Paired composite-fermion wave functions

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We construct a family of BCS paired composite-fermion wave functions 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 interelectron interactions, the ground state can be very accurately represented in this form.

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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 wave function,[2] describing p-wave pairing of composite fermions,[3] is currently the best candidate wave function for this state.[4,5] Due to the remarkable property of having quasiparticles 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 ground state at $\nu=\frac{5}{2}$, its overlap with the exact ground state in simulations of small systems is rather low[4,5] in comparison with other known trial states at different filling factors.[10] 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 unique choice for a paired state in the lowest Landau level.[3] Furthermore, several recent studies have altogether challenged the view of $\nu=\frac{5}{2}$ as being the Moore-Read state, given that one assumes that the excitation spectrum should follow from the groundstate.[7,8]

In this paper, 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 wave functions.[10,11] The Moore-Read state can be cast very accurately in this form, which reveals its connection to the pairing of CFs on top of a Fermi sea and shows how our general paired CF-BCS wave functions are adiabatically connected to the Moore-Read state. We also compare our trial states to the exact ground states of the Coulomb Hamiltonian $\mathcal{H}_C$ for electrons in the first excited Landau level (1LL), plus an arbitrary additional pseudopotential δV_1 interaction. For a very broad range of δV_1, we find a very high overlap of our trial wave functions with the exact ground state, 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 (spin polarized) 1LL. The 1LL is represented by wave functions in the LLL using appropriately modified pseudopotential coefficients.[12]

The aim of our construction is to "composite fermionize" a simple BCS state. In second quantized notation, the general form of the BCS ground state is[13] $|\Psi_{\mathrm{BCS}}\rangle=\Pi_{\mathbf{k}}(1+g_{\mathbf{k}}e^{i\varphi}c^{\dagger}_{\mathbf{k}}c^{\dagger}_{-\mathbf{k}})|0\rangle$, written in an unnormalized manner here. This wave function can be projected to a fixed number of particles by integration over $\int d\varphi \exp(-iN\varphi)$ such that we retain exactly N pair creation operators. The (inverse) Fourier transform into real space then yields[13]

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

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

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

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 wave function form is naturally generalized to spherical geometry below.

In order to obtain a LLL wave function at filling factor $\nu=\frac{1}{2}$, we follow Jain's approach[10] of multiplying a bare electron wave function with Jastrow factors and projecting the result to the LLL, yielding[14]

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

where $\mathcal{P}_{\mathrm{LLL}}$ 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 wave function (and the projection then becomes trivial). We note that the formation of CFs accommodates much of the interelectron interaction, while allowing the CFs to pair accommodates the residual interaction between the CFs. As such, our work is beyond the noninteracting CF theory.

In order to render the projection $\mathcal{P}_{\mathrm{LLL}}$ numerically tractable in general, we bring single particle Jastrow factors $J_i=\Pi_{k\neq i}(z_i-z_k)$ 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] The LLL projection of g_{ij} yields a pair wave function which is formally an *operator* acting on Jastrow factors. Thus, the proposed form overcomes a prior argument[3] that $g(z)=1/z$ is the only pairing *function* al-

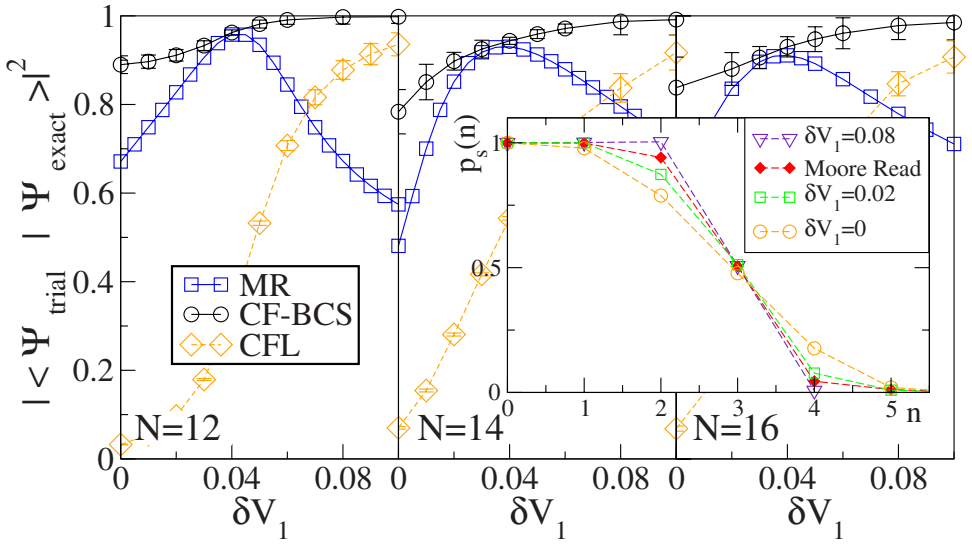

FIG. 1. (Color online) Overlaps of trial states with exact ground states as a function of the interaction parameter δV_1 for $N=12$, 14, and 16 electrons. Here, $\delta V_1=0$ corresponds to the pure Coulomb interaction in the 1LL. The optimized composite-fermionized BCS wave functions [Eq. (3), black circles] have a 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 wave function (blue squares) is also good near $\delta V_1=0.04$ but falls off substantially at other values. The CF liquid wave functions (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 wave functions over a broad range of interactions shows the large extent of the weak-pairing phase. The inset shows the occupation p_s of the CF shells n for $N=16$ electrons, as discussed in the main text.

lowed. As demonstrated in Ref. 11, modifying the projection prescription in this manner does 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 wave function. 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 wave function. Denoting $\tilde{\phi}_{\mathbf{k}}(z_i)=J_i^{-1}\mathcal{P}_{\mathrm{LLL}}[\phi_{\mathbf{k}}(z_i)J_i]$, Jastrow factors may be factored again outside the Pfaffian, and we obtain the final expression for general composite-fermionized BCS (CF-BCS) states,

$$\Psi^{\mathrm{CF}}=\mathcal{P}\mathrm{f}\left[\sum_{\mathbf{k}} g_{\mathbf{k}}\tilde{\phi}_{\mathbf{k}}(z_i)\tilde{\phi}_{-\mathbf{k}}(z_j)\right]\prod_{i<j}(z_i-z_j)^2. \qquad (3)$$

In the remainder of this study, we will focus on finite size systems with N electrons on the spherical geometry.[12] 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 CFs in one quantum of negative effective flux,[15] i.e., the (very small) effective magnetic field experienced by CFs is directed opposite to the external magnetic field. The relevant CF orbitals ($\tilde{\phi}_{\mathbf{k}}$) are given by the projected monopole harmonics $\tilde{Y}^{q=-1/2}_{n,m}$ studied in Ref. 15. 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 $\Sigma_{n,m}(-1)^{m-1/2}g_n\tilde{Y}^{q=-1/2}_{n,m}(z_i)\tilde{Y}^{q=-1/2}_{n,-m}(z_j)$. The sum over n goes from $n=0$ to $n=N-2$ since orbitals with $n\geqslant N-1$ are projected to zero. Up to a 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 wave functions 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 wave function. The definition of a "good" wave function is somewhat arbitrary and one may attempt to optimize various measures of its accuracy, e.g., the energy of the wave function, the overlap with the exact ground state, or the error in the pair correlation function compared to the exact ground state. Optimization of the chosen measure of accuracy is performed by advanced variational Monte Carlo techniques.[16]

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 wave function with our variational parameters.

Figure 1 shows overlaps between trial states and the corresponding exact ground states for different interactions obtained by modifying the first pseudopotential coefficient[12] by an amount δV_1 (with $\delta V_1=0$ being the pure Coulomb interaction in the 1LL). We have chosen to vary V_1 since it is known[5] that the most important feature of the interaction is

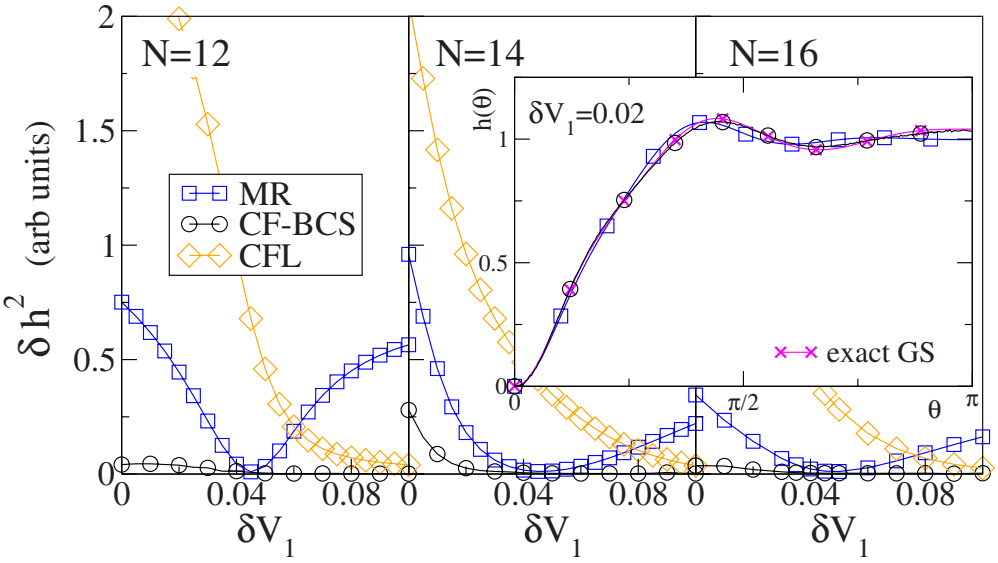

FIG. 2. (Color online) Squared error δh^2 in the pair correlation function of various trial wave functions compared with exact ground states as a function of the interaction parameter δV_1 for $N=12$, 14, and 16 electrons. Symbols are as in Fig. 1. Again, we find that composite-fermionized BCS wave functions 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 wave function along with the exact ground state at $N=14$ and $\delta V_1=0.02$. Our trial state is essentially indistinguishable from the exact ground state, whereas the Moore-Read state is slightly different.

the ratio V_1/V_3, where very large δV_1 roughly corresponds to the Coulomb interaction in the LLL.[12] In this figure, we also show overlaps of the exact ground state 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 wave functions using at most the first seven 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 wave function. 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 a very high overlap with the exact ground state 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 ground state. For larger δV_1, the CF-BCS states become even more accurate and can be continuously deformed into the CF 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 will discuss below.

Changing the interactions requires adapting the variational parameters $\vec{g}$ which, like the u and v parameters of BCS theory, effectively describe the shape of the pair wave function. However, this role is somewhat obscured by the projection to the LLL, with $\tilde{\phi}$ and g_{ij} being functions of all the z's. It is then useful to consider the notion of occupation probabilities for CF orbitals. For particles occupying orthogonal eigenstates ϕ_k and described by an N-body wave function of the form $\Psi[g_{\mathbf{k}}]=\Sigma_{\{\mathbf{k}_i\}}\Pi_i g_{|\mathbf{k}_i|}\phi_{\mathbf{k}_i}$, the probability for a particle to occupy an orbital with momentum $k=|\mathbf{k}|$ is

$$p(k) = [2n(k)dk]^{-1}\frac{\partial}{\partial(\log g_k)}\log|\Psi[g_k]|^2, \tag{4}$$

with the density of states $n(k)$. Although the CF orbitals are not orthogonal,[17] we nonetheless find that Eq. (4) allows an accurate estimate of the occupation probabilities for wave functions of the form of Eq. (3). To confirm this, it was verified that Eq. (4) reproduces to high accuracy the correct occupation numbers for 'filled shell' CFL states, where the CF occupations are defined to be 0 or 1.[18] The inset of Fig. 1 shows results for the filling of shells $p_s(n)$ for $N=16$ on the sphere. For large δV_1, we find that $p_s(n)$ is close to the values of the CFL, with $p_s(n)\approx 0$ for shells above the Fermi surface (FS) and $p_s(n)=1$ for n below Fermi surface, and there is a single valence shell where $0<p_s(n_F)<1$. As δV_1 is lowered, the distribution of occupations continually stretches out to values above the CF-FS. This makes clear the continuous connection of the paired states, including the Moore-Read Pfaffian state, to the composite-fermion Fermi liquid. Note that this occupation probability is the analog of the u and v functions of the BCS theory.

As mentioned above, overlaps are not the only possible measure of the accuracy of a wave function. In Fig. 2, we show how the pair correlation functions $h(\theta)$ of different trial states compare against those of the exact ground state. Here, θ is the angle between two particles on the sphere and we show the mean square error in the correlation function $\delta h^2 = \int d(\cos\theta)|h(\theta)-h_{\text{exact}}(\theta)|^2$. We note that if $\delta h^2=0$ for a trial

state, then it is identical to the exact ground state [this can be seen from the variational principle, noting that $h(\theta)$ fully determines the energy for a two-body interaction]. Figure 2 once more illustrates that our trial wave functions 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 wave functions have been reoptimized with respect to δh^2. The overlaps of these new wave functions with the exact ground state 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 wave functions to have over 0.99 overlaps with the Moore-Read state, we conclude that our CF-BCS wave 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 wave function in a weak-pairing phase should have the property[9] that $g(\mathbf{r})\sim 1/z$ at large distances $\mathbf{r}$. While this is not obvious from the form of Eq. (3) (particularly considering the complexity of the projected wave functions $\tilde{\phi}$), we can nonetheless establish that it is true in several ways. First, 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. Second, the property $g(\mathbf{r})\sim 1/z$ at large $\mathbf{r}$ implies that the $\mathbf{k}\rightarrow 0$ 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 by testing that increasing the value of the variational parameter g_0 does not change the wave function.

It is also worth checking that the exact ground state 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 ground state, 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 ground state of $\mathcal{H}_C'$ is adiabatically connected to the Moore-Read state, confirming that the exact ground state 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 wave functions in the same topological phase as the Moore-Read wave function. This can be thought of as the composite fermionization of a weakly paired BCS wave function. We find that over a broad range of interactions, these wave functions are very accurate—far more so than the Moore-Read wave function itself, which should be thought of only as an example of a wave function 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 wave functions,[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 ground state BCS wave functions, our approach also enables the study of excited states[16] which can then more directly address a current controversy.[7,8]

Let us now discuss how our work reflects on and relates to previous 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 wave function itself. Particle-hole symmetrizing the Moore-Read wave function 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[19] 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 ground state 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 ground state degeneracy to use as a guide. Our work, in contrast, studies only trial wave functions in the Moore-Read phase.

In contrast to all prior work, our trial wave functions 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 wave functions 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 ground state 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 ground state 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 wave function is accurate and where the CFL becomes accurate), which we describe extremely well with our wave functions, could be hard to access with typical two-dimensional electron gas samples but could likely be realized using hole-doped samples[20] or graphene.[21]

At interactions $\delta V_1<0.04$, our wave functions have substantially better performance than the Moore-Read wave function. However, near $\delta V_1\approx 0$, our wave functions do not perform as well as one might hope. This is not surprising considering that the ground state 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[22] 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 wave functions 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 ground state reasonably well with a sufficiently perturbed weak-pairing wave function, 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 CF basis without appeal to the Moore-Read wave function. Our wave function is indeed constructed in terms of CFs, retains relatively high similarity with the exact ground state, and also remains adiabatically connected to the Moore-Read state. Our work definitively shows that the gapped phase near the Coulomb point is in the topological phase of the Moore-Read state or its particle-hole conjugate.[19]

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