Landau-Level Mixing and the Emergence of Pfaffian Excitations for the 5/2 Fractional Quantum Hall Effect

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We report on exact diagonalization studies for fully spin polarized 5/2 fractional quantum Hall effect, incorporating Landau-level mixing through the Bishara-Nayak effective interaction. We find that there is an experimentally accessible region in the phase diagram where the Pfaffian model accurately describes not only the ground state but also the neutral and charged excitations. These results are consistent with the observed persistence of the 5/2 Hall effect down to very low magnetic fields; they are also relevant to the experimental attempts to detect non-Abelian braid statistics.

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The proposed route to non-Abelian braid statistics in the 5/2 fractional quantum Hall effect (FQHE) [1–4], discovered more than two decades ago [5], proceeds through a sequence of remarkable emergences. To minimize the bulk of the repulsive interaction, electrons in the second Landau level (LL) dress themselves with two vortices to transform into composite fermions [6]; composite fermions (CFs) experience a vanishing magnetic field and form a Fermi sea [7]; the CF Fermi sea, however, is unstable due to a weak residual attractive interaction between composite fermions, which causes an equal spin $p_x \pm i p_y$ pairing, thereby opening a gap and producing an FOHE state [1,2,8]; the Abrikosov vortices of the paired CF state support zero mode solutions, namely, Majorana CFs, which are symmetric combinations of the CF creation and annihilation operators [3,4]; these obey non-Abelian braid statistics [3,4] and are potential candidates for fault tolerant topological quantum computation [9].

While the decisive verification of these ideas will eventually come from laboratory experiments, we have come to expect any successful theoretical postulate in the field of FQHE to pass the test against "computer experiments," that is, exact solutions of the full many body problem for finite systems typically containing up to 16–18 particles. A concrete realization of the above physics is through the Pfaffian (Pf) model of Moore and Read [1], which has been subjected to such tests. The Pf wave function for the ground state has a moderate overlap with the exact Coulomb ground state, which can be improved either by artificially strengthening the short range part of the interaction [10–12] or by considering the effect of finite thickness [13]. The sensitivity to such slight modifications in the interaction indicates that the physical 5/2 FQHE state lies close to an instability. An adiabatic connection has been shown in finite system studies between the Coulomb and the Pf ground states [12,14,15]. The situation is less clear for excitations, however. A test of the Pf quasiholes has not found them to be satisfactory approximations of the actual quasiholes of the unperturbed Coulomb interaction [16], and an adiabatic connection between the Pf and the Coulomb quasiparticles and quasiholes has not yet been demonstrated. Given that the non-Abelian braid properties of the quasiparticles and quasiholes are of primary interest, it would appear important to ascertain the region of validity of the Pf model for the excitations as well. Our results below provide strong evidence that sufficient amount of LL mixing produces not only a ground state very close to the Pf state, but also neutral and charged excitations that are well consistent with the Pf model.

We employ the standard spherical geometry in our calculations, wherein N electrons on the surface of the sphere are exposed to a magnetic flux of 2Qhc/e, where 2Q is an integer. We consider electrons in the second Landau level coupled by the Bishara-Nayak (BN) effective interaction [17]

$$H_{\rm BN} = V_{\rm Coulomb} + \sum_{m} \delta \mathcal{V}_m + \sum_{m} \mathcal{W}_m, \qquad (1)$$

where V_{Coulomb} is the second LL Coulomb interaction and the last two terms effectively account for perturbative corrections to the interaction due to LL mixing. They are defined as $\delta \mathcal{V}_m = \delta V_m \mathcal{P}_m^{(2)}$ and $\mathcal{W}_m = W_m \mathcal{P}_m^{(3)}$, using pair and triplet amplitudes $\mathcal{P}_m^{(2)} = \sum_{ij}^{\prime} P_{ij}^{(2)} (2Q - m)$ and $\mathcal{P}_m^{(3)} = \sum_{ijk}^{\prime} P_{ijk}^{(3)} (3Q - m)$, where $P_{ij}^{(2)}(L)$ and $P_{ijk}^{(3)}(L)$ project the state of the two and three particles into the subspace of total orbital angular momentum L; δV_m is the change in the energy of a pair of electrons with relative angular momentum $m = 1, 3, 5, \cdots$, and W_m is the energy of a collection of three electrons with $m = 3, 5, 6, \cdots$. The relevant expansion parameter in the calculation of Bishara and Nayak is the ratio of Coulomb and cyclotron energies, $\kappa = (e^2/\epsilon\lambda)/(\hbar\omega_c)$, where $\lambda = \sqrt{\hbar c/eB}$ is the magnetic length and $\omega_c = eB/m_bc$ is the cyclotron frequency, m_b

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being the band mass of the electron. For GaAs, $\kappa \approx 2.5/\sqrt{B}$ (with the magnetic field *B* quoted in Tesla), which varies between $\kappa = 0.8$ and 1.8 at B = 9 to 2*T* [18]. In the following calculations we used the values of δV_m (for $m \leq 3$) and W_m (for $m \leq 8$) given in Ref. [17].

The solution of the short range three body interaction $H_{\rm Pf} = W_3$ defines the Pf model in what follows. The single zero energy eigenstate of $H_{\rm Pf}$ at 2Q = 2N - 3 is identified as the Pf ground state, the zero energy solutions at 2Q > 2N - 3 as Pf quasihole (QH) states, and the low energy solutions at 2Q < 2N - 3 as Pf quasiparticle (QP) states. As another reference we also consider the two body interaction $H_1 = V_{\rm Coulomb} + \delta V_1$, wherein we arbitrarily modify the two body pseudopotential V_1 .

A fundamental aspect of the Pf state is its lack of particle-hole (p-h) symmetry: the Pf is topologically distinct from its hole partner, called the antiPfaffian (APf) [19]. In the absence of LL mixing, the Pf and APf states are degenerate in the thermodynamic limit, and LL mixing, which enters through a three body interaction, will split the degeneracy to favor one over the other [17,20,21]. (The two have different triplet amplitudes, which guarantees an extensive energy difference in the thermodynamic limit.) In a recent work Rezayi and Simon [22] have argued that the APf has lower energy. Recent tunneling experiments [23] are closer to the expectation from the APf state, although not conclusive.

We first determine which state is favored by the BN interaction, which is different from the one used in Ref. [22]. Figure 1(a) demonstrates that increasing κ , which breaks *p*-*h* symmetry, produces a ground state that is very well approximated by the Pf wave function; the squared overlaps between the exact $H_{\rm BN}$ ground state and the Pf increase from 0.4–0.6 at $\kappa = 0$ to above 0.95 at $\kappa =$ 2 for systems with up to 18 particles. Furthermore, the Pf is a significantly better approximation than the APf, indicating that $H_{\rm BN}$ selects the Pf. An extrapolation of the $H_{\rm BN}$ energies of the Pf and the APf states is also consistent with that conclusion. We note that while W_3 , being negative, favors the APf, it is dominated by the higher W_m 's acting in favor of the Pf [24], and the total BN interaction selects the Pf phase. Further work will be required to ascertain which model is most reliable for LL mixing and which state is stabilized under realistic conditions, but we will focus on the Pf phase in what follows. We also note that another earlier work in this direction [25] used a different approach to account LL mixing, by enlarging the Hilbert space to allow a single excited electron; it considered only the APf, and was restricted to very small systems ($N \leq 8$).

Figure 1(b) reminds us that increasing the pseudopotential V_1 also produces high overlaps with the Pf wave function (also followed by a transition into the CF Fermi sea, consistent with the interpretation of the Pf as a weakly paired state of CFs) [11,12]. The increase in V_1 is not microscopically motivated, however, and also does not lift the degeneracy between the Pf and the APf.



FIG. 1 (color online). Panel (a) shows the squared overlaps of the exact ground state of $H_{\rm BN}$ with both Pf and APf as a function of κ for the indicated values of N. The top axis shows the corresponding magnetic field for GaAs. The squared overlaps of these states are also shown with the corresponding L = 0 states of noninteracting composite fermions (lines with same color and style but thinner), labeled CFFS (CF Fermi sea [32]). Panel (b) shows the squared overlaps of the exact ground state of H_1 with both Pf and CFFS. Panel (c) displays the squared overlap between the ground state of $H_{\rm BN}$ at 2Q = 2N - 3 with the hole conjugate of its ground state at 2Q = 2N + 1; the deviation from unity is a measure of the p-h symmetry breaking. The pair correlation function of the $H_{\rm BN}$ ground state is shown in panel (d) for several values of κ (with $\kappa = 0$ giving the Coulomb result) along with that of the Pfaffian wave function. Panel (e) depicts comparisons for Pf and APf (N = 16 and 14) with the $H_{\rm BN}$ ground state for a quantum well of thickness w = 3λ (three magnetic lengths).

The next three figures compare the neutral and charged excitations of $H_{\rm BN}$ with the corresponding Pf excitations. Figure 2 shows the spectra at 2Q = 2N - 3 for the Coulomb, Pf, and BN interactions (the last for $\kappa = 2$), as well as the overlaps as a function of κ and δV_1 . Figures 3 and 4 show similar comparisons for two quasiholes at 2Q = 2N - 2 and two quasiparticles at 2Q = 2N - 4. The Pf model $H_{\rm Pf}$ produces a zero energy ground state in Fig. 2(c), as well as a well-defined neutral exciton branch, which presumably represents a QP-QH excitation; it also produces a zero energy Pf QH band in Fig. 3(c), and a low energy band in Fig. 4(c) that we identify as the Pf QP states. A comparison with the exact eigenstates of the BN interaction brings out the following. First of all, the neutral and the charged excitations of V_{Coulomb} [panel (a)] are not well described by the Pf model, as indicated by the overlap values as well as the Coulomb energies of the Pf eigenstates which often lie outside the frame. With LL mixing, however, the agreement improves rapidly [panels (b) and (d)]. The overlaps become much larger, and the expectation values of $H_{\rm BN}$ with respect to the Pf eigenstates of $H_{\rm Pf}$



FIG. 2 (color online). Spectra of 16 particles at flux 2Q = 2N - 3 = 29 for (a) V_{Coulomb} , (b) H_{BN} , and (c) H_{Pf} (black as well as colored dots). The energy expectation values of the Pf wave functions are also shown for V_{Coulomb} and H_{BN} in panels (a) and (b) (dashes) except when they are so high that they fall outside the frame. The energies are given in units of e^2/λ (λ is the magnetic length) in panels (a) and (b) and in units of W_3 in (c). The numbers near the ground state (red [medium gray]) and the low energy neutral excitations (blue [dark gray]) indicate the squared overlaps with the corresponding Pf eigenstates. Panels (d) and (e) show the evolution of the overlaps of the exact states of H_{BN} and H_1 with the Pf states as a function of κ and δV_1 , respectively; results for only alternate L are shown for clarity.

(shown as dashes) are in qualitative and semiquantitative agreement with the actual band. The somewhat worse agreement at the smallest L in the exciton branch in Fig. 2 and at the largest L in Fig. 3 suggests that the Pf model is less accurate for short distance physics, because the Pf QH and the Pf QP in the exciton branch are at their closest separation at the smallest angular momentum (L =4) and the two QHs are nearest at the largest L in Fig. 3. These comparisons demonstrate that, with LL mixing, the Pf physics emerges for quasiparticles and quasiholes.



FIG. 3 (color online). Same as in Fig. 2 but for two Pf quasiholes at 2Q = 2N - 2 = 30.

(Results are only shown for the largest systems we have studied; those from smaller systems are also consistent.)

To investigate the robustness of this physics to the precise form of the interaction, we have studied the effect of a variation of the pseudopotentials. For ease of presentation, we set $\delta V_m = 0$ and retain only the dominant three body pseudopotentials of the BN model. In Fig. 5 we vary W_3 and W_6 , and take $W_5 = 0.367W_3$ (as in the BN interaction). We can conclude that there is a range of parameters where the Pf physics is valid. The slightly worse agreement for Pf QHs in this figure as well as in Fig. 3 can be attributed to the closer proximity of this system to the APf, leading to a stronger interference with the APf physics. This, however, is a finite size effect and should not be relevant in the thermodynamic limit where either the Pf or the APf ground state would be chosen.

The importance of finite quantum well width *w* has been stressed previously [13]. To assess the role of LL mixing for a system with finite thickness, we have studied an approximate model in which we modify V_{Coulomb} (assuming infinite square quantum well confinement) and rescale δV and δW by the ratio $V_{\text{Coulomb}}(m = 1, w)/V_{\text{Coulomb}}(m = 1, w = 0)$ (which is 0.91 for $w = 3\lambda$). The optimal values of κ shift downward with increasing thickness, as seen in Figs. 1(e) and 5(e)–5(g). We note that, in the absence of LL mixing, the Pf QH and Pf QP states do not improve as rapidly with increasing thickness as does the Pf ground state.

The assumption of full spin polarization is not always justified. The 5/2 FQHE has been seen at a moderately high field of B = 10 T [26], where the state is expected to be fully spin polarized, but also at very low fields [27]. There is numerical evidence that the 5/2 state remains fully polarized even at low fields [10,22,28]. Inelastic light scattering experiments suggest a lack of full spin polarization at somewhat elevated temperatures [29], but do not directly probe the 5/2 FQHE state, and can be explained [30] in terms of a polarized ground state with disorder



FIG. 4 (color online). Same as in Fig. 2 but for two Pf quasiparticles at 2Q = 2N - 4 = 28.

f+2QH

-0.05

 w/λ^2

0.00

0

(f) Pf+2QHs

 $\frac{1}{w/\lambda}^2$

W₂

(a) F

0.00 - (C)

0.00 Š

-0.03

× 8

-0.03

3

2

1

0 (e)

0

¥

1.0

0.8

0.6

0.4

0.2

0.0

-2 00

-5]

-20

0.00

W₃

(q) Pf+2QPs

 $\frac{1}{w/\lambda}^2$



value of 3.

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(b) APt

(d) Pf+2QPs

-0.05

0

aided depolarization due to e/2-charged Skyrmions. We have not considered the effect of disorder [31].

LL mixing typically results in a reduction of the gap. However, due to the strengthening of the Pf physics, the 5/2 gap in our calculations slightly increases until $\kappa \approx 1.5$ before it begins to decrease. This is nicely consistent with the observation of a robust 5/2 FQHE at very low magnetic fields (~2.5 T) [27]. Figures 5(f) and 5(g) suggest the possibility that LL mixing might actually be essential for establishing the Pf physics for the quasiparticles and quasiholes, but further theoretical and experimental work will be needed to settle this issue.

In summary, our principal result is that there exists a realistic Hamiltonian, including LL mixing, for which the Pf physics is demonstrably established not only for the ground state but for the excitations as well.

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Note added in proof.—Recent unpublished experiments by Wei Pan and collaborators have demonstrated 5/2 FQHE down to B = 0.8 T where κ assumes a large