Landau Level Mixing and the Ground State of the $\nu = 5/2$ Quantum Hall Effect

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Inter-Landau-level transitions break particle hole symmetry and will choose either the Pfaffian or the anti-Pfaffian state as the absolute ground state at 5/2 filling of the fractional quantum Hall effect. An approach based on truncating the Hilbert space has favored the anti-Pfaffian. A second approach based on an effective Hamiltonian produced the Pfaffian. In this Letter, perturbation theory is applied to finite sizes without bias to any specific pseudopotential component. This method also singles out the anti-Pfaffian. A critical piece of the effective Hamiltonian, which was absent in previous studies, reverts the ground state at 5/2 to the anti-Pfaffian.

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Topological phases of matter have been the focus of much recent theoretical interest. A prime example of such a phase [1], which is realized in experiment, is the fractional quantum Hall effect [2,3] (FQHE). The most intriguing of these quantum Hall states occurs in the half-filled first excited Landau level (1LL) [4]. Breaking the odd-denominator trend of the lowest Landau level (LLL), the state at $\nu = 5/2$ is one of the strongest FQHE states in the 1LL [5,6]. It has been the subject of numerous studies and is widely believed to be in the universality class of the Moore-Read (MR) state [7], which is a fully polarized $p_x + ip_y$ paired state [8] of composite fermions [9]. The MR state possesses richer excitations than states dominating the LLL. In particular, the presence of the neutral Majorana fermion mode results in quasiparticle excitations exhibiting non-Abelian statistics [7,10–12]. This property has greatly increased interest in the 5/2 effect, in part due to its potential for quantum information processing [13,14]. In this Letter we will assume the MR state to be the underlying phase of the 5/2 effect [15–18].

Particle-hole symmetry and the anti-Pfaffian.—Earlier studies of the 5/2 state disallowed virtual inter-LL transitions, which are only exact at infinite cyclotron energy $\hbar\omega$. In that case, because of particle-hole (p-h) symmetry, both the MR or (Pfaffian) state and its p-h conjugate [19,20] (the anti-Pfaffian) are equally valid candidates for the 5/2 state. However, they are distinct topological phases [19,20] of matter. The system will then be forced to choose one by spontaneously breaking p-h symmetry. On the other hand, the ubiquity of LL mixing provides a p-h symmetry breaking field. A measure of the mixing strength is given by the ratio of typical Coulomb energy $\varepsilon = e^2/4\pi\epsilon_0\ell$ to the cyclotron energy $\kappa = \varepsilon/\hbar\omega$, where ℓ is the magnetic length. In experiments, κ varies from 0.8 to 2.8 and either the Pfaffian (Pf) or the anti-Pfaffian (aPf) will be favored as the ground state. Until now, however, which one has not been definitively determined. What is not controversial is the more important issue of non-Abelian braiding statistics, which is shared by both [19–21].

To address the effects of p-h symmetry breaking, several studies have been carried out using different approximations. Simon and the present author [22] employed a truncated model of LL mixing, keeping only 3 LLs (3-LL model). Additionally we controlled the number of particle and hole excitations that result from inter-LL transitions. In a subsequent work by Zaletel *et al.* [23], this last restriction was completely removed, while 3-5 LLs were retained. The authors employed an infinite density matrix renormalization group (iDMRG) [24]. The method incorporates the matrix product form [25,26] of FQHE states on a cylinder of infinite length but finite radius. Both studies predict the aPf to be favored irrespective of the strength of κ.

On the other hand, Wojs *et al.* [27] and more recently Pakrouski *et al.* [28] have concluded that the Pf is the ground state. The authors used effective two-body [29] and three-body[30] pseudopotentials [31–33] that include LL-mixing corrections to the lowest order in κ. At first sight, these calculations cast doubt on the results of the 3-LL model.

In this Letter the issue is revisited in order to resolve this discrepancy and to compare the 3-LL model predictions to perturbation theory results. The recent calculations of infinite-size pseudopotentials produced a three-way agreement [31–33] on their values and are not the cause of the discrepancy.

Our approach to calculating the effective Hamiltonian closely follows the previous methods but uses the torus geometry for finite-size systems. This is the only compact geometry that avoids the shift [34] and facilitates the comparison between Pfaffian and anti-Pfaffian. A study on the sphere is also reported in this Letter which corroborates the torus results. For this and subsequent torus results we will follow the method of Wojs *et al.* and Pakrouski *et al.* and use infinite-size perturbation theory (PT) values of the two-body and the three-body pseudopotentials.

The Hamiltonian allowing inter-LL transitions is

$$\mathcal{H} = \frac{1}{2}\sum_{\{m_i\}} \langle m_1 m_2|V|m_3 m_4\rangle C^\dagger_{m_1} C^\dagger_{m_2} C_{m_3} C_{m_4}, \qquad (1)$$

where m is the combined label of LL index n, linear momentum k, and spin. $V(r)$ is the Coulomb interaction. For most of this work we will consider the electron layer width $w = 0$. The matrix elements in H, which are independent of spin, are calculated self-consistently for up to 31 LLs for each size that we studied. Another important difference with infinite-size calculations is that the three-body pseudopotential corrections are not singled out by their relative angular momentum but are automatically included in their entirety.

The effective Hamiltonian, which includes the lowest order LL-mixing corrections can be written as

$$H_{\rm eff} = H_1 + \kappa \sum_p{}' \frac{\mathcal{H}|p\rangle\langle p|\mathcal{H}}{E_0 - E_p}, \qquad (2)$$

where H_1 is the Hamiltonian for electrons in the partially filled 1LL and $|p\rangle$ is an intermediate state with kinetic energy E_p, which can have at most two electrons in the excited LLs with index $n > 1$. E_0 is the common kinetic energy of the appropriate basis states (described below) and is dropped from $H_{\rm eff}$. The prime on the sum restricts p so that $E_p \neq E_0$. In Eq. (2), the Hamiltonians are expressed in units of ε and kinetic energies are given in units of the cyclotron energy.

We will generally consider the matrix elements $\langle i|H_{\rm eff}|j\rangle$, where the set $\{|i\rangle\}$ is a relevant Slater determinant basis for N_e valance electrons in the 1LL and includes a lowest LL filled with both spins. We will choose $N_e = 2$ or 3 when calculating pseudopotentials. This form is also readily applicable when the degeneracy is not completely lifted after the action of H_1, which is the case for certain odd electron numbers on a hexagonal torus [35]. In this case, the ground state that represents the basis $\{|i\rangle\}$ is a doublet.

The last term of $H_{\rm eff}$ can be represented by Feynman diagrams, which have already appeared in print [32,33] and will not be repeated here. It is then a bookkeeping exercise; details can be found in Ref. [33]. The results are one-, two-, and three-body effective interactions for electrons in the 1LL. However, the one-body potentials, by translational symmetry, are independent of an orbital index. Since they only serve to modify the chemical potential, they will be ignored. It will be assumed throughout that the states in the 1LL are fully spin polarized, which is consistent with recent experiments [36,37] as well as with previous calculations [15,22,38]. However, virtual reversed spin excitations from the LLL are allowed. Even these make a negligible difference and can be ignored.

In the case of a doublet ground state of the H_1, we follow Landau and Lifshitz [39] and diagonalize the LL-mixing part of the H in the two-dimensional Hilbert space spanned by the doublet, which separates the Pf and the aPf components without mixing in any other state of the H_1. Figure 1 shows the difference in the energies $\Delta_0 = |E_{\rm Pf} - E_{\rm aPf}|$ as a function of the number of LLs included in the sum of Eq. (2). As observed in the 3-LL model [22,23], the aPf is favored unless only the lowest 2 LLs are kept. The inset shows Δ_0/N_e as a function of $1/N_e$. While the linear regime has not quite been reached and it is difficult to extrapolate to large sizes, the results are consistent with an extensive "gap" [23].

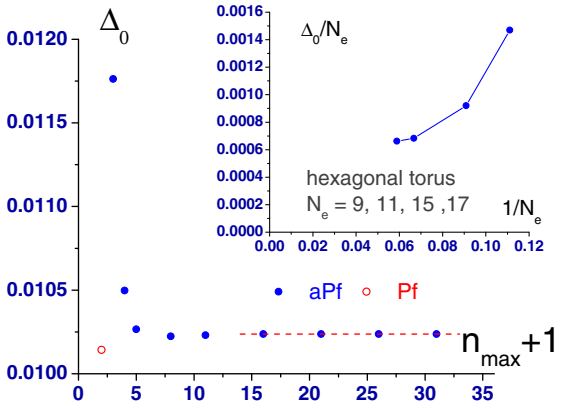

FIG. 1. Plot of Pf-aPf energy difference $\Delta_0 = |E_{\rm Pf} - E_{\rm aPf}|$ (in units of $\varepsilon\kappa$) between the aPf and Pf as a function of the number of LLs included in the present calculation ($n_{\rm max}$ is the index of the highest LL). The Pf ground state occurs only when the lowest two LLs are kept. The inset shows Δ_0 for odd sizes divided by the number of electrons plotted vs $1/N_e$.

Two-body and three-body pseudopotentials.—A very convenient way of presenting the electronic interaction potential for quantum Hall states is to express it in terms of

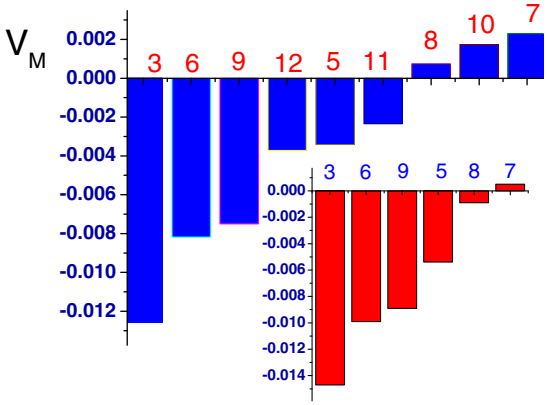

FIG. 2. The three-body pseudopotentials (in units of $\varepsilon\kappa$) for the lowest 9 relative angular momenta M on the torus for $N_\phi = 30$ and arranged in ascending order, where N_ϕ is the number of magnetic flux quanta. The values of angular momenta are indicated above the corresponding bar. The inset shows the infinite-size PT values. In contrast, the low M pseudopotentials for the first point in Fig. 1 (a 2-LL system that results in the Pf ground state) are repulsive: 0.0148 ($M = 3$), 0.0085 (6), 0.0029 (8), 0.0023 (9), etc.

TABLE I. Comparison of the differences between three-body pseudopotentials V_M for polarized electrons and finite flux sizes and their infinite size counterparts. The percent differences are given in the parentheses. For $N_\phi = 34$, the corresponding entries for $M = 7$ and 8 pseudopotentials are, respectively, 0.0152 (1.97%) [0.0152] and 0.0134 (2.90%) [0.0138]. The infinite-size values are given in brackets.

N_ϕ	$V_6 - V_3$	$V_9 - V_3$	$V_{12} - V_3$	$V_5 - V_3$
30	0.0044 (8.3%)	0.0051 (12%)	0.0088	0.0091 (2.2%)
32	0.0044 (8.3%)	0.0051 (12%)	0.0090	0.0092 (1.1%)
34	0.0045 (7.0%)	0.0052 (10%)	0.0090	0.0092 (1.1%)
∞	0.0048	0.0058	NA	0.0093

the energy (or pseudopotential) for n electrons in a state of fixed relative angular momentum. It was first introduced by Haldane [29] for the two-body case and later extended to n-body interactions by Simon *et al.* [30]. Figure 2 gives the values of the three-body pseudopotentials V_M (in units of $\varepsilon\kappa$) in an ascending order. The inset gives the results of Sodemann and MacDonald, who crucially calculated V_9. In both cases the most important pseudopotentials have relative angular momenta that are multiples of 3 [40]. The main difference between the present effective Hamiltonian and those of Wojs *et al.* and Pakrouski *et al.* is the $M = 9$ three-body pseudopotential. It will be shown that V_9 has a critical role in determining the nature of the ground state. If included, the ground state reverts to the aPf. Table I gives the differences of V_M from the $M = 3$ value for finite-size systems in the present study and compares them with their infinite-size values. Table II is the same as Table I but for two-body pseudopotentials, which already are very close to their infinite size values.

In the remainder of this Letter the effective Hamiltonian for the infinite system (see Table II and the inset of Fig. 2) will be used. While the first five pseudopotentials (in order of their relative angular momenta) are unique, the $M = 9$ has two states and a choice of basis is necessary. The Hamiltonian matrix for $M = 9$ and its corresponding basis wave functions are described by Sodemann and MacDonald [33] and Laughlin [41], respectively. It is

TABLE II. The LL-mixing corrections δv_m for two-body pseudopotentials v_m (in units of $\varepsilon\kappa$) relative to their respective δv_1 values, for three different flux sizes on the torus. For polarized electrons only odd values of relative angular momentum m are relevant. The percent differences from infinite PT results (last row) are given in parentheses.

N_ϕ	$\delta v_3 - \delta v_1$	$\delta v_5 - \delta v_1$	$\delta v_7 - \delta v_1$	$\delta v_9 - \delta v_1$
30	0.1094 (0.45%)	0.1767 (0.62%)	0.1994 (0.75%)	0.2067 (0.86%)
32	0.1094 (0.45%)	0.1769 (0.51%)	0.1996 (0.65%)	0.2069 (0.77%)
34	0.1095 (0.36%)	0.1770 (0.45%)	0.1998 (0.55%)	0.2071 (0.67%)
∞	0.1099	0.1778	0.2009	0.2085

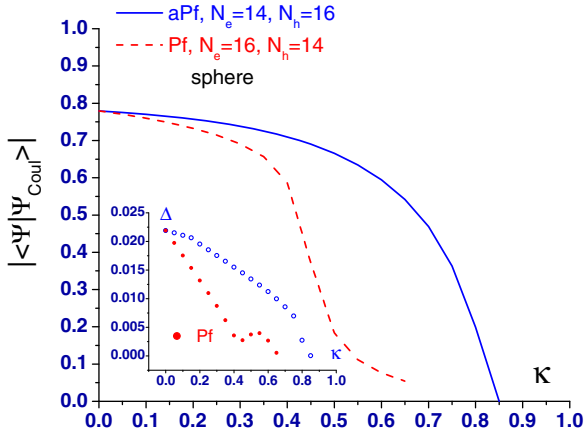

FIG. 3. Plot of overlaps of the ground state of the coulomb interaction with the aPf (solid) and Pf (dashed) vs κ. The inset is the respective energy gap (in units of ε) vs κ in each case. The sudden bends and kinks in the gaps result from level crossings of the lowest excited state.

$$H(M=9) = -0.0088|\mathbf{0},\mathbf{3}\rangle\langle\mathbf{0},\mathbf{3}| + 0.0033|\mathbf{3},\mathbf{1}\rangle\langle\mathbf{3},\mathbf{1}| + 0.0007[|\mathbf{0},\mathbf{3}\rangle\langle\mathbf{3},\mathbf{1}| + |\mathbf{3},\mathbf{1}\rangle\langle\mathbf{0},\mathbf{3}|], \quad (3)$$

where the states $|\boldsymbol{l},\boldsymbol{m}\rangle$ have relative angular momentum $M = 2l + 3m$. The relevant pseudopotentials and their projection operators are obtained by finding the eigenvalues and eigenvectors of Eq. (3). However, $H(M = 9)$ is well approximated by just the first term, which is the most dominant by far.

The effective Hamiltonian, including the $M = 9$ term, is then diagonalized. In general, the eigenvectors will have a nonlinear dependence on κ. However, the linear regime will suffice for our conclusions.

Since on the sphere the Pf and aPf have different shifts, the Pf for N_e electrons is compared to the aPf with

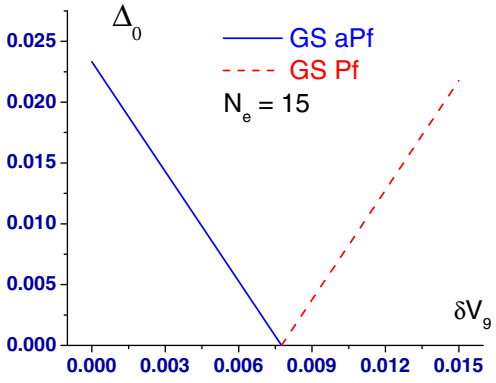

FIG. 4. Plot of the aPf-Pf energy difference for $N_e = 15$ as a function of δV_9. The solid line indicates the ground state is the aPf, while the dashed line indicates the Pf ground state. The transition point is at $\delta V_9 \approx 0.0077$. Before the transition the overlap of the ground state with the aPf is 0.70; there is no overlap with the Pf. After the transition these values are exchanged.

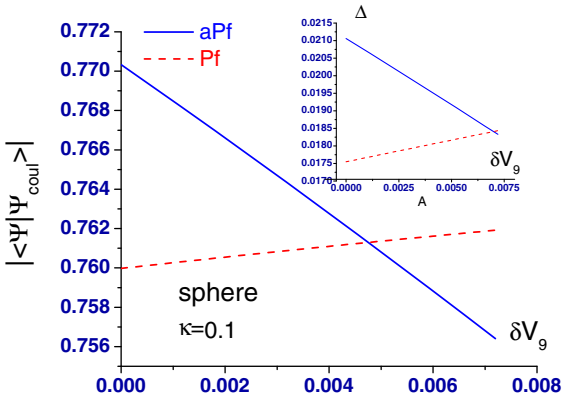

FIG. 5. Plot of overlaps and respective gaps (inset in units of ε) vs δV_9 of the aPf ($N_e = 14$) and the Pf ($N_e = 16$) on the sphere for $\kappa = 0.1$.

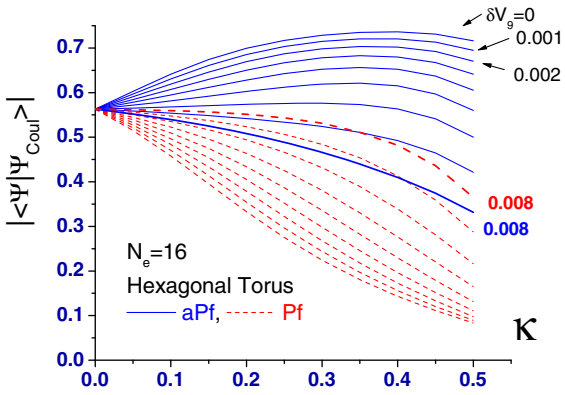

FIG. 6. Plot of overlaps for the aPf (solid line) and the Pf (dashed line) as a function of κ for a sequence of δV_9 values in increments of 0.001. The top and bottom curves are for $\delta V_9 = 0$. The second from top (and bottom) are for 0.001, etc. The system undergoes a phase transition at $\delta V_9 \approx 0.008$.

$N_e - 2$ electrons, so that the number of holes $N_h = N_e$. This introduces finite-size effects and excludes an energetic comparison of the two.

Instead we will compare overlaps and the gaps between respective ground state and the lowest excited state [28]. The gaps track the overlaps and provide another diagnostic tool. Figure 3 shows the results for $N_e = 16$ for the Pf and $N_e = 14$ for the aPf. It can be seen that now the aPf has the larger overlaps and gaps.

Transition to the Pfaffian.—Clearly, there will be a phase transition as the V_9 pseudopotential approaches zero. Making it less attractive weakens the aPf; at $V_9 \approx -0.0011$ a first order transition to the Pf is observed. The results for the $N_e = 15$ doublet on the torus is shown in Fig. 4. In this case the aPf-Pf energy difference Δ_0 displays a perfectly linear dependence on $V_9 (= -0.0088 + \delta V_9)$. It is noteworthy that to reach the point of transition the magnitude of V_9 has to be reduced by approximately 90% of its nominal value, which is a measure of how robust the ground state is.

The linear dependence on V_9 is also seen on the sphere (Fig. 5). The trend of the gaps, shown in the inset, track the corresponding overlaps. The Pf and the aPf have opposing dependence on V_9. The transition point cannot be accurately determined, but it is between the crossing points of overlaps and the gaps.

Since there is no shift on the torus, comparison of the two states is straightforward. Figure 6 shows the overlaps as a function of κ for a series of δV_9 values. The dependence on V_9 for each κ is also linear (not shown). In contrast to the sphere results for small κ, there is opposing dependence of the overlaps on κ, with the aPf increasing and Pf decreasing. Increasing δV_9 past 0.008 reverses the trend and the overlap with the Pf increases with κ.

Finally, we consider Du's experiment [42] ($\kappa = 0.8$ and layer width $w = 2.5\ell$). With these values [43] we obtain the following overlaps for $N_e = 16$: aPf 63% (55%) and Pf 9.9% (6.6%) for $\kappa = 0.7(0.8)$, which are comparable to those of Fig. 6. Also included are overlaps for $\kappa = 0.7$.

Discussion.—Entanglement properties rather than high overlaps are a better indicator of which topological phase of matter a particular state may belong. These have already been reported for the aPf ground state of the Coulomb potential, both on the cylinder [23] and on the sphere [28]. However, very high overlaps can be reached (97%, $\kappa = 2.1$ for $N_e = 14$ on the sphere and 96%, $\kappa = 1.5$ for $N_e = 16$ on the hexagonal torus) by adiabatically varying the effective Hamiltonian to include only the three (V_3, V_6, and V_9) strongest of the three-body pseudopotentials and the Bishara-Nayak two-body pseudopotentials used by Woj *et al.* This can be done without encountering a phase transition. While these parameters may seem unjustified or unphysical, they do suggest a broader phase diagram for the aPf ground state.

We have shown that under plausible experimental conditions the aPf is found to be favored for small LL mixing. The only exception is when just the lowest two LLs are kept, then the Pf is preferred.

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