Paired composite fermion wavefunctions

G. Möller[1] and S. H. Simon[2]
[1] *Theory of Condensed Matter Group, Cavendish Laboratory, J. J. Thomson Ave., Cambridge CB3 0HE, UK*
[2] *Bell Laboratories, Alcatel-Lucent, Murray Hill, New Jersey 07974*
(Dated: August 20, 2007)

We construct a family of BCS paired composite fermion wavefunctions that generalize, but remain in the same topological phase as, the Moore-Read Pfaffian state for the half-filled Landau level. It is shown that for a wide range of experimentally relevant inter-electron interactions the groundstate can be very accurately represented in this form.

The nature of the fractional quantum Hall effect at $\nu = \frac{5}{2}$ has been the subject of continued interest since its discovery roughly two decades ago [1]. The Moore-Read Pfaffian wavefunction [2], describing p-wave pairing of composite fermions [3], is currently the best candidate wavefunction for this state [4, 5]. Due to the remarkable property of having quasi-particles with non-abelian statistics, this state has recently attracted interest in the context of fault-tolerant topological quantum computation [6]. Though the Moore-Read state is a well established candidate for the groundstate at $\nu = \frac{5}{2}$, its overlap with the exact groundstate in simulations of small systems is rather low in comparison to other known trial states at different filling factors [4, 5]. This is particularly discomforting as no explicit construction for perturbations around the Moore-Read state has been previously available, and the Moore-Read state has been described as a somewhat unique choice [3]. Furthermore several recent studies have altogether challenged the view of $\nu = \frac{5}{2}$ as being the Moore-Read state [7, 8].

In this Letter, we introduce a general representation of paired composite fermion (CF) states, merging the concept of BCS Hall states [9] with the explicit construction of CF wavefunctions [10, 11]. The Moore-Read state can be cast very accurately in this form, which reveals its connection to the pairing of composite fermions on top of a Fermi-sea, and shows how our general paired CF-BCS wavefunctions are adiabatically connected to Moore-Read. We also compare our trial states to the exact groundstates of the Coulomb Hamiltonian $\mathcal{H}_C$ for electrons in the 1^{st} excited Landau level (1LL), plus an arbitrary additional pseudopotential δV_1 interaction. For a very broad range of δV_1 we find very high overlap of our trial wavefunctions with the exact groundstate, thus showing the extent of the Moore-Read phase.

For our description of the physics at $\nu = \frac{5}{2}$, we shall assume the lowest Landau level (LLL) to be entirely filled and inert, such that the relevant degrees of freedom correspond to a half filled 1LL. We assume the spin degree of freedom of these electrons to be frozen (although the experimental situation is less clear [12]). The 1LL is represented by wavefunctions in the LLL using appropriately modified pseudopotential coefficients [13].

The aim of our construction is to "composite fermionize" a simple BCS state. In second quantized notation, the general form of the BCS groundstate is [14] $|\Psi_{\rm BCS}\rangle = \prod_{\mathbf{k}} \left(1 + g_{\mathbf{k}}\, e^{i\varphi}\, c^\dagger_{\mathbf{k}} c^\dagger_{-\mathbf{k}}\right)|0\rangle$, written in an unnormalized manner here. This wavefunction can be projected to a fixed number of particles by integration over $\int \mathrm{d}\varphi\, \exp(-iN\varphi)$ such that we retain exactly N pair creation operators. The (inverse) Fourier transform into real space then yields [14]

$$\Psi_{\rm BCS}(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \mathfrak{Pf}\left[g(\mathbf{r}_i - \mathbf{r}_j)\right], \qquad (1)$$

where the Pfaffian $\mathfrak{Pf}$ is an antisymmetrized sum over all possible pairings $\mathfrak{Pf}(g_{ij}) = \mathcal{A}[g_{12}g_{34}\ldots g_{N-1,N}] = \pm\sqrt{|\det g_{ij}|}$ with $\mathcal{A}$ the antisymmetrization operator. In Eq. 1, g is constrained to be an antisymmetric function, given in terms of its Fourier components by

$$g(\mathbf{r}_i - \mathbf{r}_j) = \sum_{\mathbf{k}} g_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \equiv \sum_{\mathbf{k}} g_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{r}_i)\phi_{-\mathbf{k}}(\mathbf{r}_j). \quad (2)$$

For the last equivalence, we have identified the exponential factor as the product of two basis functions $\phi_{\mathbf{k}}(\mathbf{r}) = \exp(i\mathbf{k}\cdot\mathbf{r})$ of free electrons on the plane. This product of free wavefunctions form is naturally generalized to spherical geometry below.

In order to obtain a LLL wavefunction at filling factor $\nu = \frac{1}{2}$, we follow Jain's approach [10] of multiplying a bare electron wavefunction with Jastrow factors, and projecting the result to the LLL, yielding [15]

$$\Psi_0^{\rm CF}(z_1, \ldots, z_N) = \mathcal{P}_{\rm LLL}\left\{\mathfrak{Pf}\left[g(\mathbf{r}_i - \mathbf{r}_j)\right]\prod_{i<j}(z_i - z_j)^2\right\}$$

where $\mathcal{P}_{\rm LLL}$ is the LLL projection operator, and z_i is the complex representation of $\mathbf{r}_i$. The special case $g = 1/(z_i - z_j)$ reproduces the Moore-Read wavefunction (and the projection then becomes trivial).

In order to render the projection $\mathcal{P}_{\rm LLL}$ numerically tractable in general, we bring single particle Jastrow factors $J_i = \prod_{k\neq i}(z_i - z_k)$ inside the Pfaffian on every line i and every column j of the matrix g_{ij}, and project each of the matrix elements individually [11]. As demonstrated in Ref. [11], such slight changes in the projection prescription do not alter the accuracy of the composite fermionization procedure. It is thus expected that projecting matrix elements $[g(\mathbf{r}_i - \mathbf{r}_j)J_iJ_j]$ individually is very similar

to a projection of the full wavefunction. For further simplification, one can decompose g analogous to Eq. 2, and apply the projection separately to each of the orbitals $\phi_{\mathbf{k}}$ as suggested in Ref. [11]. Again this slight change in projection prescription is not expected to damage our wavefunction. Denoting $\tilde{\phi}_{\mathbf{k}}(z_i) = J_i^{-1}\mathcal{P}_{\rm LLL}[\phi_{\mathbf{k}}(z_i)J_i]$, Jastrow factors may be factored again outside the Pfaffian, and we obtain the final expression for general composite fermionized BCS (CF-BCS) states

$$\Psi^{\rm CF} = \mathfrak{Pf}\left[\sum_{\mathbf{k}} g_{\mathbf{k}}\,\tilde{\phi}_{\mathbf{k}}(z_i)\,\tilde{\phi}_{-\mathbf{k}}(z_j)\right]\prod_{i<j}(z_i-z_j)^2. \quad (3)$$

In the remainder of this study we will focus on finite size systems with N electrons on the spherical geometry [13]. In order for Eq. 3 to represent the Moore-Read phase, we must work at a flux of $N_\phi = 2N-3$. The orbitals $\phi_{\mathbf{k}}$ thus correspond to composite fermions in one quantum of negative effective flux [16], ie., the (very small) effective magnetic field experienced by CF's is directed opposite to the external magnetic field. The relevant CF orbitals ($\tilde{\phi}_{\mathbf{k}}$) are given by the projected monopole harmonics $\tilde{Y}^{q=-\frac{1}{2}}_{n,m}$ studied in Ref. [16]. To assure [9] that the angular momentum of a pair is $l=-1$ (the negative p-wave pairing of the Moore-Read phase) we must choose $g_{\mathbf{k}} \to (-1)^{q+m}g_n$ and we are left with only one variational parameter g_n per CF shell. Thus the term in the brackets of Eq. 3 becomes $\sum_{n,m}(-1)^{m-1/2}g_n\tilde{Y}^{q=-\frac{1}{2}}_{n,m}(z_i)\tilde{Y}^{q=-\frac{1}{2}}_{n,-m}(z_j)$. The sum over n goes from $n=0$ to $n=N-2$ since orbitals with $n \geq N-1$ are projected to zero. Thus, up to an overall normalization, there are $N-2$ variational parameters.

It is also possible to study other pairing symmetries within our approach. These would yield states at different values of the flux N_ϕ. Here, we focus on negative p-wave pairing, which appears most consistent with previous numerical data [4, 5].

The variational character of the wavefunctions we study (Eq. 3) implies that we need to optimize over the set of parameters $\vec{g} \equiv (g_0, g_1, g_2, \ldots, g_{N-2})$ to obtain a good trial wavefunction. The definition of a "good" wavefunction is somewhat arbitrary, and one may attempt to optimize various measures of its accuracy, e.g. the energy of the wavefunction, the overlap with the exact groundstate, or the error in the pair correlation function compared to the exact groundstate. The chosen measures of accuracy are evaluated by Monte-Carlo, and the variational parameters are then optimized.

It is instructive to verify that the Moore-Read state can be reproduced as a CF-BCS state (Eq. 3). Numerically we find that for a suitable set of variational parameters, $\vec{g}$, we are able to achieve overlaps in excess of 0.99 with the Moore-Read state for systems with up to 20 electrons. While this may seem a rather complicated reformulation of the Moore-Read state, we can now perturb the wavefunction with our variational parameters.

Fig. 1 shows overlaps between trial states and the corresponding exact groundstates for different interactions parametrized by the pseudopotential δV_1 (with $\delta V_1 = 0$ being the pure Coulomb interaction in the 1LL, and very large δV_1 roughly corresponding to the interaction of the LLL). We also show overlaps of the exact groundstate with the Moore-Read state and the CF liquid (CFL) (here defined to be Eq. 3 with the occupation coefficients g_n being unity below the chemical potential and zero above). Results are shown for $N = 12, 14, 16$. The dimensions of the $L=0$ Hilbert space are respectively $d = 52, 291, 2077$. Although we could in principle optimize over as many as $N-2$ variational parameters, in practice we find very good wavefunctions using at most the first 7 parameters. We remind the reader that the variational parameters are included (like the u's and v's of BCS theory) to optimize the shape of the pairing wavefunction. Note that the number of parameters used is far less than the dimension of the $L=0$ Hilbert space, so the good agreement with exact diagonalization is significant. Further we emphasize that the trial states (Eq. 3) have very high overlap with the exact groundstate for a wide range of values of δV_1.

For a particular value of $\delta V_1 \approx 0.04$ the Moore-Read state is also a very good trial state. However even at this value of δV_1, our trial states yield an improved representation of the exact groundstate. For larger δV_1 the CF-BCS states become even more accurate and can be continuously deformed into the composite fermion liquid at large δV_1. As shown in Fig. 1 when δV_1 gets close to zero (or negative, not shown) the overlap drops. This behavior could be expected considering prior work [5] showing a nearby phase transition, as we discuss below.

As mentioned above, overlaps are not the only possible measure of the accuracy of a wavefunction. In Fig. 2, we show how the pair correlation functions $h(\theta)$ of different trial states compare against those of the exact groundstate. Here θ is the angle between two particles on the sphere, and we show the mean square error in the correlation function $\delta h^2 = \int {\rm d}(\cos\theta)\,|h(\theta) - h_{\rm exact}(\theta)|^2$. We note that if $\delta h^2 = 0$ for a trial state, then it is identical to the exact groundstate (this can be seen from the variational principle, noting that $h(\theta)$ fully determines the energy for a two-body interaction). Fig. 2 once more illustrates that our trial wavefunctions are extremely accurate – far more so than either the Moore-Read or CFL trial states. Again, we find that near $\delta V_1 = 0$ our trial state fails to match the exact pair correlation function to some extent.

In Fig. 2, the trial wavefunctions have been reoptimized with respect to δh^2. The overlaps of these new wavefunctions with the exact groundstate, would generally be found to be slightly lower than those in Fig. 1, but still remain very high (except in the vicinity of $\delta V_1 = 0$).

Since, as mentioned above, we can continuously deform our wavefunctions to have over .99 overlaps with the Moore-Read state, we conclude that our CF-BCS wave-

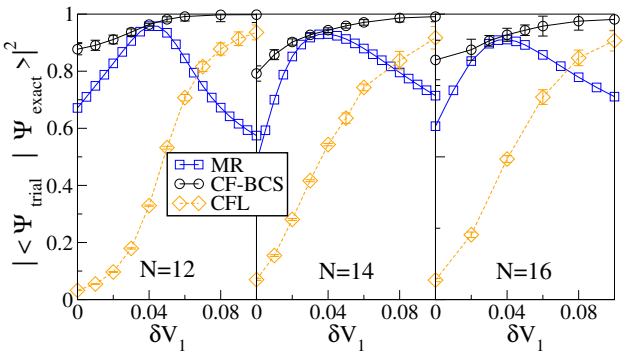

FIG. 1: (color online) Overlaps of trial states with exact groundstate as a function of the interaction parameter δV_1 for $N = 12, 14$ and 16 electrons. Here, $\delta V_1 = 0$ corresponds to the pure Coulomb interaction in the 1LL. The optimized composite-fermionized BCS wavefunctions (Eq. 3, black circles) have very high overlap except close to $\delta V_1 = 0$, where the system is thought to be close to a phase transition. The Moore-Read wavefunction (blue squares) is also good near $\delta V_1 = 0.04$, but falls off substantially at other values. The composite fermion liquid wavefunctions (orange diamonds) are accurate at very high δV_1 only. Error bars indicate statistical errors where a Monte-Carlo algorithm was employed for the evaluation of the overlaps. The high accuracy of the BCS wavefunctions over a broad range of interactions shows the large extent of the weak-pairing phase.

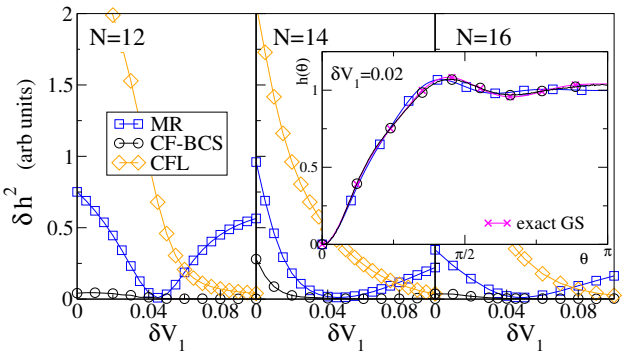

FIG. 2: (color online) Squared error δh^2 in the pair correlation function of various trial wavefunctions compared with exact groundstates as a function of the interaction parameter δV_1 for $N = 12, 14$ and 16 electrons. Symbols are as in Fig. 1. Again we find that composite-fermionized BCS wavefunctions are far more accurate than either Moore-Read or the CF liquid. Inset: Pair correlation functions $h(\theta)$ of the Moore-Read state and our trial wavefunction along with the exact groundstate at $N = 14$ and $\delta V_1 = 0.02$. Our trial state is essentially indistinguishable from the exact groundstate, whereas the Moore-Read state is slightly different.

functions are generally in the same so-called weak-pairing phase as the Moore-Read state. To further emphasize this point, we note that a wavefunction in a weak-pairing phase should have the property that $g(\mathbf{r}) \sim 1/z$ at large distances $\mathbf{r}$ [9]. While this is not obvious from the form of Eq. 3 (particularly considering the complexity of the projected wavefunctions $\tilde{\phi}$) we can nonetheless establish it is true in several ways. Firstly, we have tried making the $1/z$ tail of the pair correlation function explicit, writing $g(\mathbf{r}_i - \mathbf{r}_j) = a/(z_i - z_j) + f(\mathbf{r}_i - \mathbf{r}_j)$ before projection, decomposing only the function f into orbitals as in Eq. 2 and projecting these orbitals. We have found that this procedure leads to equivalent results. Secondly, the property $g(\mathbf{r}) \sim 1/z$ at large $\mathbf{r}$ implies that the $\mathbf{k} \to 0$ orbitals are occupied with probability approaching unity [9] (which would not be true of a strong pairing phase). It is easy for us to establish numerically that the lowest orbitals ($n = 0$) are indeed fully occupied unity by testing that increasing the value of the variational parameter g_0 does not change the wavefunction.

It is also worth checking that the exact groundstate is indeed adiabatically connected to the Moore-Read state. To this end, we analyze the evolution of the energy gap for a family of Hamiltonians that interpolate between the three-body contact interactions $\mathcal{V}_3$, which yield the Moore-Read state as its exact groundstate, and a two-body interaction Hamiltonian $\mathcal{H}'_C$ corresponding to $\delta V_1 = 0.04$. In particular, for any of the interactions $\mathcal{H}(x) = x\mathcal{V}^3 + (1-x)\mathcal{H}'_C$, we find no indication that in the thermodynamic limit the energy gap closes (data not shown). We conclude that the exact groundstate of $\mathcal{H}'_C$ is adiabatically connected to the Moore-Read state, confirming that the exact groundstate of $\delta V_1 = 0.04$ is in the weak pairing phase [9].

The main result of this work is the construction of a family of accurate wavefunctions in the same topological phase as the Moore-Read wavefunction. This can be thought of as the composite fermionization of a weakly paired BCS wavefunction. We find that over a broad range of interactions these wavefunctions are very accurate – far more so than the Moore-Read wavefunction itself, which should be thought of only as an example of a wavefunction in a broad phase of matter. Indeed, the Moore-Read state may be approximated extremely precisely by the form we propose, and when doing so, the result does not particularly stand out from other possible CF-BCS states. Although from a topological standpoint, it is sufficient to identify the phase of matter, from a practical standpoint, it is still valuable to have explicit forms of wavefunctions [10, 11], as this is important for performing detailed calculations of excitation spectra and other physical properties. Although we have currently only analyzed the composite fermionization of groundstate BCS wavefunctions, it is natural to consider a similar procedure for excited states, which we will consider in future work.

Let us now discuss how our work reflects on and relates to previously results. Prior work on the torus [5] found a first order phase transition from a charge density wave (CDW) state to a phase presumed to be the Moore-

Read phase at roughly the Coulomb point $\delta V_1 = 0$. This phase had the required degeneracy of a weak pairing (Moore-Read) phase, but had relatively low overlaps with the Moore-Read wavefunction itself. Particle-hole symmetrizing the Moore-Read wavefunction increased the overlap to 97% for $N = 10$ at one particular value of δV_1 but remained somewhat lower at other values. We note that the Moore-Read phase and its particle-hole conjugate are distinct phases [17] and the effect of symmetrization is unclear and remains a topic of current interest. In our work on the sphere, there is no possible mixing of states with their conjugates, although we cannot determine whether a state or its conjugate would occur in an experimental system. On the sphere, it was previously known [4] that the overlap of the exact groundstate with the Moore-Read state has a peak at $\delta V_1 \approx 0.04$, and also drops strongly near $\delta V_1 = 0$. However, on the sphere, it was hard to distinguish the thermodynamic phase since there is no groundstate degeneracy to use as a guide. Our work, in contrast, studies only trial wavefunctions in the Moore-Read phase.

In contrast to all prior work, our trial wavefunctions have high overlaps over a very broad range of δV_1, confirming that the weak pairing phase is robust to large changes in the interaction. Our wavefunctions make a smooth transition between the Moore-Read phase and the CF liquid at large δV_1. It is difficult to distinguish numerically if the groundstate of the LLL still has some amount of pairing. To determine if at large δV_1, the putative CFL still pairs (as previously suggested [5]), a more careful study of the groundstate for the LLL interactions would be required. We note in passing that the wide region of intermediate values of δV_1 (between where the Moore-Read wavefunction is accurate and where the CFL becomes accurate) which we describe extremely well with our wavefunctions, could be hard to access with typical 2DEG samples but could likely be realized using hole-doped samples [18] or graphene [19].

At interactions $\delta V_1 < 0.04$ our wavefunctions have substantially better performance than the Moore-Read wavefunction. However, near $\delta V_1 \approx 0$ our wavefunctions do not perform as well as one might hope. This is not surprising considering that the groundstate of $\delta V_1 = 0$ on the torus is a CDW state [5]. However, experiments, which see a quantum Hall plateau, do not correspond to the pure Coulomb interaction ($\delta V_1 = 0$) due to finite well width effects and Landau-level mixing. It has also been noted [5] that a more realistic interaction puts the physical system just slightly on the quantum Hall side of the transition. Indeed, it is known experimentally [20] that modifying the electron interaction slightly by tilting the field pushes the system from a quantum Hall state into a CDW state. Being that pure Coulomb is thought to be on the other side of this phase transition, the fact that our wavefunctions remain so good is perhaps surprising. However, one might argue that since the CDW is frustrated by the geometry of the sphere we can still match the groundstate reasonably well with a sufficiently perturbed weak pairing wavefunction, which remains adiabatically connected to the Moore-Read state.

In Ref. [7] it was suggested that the gapped state near the Coulomb point is best constructed within a composite fermions basis without appeal to the Moore-Read wavefunction. Our wavefunction is indeed constructed in terms of composite fermions, retains relatively high similarity with the exact groundstate, and also remains adiabatically connected to Moore-Read. We believe this result should put to rest concerns that the gapped phase near the Coulomb point is not in the topological phase of the Moore-Read state or its particle-hole conjugate [17].

We are grateful to N. Regnault for generously sharing data. The authors acknowledge helpful discussions with E. H. Rezayi and N. R. Cooper, and thank the Aspen Center for Physics for its hospitality. G.M. acknowledges support by EPSRC Grant No. GR/S61263/01.

[1] R. Willett, et al, Phys. Rev. Lett. **59**, 1776 (1987).
[2] G. Moore and N. Read, Nucl. Phys. **B360**, 362 (1991).
[3] M. Greiter, X. G. Wen, and F. Wilczek, Nucl. Phys. B **374**, 567 (1992).
[4] R. H. Morf, Phys. Rev. Lett. **80**, 1505 (1998).
[5] E. H. Rezayi and F. D. M. Haldane, Phys. Rev. Lett. **84**, 4685 (2000).
[6] See for example, S. DasSarma, M. Freedman, C. Nayak, S. H. Simon and A. Stern arXiv:0707.1889.
[7] C. Tőke and J. K. Jain, Phys. Rev. Lett. **96**, 246805 (2006).
[8] C. Tőke, N. Regnault, and J. K. Jain, Phys. Rev. Lett. **98**, 036806 (2007).
[9] N. Read and D. Green, Phys. Rev. B **61**, 10267 (2000).
[10] See for example O. Heinonen (ed.), *Composite Fermions* (World Scientific, 1998), and therein.
[11] J. K. Jain and R. K. Kamilla, Phys. Rev. B **55**, R4895 (1997).
[12] R. L. Willett, K. W. West, and L. N. Pfeiffer, Phys. Rev. Lett. **88**, 066801 (2002).
[13] F. D. M. Haldane, Phys. Rev. Lett. **51**, 605 (1983).
[14] P. G. de Gennes, *Superconductivity of Metals and Alloys* (Benjamin, New York, 1966).
[15] We omit Gaussian factors $\exp(-\sum_i |z_i|^2/4\ell_0^2)$.
[16] G. Möller and S. H. Simon, Phys. Rev. B **72**, 045344 (2005).
[17] M. Levin, B. I. Halperin and B. Rosenow, arXiv:0707.0483; S.-S. Lee, S. Ryu, C. Nayak and M. P. A. Fisher, arXiv:0707.0478.
[18] M. J. Manfra, et al, Phys. Rev. Lett. **98**, 206804 (2007).
[19] C. Tőke, P. E. Lammert, V. H. Crespi, and J. K. Jain, Phys. Rev. B **74**, 235417 (2006); M. O. Goerbig, R. Moessner, and B. Doucot, Phys. Rev. B **74**, 161407 (2006)
[20] M. P. Lilly, et al, Phys. Rev. Lett. **83**, 824 (1999); W. Pan, et al, Phys. Rev. Lett. **83**, 820 (1999); T. Jungwirth, et al, Phys. Rev. B **60**, 15574 (1999).