Study of composite fermions: Beyond few particle systems

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Abstract

We construct a new representation of composite fermion wave functions in the lowest Landau level which enables Monte Carlo computations at arbitrary filling factors for a fairly large number of composite fermions, thus clearing the way toward a more detailed quantitative investigation of the fractional quantum Hall effect. As an illustrative application, thermodynamic estimates for the transport gaps of several spin polarized incompressible states have been obtained.

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Interacting electrons confined to two dimensions and subjected to a strong magnetic field exhibit spectacular phenomena, e.g., the fractional quantum Hall effect (FQHE) [1]. A rather simple and succinct qualitative explanation of these phenomena is given in terms of objects called composite fermions [2], which are electrons bound to an even number of vortices of the many body wave function. The FQHE is a manifestation of the Landau level (LL) structure of composite fermions, and several recent experiments [3] have produced striking additional evidence for composite fermions by detecting their semiclassical cyclotron orbits in the vicinity of the half filled LL [4].

A detailed quantitative description of the FQHE and related phenomena is less than satisfactory, however. It relies largely on exact diagonalization studies [5,6], which have played an extremely useful role in testing and confirming various theoretical postulates, but whose predictive power is rather limited as they typically deal with systems containing fewer than 10-12 electrons. Not only is this insufficient for making reliable thermodynamic estimates in most cases, a large region of filling factors is totally inaccessible in such small systems. To see this, take the conventional spherical geometry. Here, the $n/(2n+1)$ FQHE state requires at least $n^2$ electrons (which is the minimum number of composite fermions needed to fill $n$ LLs). As a result, only two data points are available for $3/7$ ($N = 9$ and 12) in present exact diagonalization studies, and $4/9$, $5/11$, etc. do not show up at all. The situation is worse for the $n/(4n+1)$ sequence – even $3/13$ is out of reach. Due to an exponential increase with the number of electrons in the computer time and memory requirements, it is unlikely that exact diagonalization studies will tell us much more in the future.

A more promising approach toward the goal of a better quantitative description of the FQHE is to work with the composite fermion (CF) wave functions, which have been shown to be remarkably close to the exact solutions [7] and are expected to yield thermodynamic estimates for various quantities correct to within a few percent. Due to technical difficulties, however, it has not been possible in the past to work with these wave functions for more than $\sim 10$ composite fermions [8] and, as a result, the CF theory has also in general failed
to provide quantitative information beyond what was known from exact diagonalization studies. In this Letter, we develop a new representation of the CF wave functions which enables computations for rather large CF systems. We report below results for as many as 40 composite fermions; treatment of much bigger systems should be possible in the future. This constitutes a significant step in our ability to achieve detailed quantitative predictions for the FQHE. As a first application of this method, we have computed the transport gaps for several FQHE states of interest.

The approach described below has been tested in both the disk (planar) and spherical geometries; here we will discuss only the latter due to space constraint. This geometry considers \( N \) electrons on the surface of a sphere moving under the influence of a radial magnetic field. The single particle eigenstates are the monopole harmonics \( Y_{q,n,m} \), which, after a bit of algebra, can be expressed as

\[
Y_{q,n,m}(\Omega_j) = N_{qnm}(-1)^{q+n-m}2^m e^{iq\phi_j} u_j^{q+m} v_j^{q-m} \sum_{s=0}^{n} (-1)^s \binom{n}{s} \binom{2q+n}{q+n-m-s} (v_j^* v_j)^{n-s} (u_j^* u_j)^s ,
\]

where \( \Omega_j \) represents the angular coordinates \( \theta_j \) and \( \phi_j \) of the \( j \)th electron, the total flux through the sphere is equal to \( 2q\phi_0 \) (\( 2q \) is an integer and \( \phi_0 = hc/e \)), \( n = 0, 1, 2, \ldots \) is the LL index, \( m = -q-n, -q-n+1, \ldots, q+n \) labels the degenerate states in the \( n \)th LL, and \( l = q+n \). It is understood here and below that the binomial coefficient \( \binom{\gamma}{\beta} \) vanishes if either \( \beta > \gamma \) or \( \beta < 0 \). The spinor coordinates are defined as \( \left[12\right] u_j \equiv \cos(\theta_j/2) \exp(-i\phi_j/2) \) and \( v_j \equiv \sin(\theta_j/2) \exp(i\phi_j/2) \) \( [13] \).

The CF theory postulates that the strongly correlated liquid of interacting electrons is equivalent to a weakly interacting gas of composite fermions. The \( (2p) \) vortices bound to electrons have the effect of partly cancelling the external field, and the composite fermions effectively experience a reduced magnetic field, given by \( B^* = B - 2\rho p \phi_0 \), where \( B \) is the external field, and \( \rho \) is the electron density. Equivalently, the effective filling factor of
composite fermions ($\nu^*$) is related to the electron filling factor $\nu$ by $\nu = \nu^*/(2p\nu^* + 1)$ and, in particular, the FQHE of electrons at $\nu = n/(2pn + 1)$ is a manifestation of the $\nu^* = n$ integer QHE (IQHE) of composite fermions. The (unprojected) wave function for the CF state at $\nu^*$, $\Phi'_{CF}$, is related to that of the electron state at $\nu^*$, $\Phi$, as

$$\Phi'_{CF} = J\Phi,$$

where the Jastrow factor is given by

$$J \equiv \prod_{j<k} (u_j v_k - v_j u_k) \exp[ip(\phi_j + \phi_k)].$$

One problem with $\Phi'_{CF}$ is that it is, in general, not strictly in the lowest LL (LLL), and thus cannot be used as a good quantitative representation of the electron state at $\nu$ in the high $B$ limit. This is remedied by simply throwing away the part of the wave function that involves higher Landau levels and working with the remaining wave function $\mathcal{P}\Phi'_{CF}$, where $\mathcal{P}$ is the LLL projection operator. It has been demonstrated to be very accurate by comparison with exact solutions available numerically for small systems [7]. However, in spite of several attempts, it has not been possible to compute with $\mathcal{P}\Phi'_{CF}$ for large CF systems, as would be necessary for exploiting the full quantitative potential of the CF theory.

Let us outline the basic philosophy behind our approach. There are compelling theoretical and experimental reasons to believe that $\Phi'_{CF}$ contains the correct physics and is adiabatically connected to the true electron wave function in the lowest LL. Moreover, it has only a small fraction of electrons outside of the lowest LL [14]. Therefore, the objective is to obtain a LLL wave function from $\Phi'_{CF}$ without disturbing it violently. There is nothing a priori to choose from between various methods that accomplish this goal; of course the accuracy of the resulting LLL wave function must be established by comparison with exact solutions. The principal result of this work is that we have constructed a LLL wave function for composite fermions different from $\mathcal{P}\Phi'_{CF}$ but comparably accurate and, most importantly, much easier to compute with.

For simplicity, we will consider below only states for which $\Phi$ is a single Slater determinant, $\Phi = Det[Y_i(\Omega_j)]$; generalization to the case where $\Phi$ is a linear superposition of Slater
determinants is straightforward. Then,

\[ \Phi'_\text{CF} = J \, \text{Det}[Y_i(\Omega_j)] \]  

(5)

We write the Jastrow factor as

\[ J = \prod_{j \neq k} (u_j v_k - v_j u_k)^p \exp[i \frac{P}{2}(\phi_j + \phi_k)] = \prod_j J_j^p, \]  

(6)

with

\[ J_j = \prod_k (u_j v_k - v_j u_k) \exp[i(\phi_j + \phi_k)] , \]  

(7)

where the prime denotes the condition \( j \neq k \). \( J_j \) has the property that when expanded in terms of a linear superposition of single particle eigenstates of the \( j \)th electron, all eigenstates correspond to the same monopole strength \( q' = (N - 1)/2 \) (although with different \( m' \)). The Jastrow factor can now be incorporated into the Slater determinant to give

\[ \Phi'_\text{CF} = \text{Det}[Y_i(\Omega_j) J_j^p] . \]  

(8)

Now, instead of projecting the determinant on to the lowest LL, as had been done previously, we project each matrix element individually to write

\[ \Phi_{\text{CF}} = \text{Det}[\mathcal{P} Y_i(\Omega_j) J_j^p] . \]  

(9)

Since the product of two LLL wave functions is also in the lowest LL, \( \Phi_{\text{CF}} \) is guaranteed to be in the lowest LL. In order to evaluate the projection \( \mathcal{P} Y_{q,n,m}(\Omega_j) J_j^p \), we first show that there exists an operator \( \mathcal{Y}_{q,n,m} \) satisfying the property that

\[ \mathcal{P} Y_{q,n,m} = \mathcal{Y}_{q,n,m} \mathcal{Y}_{q',0,m'} - \mathcal{Y}_{q',0,m'} \mathcal{Y}_{q,n,m} , \]  

(10)

where \( Y_{q',0,m'} \sim e^{i q' \phi_j} u_{j}^{q'+m'} v_{j}^{q'-m'} \) is a LLL wave function at monopole strength \( q' \). For the present purposes, it is important that \( \mathcal{Y}_{q,n,m} \) be independent of \( m' \). To this end, we multiply one of the terms on the right hand side of Eq. (10) by the LLL wave function \( Y_{q',0,m'} \) and write (with \( Q \equiv q + q' \), \( M \equiv m + m' \), and the subscript \( j \) suppressed):

5
For $|M| > Q$, $a_0$ must vanish, since $|M| \leq Q$ in the lowest LL. Let us first consider the case $|M| \leq Q$. Multiplying both sides by $e^{-iQ\phi}u^{*Q+M}v^{*Q-M}$ and integrating over the angular coordinates gives

$$a_0 = \frac{(Q - M + n - s)!(Q + M + s)!(2Q + 1)!}{(Q + M)!(Q - M)!(2Q + n + 1)!}.$$  (12)

This shows that, apart from an $m'$-independent multiplicative constant $(2Q + 1)!/(2Q + n + 1)!$, the LLL projection of the left hand side of Eq. (11) can be accomplished by first bringing all $u^*$ and $v^*$ to the left and then making the replacement

$$u^* \rightarrow \frac{\partial}{\partial u}, \ v^* \rightarrow \frac{\partial}{\partial v}.$$  (13)

While this prescription is not valid in general for $|M| > Q$, it can be shown to produce the correct result (i.e., zero) even for $|M| > Q$ for the LLL projection of states of the form $Y_{q,n,m}Y_{q',0,m'}$: all terms with non-zero binomial coefficients have the form $(\frac{\partial}{\partial u})^\alpha u^\beta (\frac{\partial}{\partial v})^\gamma v^\delta$ with either $\alpha > \beta$ (for $M < Q$) or $\gamma > \delta$ (for $M > Q$), and consequently vanish. Thus,

$$Y'_{q,n,m} = \frac{(2Q + 1)!}{(2Q + n + 1)!} N_{qnm}(-1)^{q+n-m}2^m e^{iq\phi},$$

$$\sum_{s=0}^n (-1)^s \binom{n}{s} \binom{2q + n}{q + n + m - s} \left(\frac{\partial}{\partial u}\right)^s u^{q+m+s} \left(\frac{\partial}{\partial v}\right)^{n-s} v^{q-m+n-s}.$$  (14)

A delightful simplification occurs when one brings all the derivatives to the right in Eq. (14) using

$$\left(\frac{\partial}{\partial v}\right)^\gamma v^\gamma = \sum_{\alpha=0}^\beta \frac{\beta!}{\alpha!} \left(\frac{\partial}{\partial v}\right)^{\gamma-\beta+\alpha},$$  (15)

and a similar equation for the derivative with respect to $u$ (with the summation index $\alpha'$).

The sum over $s$ in Eq. (14) then takes the form

$$\sum_{s=\alpha'}^{n-\alpha} (-1)^s \binom{n - \alpha - \alpha'}{s - \alpha'} = \sum_{s'=0}^{n-\alpha-\alpha'} (-1)^{\alpha'+s'} \binom{n - \alpha - \alpha'}{s'},$$  (16)

which is equal to $(-1)^{\alpha'}(1 - 1)^{n-\alpha-\alpha'}$ and vanishes unless $n = \alpha + \alpha'$. The only term satisfying this condition is one with $\alpha = n - s$ and $\alpha' = s$. Consequently, the derivatives
in Eq. (14) can be moved to the extreme right and act only on the following LLL wave function. Specializing to the case where \( Y_{q,n,m} \) acts on \( J^p_j \), we write

\[
\left( \frac{\partial}{\partial u_j} \right)^s \left( \frac{\partial}{\partial v_j} \right)^{n-s} J^p_j = J^p_j R^{s,n-s}_j ,
\]

where

\[
R^{s,n-s}_j = U^s_j V^{n-s}_j ,
\]

\[
U_j = J^{-p}_j \frac{\partial}{\partial u_j} J^p_j = p \sum_k \frac{v_k}{u_j v_k - v_j u_k} + \frac{\partial}{\partial u_j} ,
\]

\[
V_j = J^{-p}_j \frac{\partial}{\partial v_j} J^p_j = p \sum_k \frac{-u_k}{u_j v_k - v_j u_k} + \frac{\partial}{\partial v_j} .
\]

Substituting in Eq. (9) and factoring out the mini-Jastrow factors \( J_j \) to produce back the full Jastrow factor finally gives

\[
\Phi_{CF} = J \text{Det}[\tilde{Y}_i(\Omega_j)] ,
\]

which has the same form as the unprojected wave function \( \Phi'_{CF} \) in Eq. (5) except that each \( Y \) has been replaced by \( \tilde{Y} \), given by

\[
\tilde{Y}_{q,n,m}(\Omega_j) = N_{qnm} (-1)^{q+n-m} 2^m (2Q + 1)! (2Q + n + 1)! e^{iq \phi_j} u^{q+m}_j v^{q-m}_j \sum_{s=0}^{n} (-1)^s \binom{n}{s} \binom{2q + n}{q + n - m - s} v^{n-s}_j u^{s}_j R^{s,n-s}_j .
\]

A consequence of the LLL projection is that changing the coordinates of one particle alters all elements of the Slater determinant in \( \Phi_{CF} \), as \( R_j \) depends on all particle coordinates. As a result, certain time saving tricks for updating the Slater determinant [15] at each step of the Monte Carlo cannot be used here and the full determinant must be evaluated at each step. This increases the computation time enormously (as compared to Monte Carlo on \( \Phi'_{CF} \)), but it is still possible to deal with much bigger systems than before.

Of course, the usefulness of \( \Phi_{CF} \) hinges critically on how precisely it approximates the true electron state. We resort to small systems to answer this question. Here and below, we
will assume fully polarized electrons confined to the lowest LL. The Coulomb energy of $\Phi_{CF}$, obtained by Monte Carlo, along with the corresponding exact ground state energy is given in Table I for several incompressible states. A comparison establishes the extreme accuracy of $\Phi_{CF}$.

We are now in a position to make detailed quantitative predictions for a number of experimentally measurable quantities in the FQHE. We consider in this paper the (transport) gaps of FQHE states belonging to the principal sequence $\nu = n/(2n + 1)$. The gaps of the 1/3 and 2/5 states have been known quite well from exact diagonalization studies \[5,6\]; the gap of 3/7 is known with a large (40%) uncertainty \[6\]; and no estimates exist for 4/9, 5/11, etc. From a different perspective, Halperin et al. \[4\] have suggested, based on particle-hole symmetry in the lowest LL and the earlier known numerical results, that the gaps of the $n/(2n + 1)$ states are given by the equation

$$E_g = C \left| \frac{2n + 1}{2n + 1} \right| e^2\ell,$$

with $C \approx 0.31$. There is also experimental support for such behavior \[16\]. Equating $E_g$ to the effective cyclotron energy of composite fermions, $\hbar eB^*/m^*c$, motivated by a mean-field description of composite fermions, produces an effective mass of composite fermions that scales as $m^* \sim \sqrt{B}$ \[4\].

The gap of the FQHE state at $\nu = n/(2n + 1)$ is equal to the energy required to create a far separated CF particle-hole pair. The ground state has $n$ filled LL’s of composite fermions and the excited state is obtained by taking one composite fermion out from the south pole of the $n$th CF-LL and placing it on the north pole of the $(n + 1)$th CF-LL (to maximize the distance between the CF-particle-hole pair). Since the gap, an $O(1)$ energy, is obtained as the difference between two large $O(N)$ energies, its accuracy is expected to be much less than that of either the ground state or the excited state energy. To get a feel for how well the CF theory does here, Table II quotes the gaps predicted by the CF theory for some of the largest systems for which exact gaps are also known; a comparison indicates that the error in the thermodynamic limit is expected to be within a few percent, typically much smaller.
than the statistical uncertainty of our Monte Carlo. We proceed to compute the gaps for 2/5, 3/7, 4/9 and 5/11 as a function of \( N \) [17]. Fig. 1 shows the results for 3/7 and 4/9. Each error bar signifies one standard deviation, as determined from the average gaps from ten Monte Carlo runs. The thermodynamic estimates, shown in Fig. 2, have been obtained using a chi-square fitting that biases the points by their error bars. For \( \nu = 3/7 \) the gap is consistent with the earlier estimate, although with much smaller uncertainty. The overall behavior of the gaps is in good agreement with Eq. (23), as seen in Fig. 2. It should be noted that the experimental values of the gaps are reduced by various unavoidable effects, e.g., finite width of the quantum well [18], LL mixing [19] and disorder, and the present estimates are actually only the upper bounds. The finite well width softens the Coulomb interaction at short distances, which is straightforward to incorporate into our Monte Carlo and will be the subject of a future work. LL mixing is harder to deal with. Fixed phase Monte Carlo [20] or a variational approach considering a linear combination of \( \Phi'_CF \) and \( \Phi_{CF} \) [21] may be useful in this context.

In summary, we have developed an approach that permits an investigation of large CF systems and thereby makes accessible previously unexplored regions of the FQHE. We believe that it will prove extremely useful toward a better quantitative understanding of the FQHE.

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that in Eq. (1) for which a number of simplifications are obtained.

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Table Caption

Table I. Comparison between the energy per particle of the CF wave function $\Phi_{CF}$ and the exact Coulomb energy for the ground states at $\nu = 2/5$ and $3/7$. The energies are in units of $e^2/\epsilon\ell$, where $\ell$ is the magnetic length and $\epsilon$ is the background dielectric constant, and include interaction with the uniformly charged positive background. The energy of $\Phi_{CF}$ has been evaluated by Monte Carlo, with the statistical uncertainty in the last two digits shown in brackets. The exact results for $N = 12$ and $\nu = 3/7$ are taken here and in Table II from S. He, S.H. Simon and B.I. Halperin, Phys. Rev. B 50, 1823 (1994).

Table II. The gap to create a CF-particle-hole excitation in which a composite fermion is removed from the south pole of the topmost filled CF-LL and placed on the north pole of the lowest empty CF-LL. The exact gaps are also given; the gap at $\nu = 2/5$ for $N = 10$ has been read off from the spectrum in Ref. [6].

Figure Captions

Fig. 1. The energy gaps (in units of $e^2/\epsilon\ell$) at $3/7$ and $4/9$ for several $N$. In order to minimize finite size effects, the interaction energy of two appropriately charged pointlike particles situated at the two poles has been subtracted from the gaps here (compared to those quoted in Tables I and II), following [5,6].

Fig. 2. Thermodynamic values of the gaps plotted as a function of $1/(2n + 1)$. The gap for $\nu = 1/3$ is taken from Ref. [8]. The straight line is a chi-square fit, given by $E_g = -0.001(5) + 0.320(2)(2n + 1)^{-1}$. 
| $\nu$ | $N$ | CF energy   | exact energy |
|-------|-----|-------------|--------------|
| 2/3   | 6   | -0.500339(42) | -0.5004002   |
|       | 8   | -0.480216(33) | -0.4802436   |
| 3/7   | 9   | -0.499138(71) | -0.4991843   |
|       | 12  | -0.482507(49) | -0.4826388   |

**TABLE I**

| $\nu$ | $N$ | CF gap     | exact gap   |
|-------|-----|------------|-------------|
| 2/3   | 6   | 0.07615(61) | 0.07505     |
|       | 8   | 0.07021(87) | 0.06809     |
|       | 10  | 0.0681(12)  | 0.0673(7)   |
| 3/7   | 9   | 0.0691(14)  | 0.0681      |
|       | 12  | 0.0518(12)  | 0.0525      |

**TABLE II**
