Single-parameter variational wave functions for quantum Hall bilayers

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Bilayer quantum Hall states have been shown to be described by a BCS-paired state of composite fermions. However, finding a qualitatively accurate model state valid across all values of the bilayer separation is challenging. Here, we introduce two variational wave functions, each with a *single* variational parameter, which can be thought of as a proxy for the BCS order parameter. Studying systems of up to $9+9$ electrons in a spherical geometry using Monte Carlo methods, we show that the ground state can be accurately described by these single-parameter variational states. In addition, we provide a numerically exact wave function for the Halperin-111 state in terms of composite fermions.

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I. INTRODUCTION

Non-Fermi liquids have been attracting an increasing amount of interest as a gapless phase of matter that challenges the paradigm of Fermi-liquid theory [1]. One example of a non-Fermi liquid is the compressible liquid arising at half filling of a Landau level (LL) in the quantum Hall effect. Quantum Hall bilayers offer a platform for studying pairing instabilities of this non-Fermi liquid.

The quantum Hall effect arises when electrons confined to two dimensions are subjected to a strong magnetic field. For particular values of the filling factor $\nu = N_e/N_\phi$, where N_e is the number of electrons and N_ϕ is the number of magnetic flux quanta, a gapped state with a quantized Hall response is observed. The first experiments [2] observed quantized Hall plateaus at integer ν, i.e., the integer quantum Hall effect (IQHE). However, soon thereafter further plateaus at fractional ν were observed [3], marking the discovery of the fractional quantum Hall effect (FQHE). Whereas the IQHE can be described effectively as a band insulator of noninteracting electrons, the FQHE fundamentally requires electron-electron interactions in order to open up a gap.

One of the most successful approaches to the quantum Hall effect consists of thinking in terms of composite fermions (CFs)—composite objects of electrons bound to an even number of flux quanta [4,5]—since this allows one to bridge the gap between the IQHE and FQHE. At the mean-field level, the CFs experience a different effective magnetic field than the electrons such that integer values of their effective filling factor ν_{CF} correspond to fractional values of ν. This unifying framework allows one to describe the fractional quantum Hall effect of strongly interacting electrons as an integer quantum Hall effect of weakly interacting CFs. Furthermore, the compressible state observed at $\nu = 1/2$ [6] can be viewed as a CF Fermi liquid (CFL). However, the CFs experience a fluctuating gauge field which can lead to non-Fermi-liquid behavior [7] and the residual interactions between the CFs are still able to generate instabilities such as pairing instabilities and open up a gap. Paired states of composite fermions such as the Moore-Read state are indeed candidates for the elusive gapped $\nu = 5/2$ state [8,9].

Another platform to study pairing of composite fermions is a quantum Hall bilayer with total filling factor $\nu = 1$. The electrons are confined to two layers with layer separation d, with each layer at half filling $\nu = 1/2$. The typical distance between electrons in the same layer is given by the magnetic length $\ell_B = \sqrt{\hbar/eB}$ and therefore the ratio of interlayer to intralayer interaction strength is roughly $\frac{1}{d/\ell_B}$. By tuning the ratio d/ℓ_B, the two competing interactions can be tuned. At large d/ℓ_B the composite fermions form two decoupled composite Fermi liquids in the two layers [7], for which numerically exact wave functions can be written. At small d/ℓ_B, electron-hole pairs form an exciton condensate, the so-called 111 state [10,11]. The limits $d \to 0$ and $d \to \infty$ of the quantum Hall bilayer are thus well understood. However, one difficulty is that the two limits are described in terms of different quasiparticles (electrons at $d \to 0$ vs CFs at $d \to \infty$). Much theoretical work has been devoted to understanding the nature of the state at intermediate distances and the connection between these two well-understood limits [12–44].

Recently, it has been proposed that at intermediate distances the composite fermions in a quantum Hall bilayer pair up in a BCS-like fashion and undergo a BEC-BCS crossover, from a BCS-like state at large d/ℓ_B to a BEC-like state at small d/ℓ_B [35,45,46]. Experiments on double layers of graphene have shown that as d/ℓ_B decreases, one goes from a regime where the pairing temperature and the condensation temperature coincide (BCS regime) to a regime where the pairing temperature lies significantly above the condensation temperature (BEC regime), as expected for the BEC-BCS crossover [45]. Besides this experimental evidence, exact diagonalization results show that an s-wave BCS trial state with CFs in one layer paired with anti-CFs in the other layer has high overlaps with the exact ground state [47] for any interlayer separation. An Eliashberg calculation of the pairing of CFs and anti-CFs mediated by the fluctuating gauge field they experience indeed finds a dominant s-wave pairing channel [48].

In the present paper, we study trial wave functions for the BEC-BCS crossover in quantum Hall bilayers. In contrast to previous work, we use trial wave functions with a *single* variational parameter. Given that the Hilbert space size is exponentially increasing with the number of electrons, the fact we can capture the ground state with a single variational parameter shows that the wave function describes the correct physics. Moreover, our trial state captures the Halperin-111 state, which is known to be the exact ground state of the quantum Hall bilayer at $d = 0$. The 111 state is usually understood as a condensate of interlayer electron/hole excitons. However, we show that it can also be represented as a condensate of CF/anti-CF excitons up to numerical precision. Therefore, we find that the quantum Hall bilayer at $\nu = 1/2 + 1/2$ can be *entirely* described in terms of CFs irrespective of d.

II. METHODS

The starting point for our analysis is a trial wave function for the quantum Hall bilayer introduced in Ref. [47]. This wave function describes s-wave BCS pairing of CFs in one layer with anti-CFs in the other layer. The CFs are organized in CF LLs ("Λ levels"). For each of these Λ levels a separate pairing parameter g_n is introduced, where $n = 0, 1, \ldots, N_\Lambda$ is the Λ-level index. N_Λ is the maximum Λ level that is included and in the following we will always set $N_\Lambda = N_1 - 1$ which is required to capture the 111 state as explained below. N_1 is the number of electrons in each layer. The trial wave function written as appropriate for the spherical geometry that we use here is [47]

$$\Psi_{\mathrm{BCS}} = \prod_{i<j} (\Omega_i - \Omega_j)^2 (\varpi_i - \varpi_j)^{*2} \det(G),$$
$$G(\Omega_i, \varpi_j) = \sum_{n,m} g_n \tilde{Y}_{q,n,m}(\Omega_i) \tilde{Y}^*_{q,n,m}(\varpi_j), \tag{1}$$

where $\Omega_j = (\theta_j, \varphi_j)$ is the spinor coordinate of the jth electron in the top layer, ϖ_i is the spinor coordinate of the ith hole in the bottom layer, and the notation $(\Omega_i - \Omega_j)$ is shorthand notation for a Jastrow factor. $\tilde{Y}_{q,n,m}$ are the Jain-Kamilla projected monopole harmonics [49], $2q$ is the net flux experienced by the CFs, and m is the L_z angular momentum quantum number. We consider the case of a balanced bilayer with N_1 electrons per layer and a total number of flux quanta $N_\phi = 2N_1 - 1$, which corresponds to a filling factor $\nu = 1/2 + 1/2$ in the thermodynamic limit, with a shift appropriate for observing the CFL in each individual layer when they are decoupled.

In Ref. [47], the number of Λ levels that are included—and hence the number of variational parameters—is proportional to the system size N_1: $N_\Lambda = N_1 - 1$. In the present work, we use the same trial wave function (1), however, we use an ansatz for the parameters g_n such that there is only one variational parameter. We use two different types of ansatz: (i) We use the BCS order parameter Δ as the variational parameter. The BCS prediction for the occupation probability of the composite fermion orbitals with index n and energy ε_n is [31]

$$p_n = \frac{1}{2}\left(1 - \frac{\varepsilon_n}{\sqrt{\varepsilon_n^2 + \Delta^2}}\right), \tag{2}$$

and by solving the inverse problem we may deduce the parameters g_n corresponding to a given Δ. We measure ε_n in units of the Fermi energy such that Δ is dimensionless. Note that the Λ-level index n of the CFs can be thought of as a momentum $\mathbf{k}$, which allows one to compute ε_n (see Supplemental Material [50]). (ii) We use a parameter α as the variational parameter such that

$$g_n = e^{\alpha n}. \tag{3}$$

In order to study larger systems than are accessible with exact diagonalization, we use Monte Carlo methods to minimize variational energies. In Ref. [47] it was shown that for systems of up to $7 + 7$ electrons, the BCS trial state with $N_\Lambda = N_1 - 1$ always has at least a 0.95 overlap squared with the exact diagonalization ground state. In the present work, therefore, the same number of variational parameters are used for energy minimization and the resulting BCS state is chosen as the reference ground state. Using the fact that having large overlaps is a transitive feature, we may deduce that the single-parameter optimized variational state has high overlaps with the exact ground state (provided it has high overlap with the reference state).

Since the optimization at large interlayer separation is trivial (the BCS trial state exactly reduces to the CFL state in a certain limit), whereas at small interlayer separation the optimization can have difficulties converging, we pick the 111 state for the importance sampling of the Monte Carlo samples.

III. RESULTS FOR Δ OPTIMIZATION

We first attempt to use the BCS order parameter Δ as a variational parameter. From a given set of BCS coupling constants g_n we can extract the CF orbital occupation numbers via the prescription outlined in Ref. [31]. These are related via Eq. (2) to Δ. Since the wave function is written in terms of g_n, to evaluate the wave function for a given Δ we need to first solve an optimization problem to find the corresponding g_n. We can then optimize Δ to find the lowest-energy configuration. Since we have two nested variational problems, this is a computationally intensive method, which motivates us to later investigate a different ansatz which directly gives the g_n coefficients.

As shown in Fig. 1, for $\Delta \to 0$ we recover the CFL wave function which has extremely high overlaps (>0.999 for $N_1 = 6$) with the exact diagonalization ground state at $d \to \infty$. For $\Delta \to \infty$ we recover a state that has a very high overlap (>0.947 for $N_1 = 6$) with the 111 state, which is consistent with the picture from the Chern-Simons theory of this trial state [45]: For tightly bound CF/anti-CF pairs, the fluxes attached to the CF and anti-CF cancel, making this CF/anti-CF exciton equivalent to an electron/hole exciton, whose condensation leads to the 111 state. A very similar calculation is performed for the torus geometry and the overlap is also fairly high (>0.991 for $N_1 = 6$). We note however that our implementation of the lowest Landau level projection

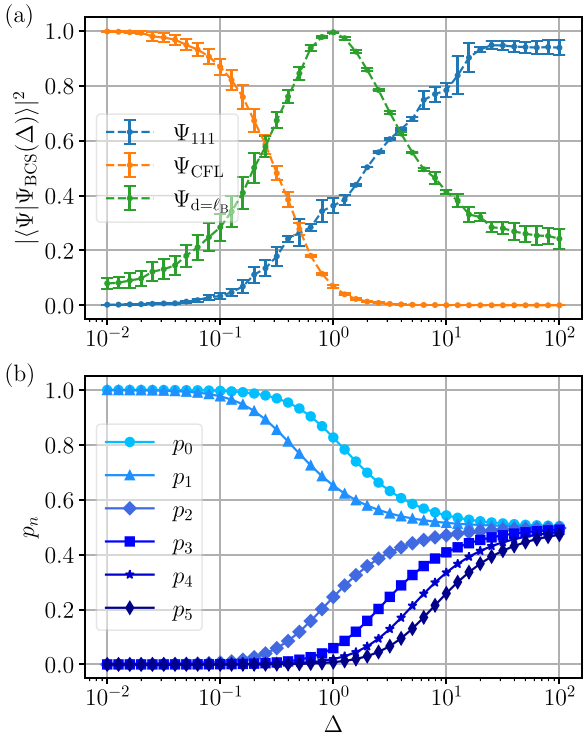

FIG. 1. Variational results for Δ optimization. (a) Overlaps with three representative states [the two model states and the (energy-optimized) ground state at $d/\ell_B = 1$] for $-2 \leqslant \log_{10}(\Delta) \leqslant 2$ in a $6+6$ system. The CFL is described by the limit $\Delta \to 0$ (BCS regime), while the 111 state is well described by the limit $\Delta \to \infty$ (BEC regime). At intermediate distances $d \sim \ell_B$ we have the best overlap with a state having $\Delta \sim 1$. (b) Orbital occupation probability for variational states. Occupation probabilities are analytical results evaluated according to Eq. (2). In the limit $\Delta \to 0$ only the lowest two CF shells are filled, while at $\Delta \to \infty$ all CF shells have equal occupation.

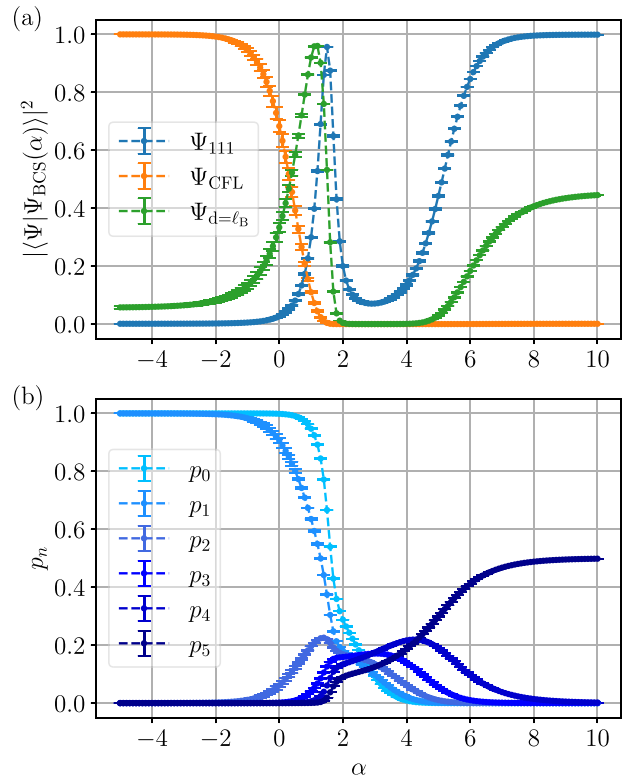

FIG. 2. Variational results for α optimization. (a) Overlaps with three representative states [the two model states and the (energy-optimized) ground state at $d/\ell_B = 1$] for $-5 \leqslant \alpha \leqslant 10$ in a $6+6$ system. The CFL state has maximum overlap with the $\alpha \to -\infty$ state, and the 111 state has maximum overlap with the $\alpha \to \infty$ state. At intermediate $d \sim \ell_B$, the optimum value is $\alpha \sim 1$. (b) Orbital occupation probability for variational states. For $\alpha \sim 1$ we have roughly equal occupation of all CF orbitals (corresponding to $\Delta \to \infty$). The overlap with the 111 state has a local maximum at this value, however, for larger system sizes this local maximum decreases showing that the 111 state is truly captured by the $\alpha \to \infty$ limit [see Fig. 3(a)]. In the limit $\alpha \to \infty$ which corresponds to the 111 state, only the highest CF orbital is occupied.

on the torus does not preserve periodic boundary condition, and a more precise implementation is left to future work. The results are summarized in the Supplemental Material [50]. For intermediate distances $d \sim \ell_B$ we find $\Delta \sim 1$.

By minimizing the energy as a function of Δ, we find $\Delta \propto d^{-3.4}$ scaling for $d \gtrsim \ell_B$. This is consistent with the BEC-BCS crossover picture where Δ increases as we approach the small-d BEC limit. A renormalization group (RG) calculation for quantum Hall bilayers predicts $\Delta \propto d^{-2}$ [35], however, this was derived for pairing of CFs with CFs whereas we are considering pairing of CFs with anti-CFs.

IV. RESULTS FOR α OPTIMIZATION

We now turn to a computationally more manageable approach, namely the ansatz $g_n = e^{\alpha n}$. This ansatz is motivated by the fact that when variationally optimizing the g_n parameters at small d, they show an exponential dependence on n. (see Fig. S2 in Supplemental Material [50]).

As shown in Fig. 2, the limit $\alpha \to -\infty$ leads to only the lowest CF orbitals being occupied, which again reduces to the CFL wave function. The regime $\alpha \sim 1$ has high overlaps with the 111 state (>0.989 for $N_1 = 4$). This regime leads to occupation numbers that are almost constant as a function of n. This can be understood as a consequence of the lowest LL (LLL) projection of the CF orbitals: Those with large n have small weight in the LLL and therefore need exponentially large coefficients g_n [49]. Furthermore, this corresponds to the regime $\Delta \to \infty$ that was previously identified as having a large overlap with the 111 state. However, we find that increasing α even further leads to a state with only the highest CF shell being occupied which has an even better overlap with the 111 state (>0.999 for $N_1 = 4$). States in this regime are far outside the Hilbert space captured by the variational ansatz with Δ where the lowest CF shells are always occupied. We note that there is a discontinuous change in the optimum value of α as a function of d as seen in Fig. 3(b). This discontinuous jump is a consequence of the variational principles, so even though the wave function evolved continuously, the optimized variational parameter may change discontinuously.

In the limit $\alpha \to \infty$, we find a wave function that almost exactly reproduces the 111 state within the numerical accuracy for all system sizes up to $9+9$ particles. As shown in Fig. 3(a), the overlaps with the 111 state are better than 0.993

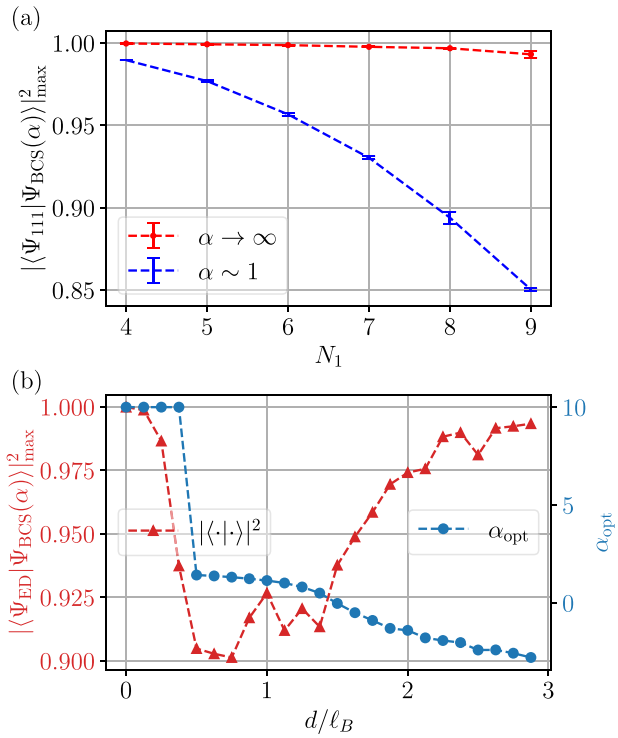

FIG. 3. Overlaps of the α trial state for different system sizes and interlayer separations. The maximum overlap of α-ansatz trial state Eq. (3) (a) with Ψ_{111} for different system sizes N_1 and (b) for different interlayer distances d for $6+6$ electrons. The one-parameter ansatz captures the 111 state accurately for all system sizes shown and captures the state at intermediate distances d well too. We also show the optimum value of α as a function of interlayer separation. The optimum α value increases as d decreases and jumps discontinuously to its maximum value in the optimization range ($\alpha = 10$) around $d \sim 0.5\ell_B$.

for all system sizes up to and including $9+9$. The 111 state is thus described by the wave function Eq. (1) with $g_n = \delta_{n,N_1-1}$. The CFs in each layer half fill the Λ level with $n = N_1 - 1$ and there is s-wave pairing between the CFs in one layer and the anti-CFs in the other layer. In the 111-state description in terms of electrons and holes, electrons half fill the LLL in each layer and there is s-wave pairing between the electrons in one layer and the holes in the other layer. The correspondence between the two descriptions makes sense intuitively: Eq. (1) describes s-wave pairing of CFs and anti-CFs. If we have tightly bound CF/anti-CF pairs, then the set of coordinates $\{\Omega_i\}$ of the CFs coincides with the set of coordinates $\{\varpi_i\}$ of the anti-CFs and therefore the Jastrow factors in Eq. (1) cancel. The Jastrow factors describe the flux attachment procedure and removing the Jastrow factors reduces the pairing of CFs and anti-CFs to that of electrons and holes—which is precisely the 111 state. For system sizes of $10+10$ electrons and above, the overlap of the $\alpha\to\infty$ state with the 111 state becomes small [see Fig. S1(f) in Supplemental Material [50]]. However, in that case we are dealing with orbitals with a high LL index and we caution that in that case the approximate LLL projection we use may not be accurate. Furthermore, the evaluation of CF orbitals with a high LL index may suffer from numerical precision issues [51].

In Fig. 3(a) we also show the overlap of the 111 state with the state with $\alpha \sim 1$ as a function of system size N_1. As can be seen from Fig. 2, this is a local maximum of the overlap. However, we can see that this state performs significantly worse, when the system size is increased.

As shown in Fig. 3(b), the trial state with a single variational parameter captures the entire crossover from large to small d very well. The limits of large and small d are captured exactly to within numerical precision, while at intermediate distances, the overlap squared with the exact diagonalization ground state is always better than 0.90 for a system of $6+6$ electrons.

V. CONCLUSION

We have investigated a BCS trial wave function for quantum Hall bilayers which consists of pairing CFs in one layer with anti-CFs in the opposite layer. Previous work [47] used trial wave functions with the number of variational parameters growing proportional to the system size. Here, in contrast, we achieve high overlaps squared of better than 0.94 for up to $6+6$ electrons with a single variational parameter. Overall these are extremely high overlaps considering we are only using a single variational parameter. A single-parameter wave function has also been developed for bosonic quantum Hall bilayers [52], where a transition to a non-Abelian state is possible.

In particular, we show that for a particular choice of variational parameters, the BCS trial state which is entirely written in terms of CF orbitals has unity overlap with the 111 state (within numerical precision). The 111 state is known to be the exact ground state of the quantum Hall bilayer system at $d = 0$, however, it is usually written in terms of electrons. Here, we provide the expression for the 111 state in terms of composite fermions.

One of the interesting features of the quantum Hall bilayer system is that the large d physics is most simply understood in terms of CFs, while the small d physics is most simply understood in terms of electron-hole excitons. We have now shown that CFs offer an accurate description of the system for all d. It would be very interesting to confirm experimentally that this is the case. Experimental evidence for a composite fermion description can come from geometric resonance experiments, as have been performed on the $\nu = 1/2$ system [53] and more recently on the $\nu = 5/2$ system [54]. Geometric resonance experiments on quantum Hall bilayers have indeed revealed the presence of CFs [55]. It would be fascinating to perform such experiments on a quantum Hall bilayer as a function of the interlayer separation d/ℓ_B to confirm at which interlayer separation (if any) signatures of CFs disappear.

Recent work has shown that imbalanced bilayers at filling $\nu = 1/3 + 2/3$ also undergo a continuous transition [56,57] and it would be interesting to investigate the trial wave functions for that scenario. We leave that to future work.

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