momentum quantum numbers. It is also convenient to define the spinor coordinates $u_i = \cos[\theta_i/2]\exp[i\phi_i/2]$ and $v_i = \sin[\theta_i/2]\exp[-i\phi_i/2]$ where θ_i and ϕ_i are the usual spherical coordinates. For spin singlet states it will be assumed that a particle is spin up if $i \leq N/2$ and spin down if $i > N/2$. For a given ν the relationship between the number of flux quanta and the number of particles is $2Q = \nu^{-1}(N-1) - S$ where the order-unity shift S depends on the state being considered.

The CF states are the lowest LL projections of wave functions of the form (Jastrow Factor) $\times$ (Slater Determinant):

$$\psi = \mathcal{P}_{LLL}\Phi_1^2\Phi = \Phi_1^2\tilde{\Phi}. \tag{1}$$

Here, $\Phi_1 = \Pi_{i<j}(u_iv_j - v_iu_j)$, $\mathcal{P}_{LLL}$ is the lowest LL projection operator, and Φ is the $N \times N$ Slater determinant state of electrons at effective flux $q = Q - N + 1$, made of one-body eigenstates $Y_{q,l_i,m_i}(\theta_j, \phi_j)$. The lowest LL projection is car-

TABLE I. Correlation energies of the five states considered in this paper for both $\nu = 1/2$ and $\nu = 5/2$. All results have been extrapolated to the thermodynamic limit and are given in units of $e^2/\epsilon l_0$.

ν	Pfaffian (Polarized)	Composite Fermi Sea (Polarized)	Composite Fermi Sea (Singlet)	Haldane-Rezayi (Singlet)	Belkhir-Jain (Singlet)
$\frac{1}{2}$	$-0.4569(2)$	$-0.46557(6)$	$-0.46953(7)$	$-0.3147(3)$	$-0.4169(3)$
$\frac{5}{2}$	$-0.362(2)$	$-0.3492(5)$	$-0.2952(3)$	$-0.303(3)$	$-0.287(2)$

ried out following the procedure devised by Jain and Kamilla,[17] which amounts to replacing the monopole harmonics in Φ by the *projected* monopole harmonics $\widetilde{Y}_{q,l_i,m_i}(\theta_j, \phi_j)$, defined by

$$\widetilde{Y}_{q,l,m} = \mathcal{J}_i^{-1} \mathcal{P}_{LLL} \mathcal{J}_i Y_{q,l,m} \qquad (2)$$

where $\mathcal{J}_i = \Pi_{k(\neq i)}(u_i v_k - v_i u_k)$. This changes Φ into $\widetilde{\Phi}$ to give the last equality of Eq. (1). Explicit analytic expressions for $\widetilde{Y}_{q,l,m}$ are given in Ref. 17.

The spin polarized and spin singlet CF sea states have the form

$$\psi = \mathcal{P}_{LLL} \Phi_1^2 \Phi_{F.S.} \qquad (3)$$

where $\Phi_{F.S.}$ is the $N \to \infty$ limit of the $N \times N$ Slater determinant ground state of electrons at ''zero effective flux'' ($q = 0$), chosen appropriately to be either fully polarized or unpolarized. For the spin-polarized case states of progressively higher l values are filled until a closed shell configuration is reached. This occurs when $N = p^2$ where p is an integer and results have been obtained for $N = 4, 9, 16, 25,$ and 36. For the spin-singlet case each state is doubly occupied by a spin up and spin down composite fermion. The closed shell configurations then occur when $N = 2p^2$ and results have been obtained for $N = 8, 18, 32,$ and 50 electrons. The quantities for the CF sea have been obtained by an extrapolation of the finite system results.

The Haldane-Rezayi state[2] is given by $\Phi_1^2 \det M$, where M is the $N/2 \times N/2$ matrix with components $M_{ij} = (u_i v_{j+N/2} - v_i u_{j+N/2})^{-2}$ where $i,j = 1, \cdots N/2$. The other incompressible spin-singlet state we have considered is the Belkhir-Jain state,[14] $\Phi_1 \Phi_{1,1} \Phi_2$, where $\Phi_{1,1}$ is the wave function of the lowest LL with both spin up and spin down states fully occupied, and the matrix Φ_2 is an $N \times N$ Slater determinant corresponding to two filled LLs, at effective flux $2q = 2Q - (3N/2 - 2) = (N-4)/2$, constructed as if the electrons were spinless. The lowest LL projection is carried out by writing it as $\Phi_{1,1} \Phi_1^{-1} \mathcal{P}_{LLL} \Phi_1^2 \Phi_2 = \Phi_{1,1} \Phi_1 \widetilde{\Phi}_2$.

Finally, the Pfaffian state is a spin polarized FQHE state[8] which can be written as

$$\psi_{Pf} = \Phi_1^2 \mathrm{Pf}\, M \qquad (4)$$

where $\mathrm{Pf}\, M$ is the Pfaffian of the $N \times N$ antisymmetric matrix M with components $M_{ij} = (u_i v_j - v_i u_j)^{-1}$. As pointed out by Greiter *et al.*,[7] $\mathrm{Pf}\, M$ is a real space Bardeen-Cooper-Schrieffer (BCS) wave function and so ψ_{Pf} can be viewed as a p-wave paired quantum Hall state.

All of these wave functions, with the exception of the Pfaffian state, are of the form (Jastrow Factor) $\times$ (Determinant), and can be studied by standard variational Monte Carlo methods. For the Pfaffian state the identity $|\mathrm{Pf}\, M|^2 = |\det M|$ (up to an irrelevant normalization factor) can be used, and, again, standard variational Monte Carlo techniques can be applied. For each of these states the correlation energy per particle $E = (n/2) \int [g(r) - 1] V(r) d^2 r$, where n is the carrier density, $g(r)$ is the pair correlation function and $V(r)$ is the electron-electron interaction, has been calculated for systems containing up to 50 particles and the results extrapolated to the $N \to \infty$ limit.

$\underline{\nu = 1/2}$. The extrapolated Coulomb energies per particle obtained for the five states we have studied are given in Table I. Results are in units of $e^2/\epsilon l_0$ where ϵ is the dielectric constant and $l_0 = (\hbar c/eB)^{1/2}$ is the magnetic length. At $\nu = 1/2$, the lowest energy state is the singlet CF sea state, closely followed by the polarized CF sea and the Pfaffian states. The Haldane-Rezayi and Belkhir-Jain states have significantly higher energies and shall not be considered further.

The difference between the energies (per particle) of the polarized and unpolarized CF sea states is $\approx 0.004 e^2/\epsilon l_0$. In a model of noninteracting composite fermions with an effective mass m_p^* (the ''polarization mass''), this is equated to the kinetic energy difference between the polarized and unpolarized CF seas to give

$$\frac{1}{8} \frac{\hbar e B}{m_p^* c} = 0.004 \frac{e^2}{\epsilon l_0}. \qquad (5)$$

In contrast, the ''activation mass'' m_a^* of composite fermions, defined by equating the excitation gap to an effective cyclotron energy gives

$$\frac{\hbar e B}{m_a^* c} = 0.32 \frac{e^2}{\epsilon l_0},$$

implying that $m_p^*/m_a^* \approx 10$, roughly consistent with the result in Ref. 18. For typical magnetic fields, the actual ground state will be a partially polarized CF sea.

It is remarkable that the Pfaffian and polarized CF sea states are so close in energy given their qualitatively different natures. This difference can be seen in Fig. 1 in which the pair correlation functions for these two states are shown for a system with 36 electrons plotted as a function of $r k_F$ where r is the chord distance on the sphere and $k_F = l_0^{-1}$ is the Fermi wave vector of the polarized CF sea. For the pair correlation function of the CF sea one sees $2 k_F$ oscillations which fall off as a power law for large r (Refs. 19 and 20) consistent with the existence of a sharp ''Fermi surface'' of composite fermions. Similar oscillations are strongly damped for the pair correlation function of the Pfaffian state[21] which presumably approaches the asymptotic value of unity exponentially with increasing r. In going from the polarized CF
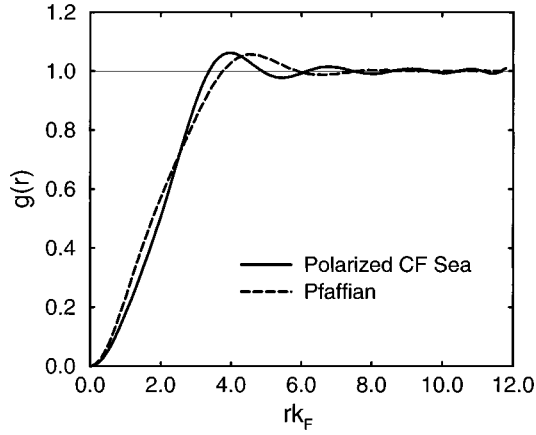
FIG. 1. Pair correlation functions for the Pfaffian and spin polarized composite Fermi sea wave functions. Results are for systems with 36 electrons.

sea to the Pfaffian state there is an increase in $g(r)$ for small r which we interpret as a signature of real space pairing correlations.

The fact that the correlation energy of the Pfaffian state is close to that of the CF sea, which in turn is believed to be an excellent representation of the true Coulomb ground state in the lowest LL, makes it plausible that the former may be relevant for an interaction not too different from the pure Coulomb interaction. (Strictly speaking, a variational study is too crude to distinguish between states with small energy differences and cannot rule out the possibility that even for the Coulomb interaction the true ground state is paired, as argued in Ref. 12, but we will assume this not to be the case in view of the facts that no FQHE is observed at $\nu = 1/2$ and that there is experimental evidence for a Fermi sea at $\nu = 1/2$.) It would be of interest to explore if a transition from the compressible CF sea to the Pfaffian may be induced at $\nu = 1/2$ by tuning some experimentally controllable parameter, e.g., the thickness of the two-dimensional electron system, which alters the detailed form of the interaction potential. To investigate this possibility we have modeled the effect of finite thickness by replacing the pure Coulomb interaction by the effective interaction,[22]

$$V(r) = \frac{e^2}{\epsilon \sqrt{r^2 + \lambda^2}}. \qquad (6)$$

The energy differences between the unpolarized CF sea and the polarized CF sea and the Pfaffian state are plotted as a function of λ/l_0 in Fig. 2. To account for the reduction of the characteristic energy scale with increasing thickness the energy difference is given in units of $e^2/\epsilon(l_0^2 + \lambda^2)^{1/2}$. For $\lambda \gtrsim 4l_0$ we find that the Pfaffian has lower energy than the fully polarized CF sea, and for $\lambda \gtrsim 5l_0$ its energy is below even that of the unpolarized CF sea. Thus we expect that, independent of whether the CF sea is fully or partially spin polarized, it should be possible to induce a transition to the Pfaffian state by increasing the thickness.

$\underline{\nu = 5/2}$. While it is conceptually straightforward to promote the above wave functions to the first excited LL, a computation of the energy is difficult due to a lack of an explicit form. We instead proceed by working with an *effec-*
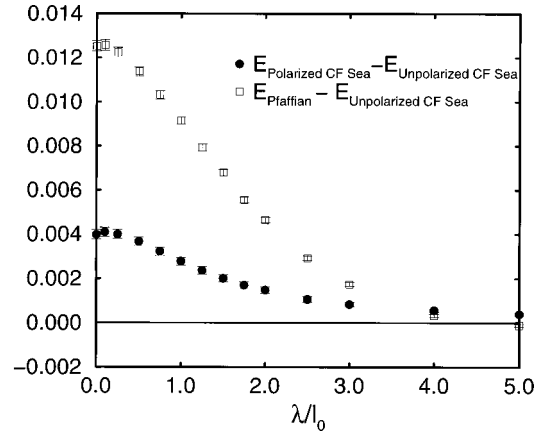

FIG. 2. Energy difference between the Pfaffian state and the unpolarized composite Fermi sea (open squares) and between the polarized and unpolarized composite Fermi sea (solid circles) vs λ/l_0 where λ characterizes the thickness of the two-dimensional electron system. Energy differences are given in units of $e^2/\epsilon(l_0^2 + \lambda^2)^{1/2}$.

tive interaction in the lowest LL, which is equivalent to the Coulomb interaction in the second LL. This interaction is derived by requiring that its pseudopotentials in the lowest LL are the same as the pseudopotentials of the Coulomb interaction in the second LL. We remind the reader that the Haldane pseudopotentials V_m (Ref. 15) are simply the correlation energies of pairs of particles in a given LL with relative angular momentum m. We have used the following effective potential,

$$V_{eff}(r) = \frac{e^2}{\epsilon} \left(\frac{1}{r} + a_1 e^{-\alpha_1 r^2} + a_2 r^2 e^{-\alpha_2 r^2} \right). \qquad (7)$$

The parameters a_1, a_2, α_1, and α_2 have been fixed by requiring that the first four pseudopotentials of $V_{eff}(r)$ for $n = 0$ be exactly equal to the first four pseudopotentials of the Coulomb repulsion for $n = 1$ (the results of this procedure are $a_1 = 117.429$, $a_2 = -755.468$, $\alpha_1 = 1.3177$ and $\alpha_2 = 2.9026$). The remaining pseudopotentials are asymptotically correct because $V_{eff}(r) \simeq e^2/\epsilon r$ for large r. The pseudopotentials for the Coulomb interaction in the $n = 1$ LL and for V_{eff} in the $n = 0$ LL are shown in Fig. 3. It can be seen clearly that the effective potential V_{eff} does an excellent job of characterizing the Coulomb interaction in the $n = 1$ LL.

The energies of various wave functions at $\nu = 5/2$ are now straightforwardly computed as before, with the results also shown in Table I. The lowest energy state here is the Pfaffian, with the spin-polarized CF sea having only slightly higher energy and all three singlet wave functions having much higher energy. The correlation energy per particle we obtain for the Pfaffian, $-0.362(2)e^2/\epsilon l_0$, is remarkably close to the extrapolated exact diagonalization calculations of Morf[6] of $-0.366e^2/\epsilon l_0$ [although it should be noted while comparing these numbers that the $V_{eff}(r)$ used in our calculations is slightly less repulsive than the actual Coulomb interaction (Fig. 3)]. We stress, however, that while the above variational calculations make the Pfaffian state plausible, more work will be required to definitively establish its relevance to the true FQHE state at $\nu = 5/2$. This is in contrast
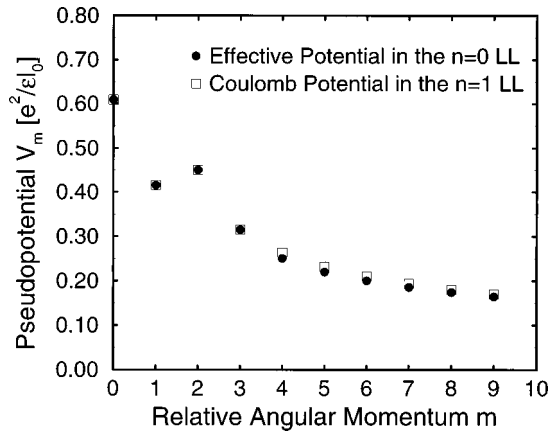
FIG. 3. Haldane pseudopotentials for the effective potential V_{eff} discussed in the text in the $n = 0$ Landau level (solid circles) and for the Coulomb potential in the $n = 1$ Landau level (open squares).

to the situation in the lowest LL FQHE where the CF wave functions have been found to have close to 100% overlap with the exact ground states.

The state which lies lowest in energy for a given potential is determined by the relative strengths of the various pseudo-potentials. The superiority of the Pfaffian wave function over the fully polarized CF sea for large thickness at $\nu = 1/2$ and for zero thickness at $\nu = 5/2$ are somewhat analogous: in both cases, the short-range part of the interaction is suppressed relative to pure Coulomb interaction. Also, the tendency for full spin polarization in the second LL may be attributed to the relatively high Coulomb energy cost of having pairs of particles with relative angular momentum $m = 2$ (Fig. 3).

To summarize, we have presented a variational Monte Carlo study of several wave functions both for $\nu = 1/2$ and $5/2$. Of the states we have considered we find that for the pure Coulomb repulsion, the spin (un)polarized CF sea is the ground state at (zero) large Zeeman coupling at $\nu = 1/2$, and the incompressible spin-polarized Pfaffian state lies lowest at $\nu = 5/2$. The possibility of a transition at $\nu = 1/2$ from the CF sea to the Pfaffian state as a function of the thickness of the two-dimensional electron system has been investigated.

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