Landau-level-mixing and the ground state of the $\nu = 5/2$ quantum Hall effect

Edward H. Rezayi
Department of Physics, California State University Los Angeles, Los Angeles, CA 90032, USA

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 pseudo-potential 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.

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 [4, 5]. It has been the subject of numerous studies and is widely believed to be in the universality class of the Moore-Read (MR) state [6], which is a fully polarized $p_x + ip_y$ paired state of composite fermions [7]. The MR state possesses richer excitations than states dominating the LLL. In particular, the presence of the neutral Majorana fermion mode results in quasi-particle 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, while both states display non-Abelian statistics, 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 $\ell$ is the magnetic length. In experiments, $\kappa$ 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.

To address the effects of P-H symmetry-breaking, several studies have been carried out using different approximations. Simon and the present author [21] employed a truncated model of LL-mixing by 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. [22] this last restriction was completely removed. The authors employed an infinite density matrix renormalization group (iDMRG) [23]. The method incorporates the matrix product form [24, 25] of FQHE states on a cylinder of infinite length but finite radius. The iDMRG also kept a finite number of LLs (3-5), but could reach cylinder circumferences of 20 magnetic lengths. A square torus of this dimension would include about 30 electrons, which is a considerable increase in system size over previous studies. Both approaches predict the aPf to be favored irrespective of the strength of $\kappa$.

On the other hand, Wojs et al. [26] and more recently Pakrouski et al. [27] have concluded that the Pf is the ground state. The authors used the effective 2-body [28] and 3-body [29] pseudo-potentials [30–32] that include LL-mixing corrections to the lowest order in $\kappa$. At first sight, these calculations have 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 pseudo-potentials produced a 3-way agreement [30–32] 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 [33] 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 2-body and the 3-body pseudo-potentials.

The Hamiltonian allowing inter-LL transitions is

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

where $m$ is the combined label of LL index $n$, linear
momentum \( k \), and spin. \( V(r) \) is the Coulomb interaction. We will consider the electron layer to have zero width. The matrix elements in \( \hat{H} \), 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 3-body pseudo-potential 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:

\[
H_{\text{eff}} = H_1 + \kappa \sum_p \frac{\hat{H}(p)\langle p|\hat{H}}{E_0 - E_p},
\]

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 kinetic energy of the appropriate basis states (described below) and is dropped from \( H_{\text{eff}} \). The prime on the sum restricts \( p \) so that \( E_p \neq E_0 \). In Eq. 2, the Hamiltonians are expressed in units of \( \varepsilon \) and kinetic energies are given in units of the cyclotron energy.

We will generally consider the matrix elements \( \langle i|H_{\text{eff}}|j\rangle \), where the set \( \{|i\} \) is a relevant Slater determinant basis for \( N_e \) valence electrons in the 1LL and includes a lowest LL filled with both spins. We will choose \( N_e = 2 \) or 3 when calculating pseudo-potentials. 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[34]. In this case, the ground state that represents the basis \( \{|i\} \) is a doublet. Extra degeneracies of this type result from the combination of anti-unitary P-H conjugation and unitary discrete rotational symmetries[35].

It can be seen from the definition of the basis states that the two creation operators of the right \( \hat{H} \) acting on \( |i\rangle \) (and destruction operators of the left \( \hat{H} \) acting on \( |j\rangle \) will have LL indices of either 0 or 1. It is therefore convenient to organize \( \hat{H} \) in terms of the number of LL holes \( (0, 1, 2) \) in \( |p\rangle \). For example, in the case of two holes, one can ignore the intermediate states \( |n_1, n_2\rangle \), where \( n_i > 1 \) are excited LL indices, since these terms do not depend on the specifics of \( |i\rangle \) and \( |j\rangle \) and amount to an overall constant in Eq. 2. The last term of \( H_{\text{eff}} \) can be represented by Feynman diagrams, which have already appeared in print[31, 32] and will not be repeated here. It is then a bookkeeping exercise; some relevant details can be found in the appendices B and C of Sodemann and MacDonald. The results are 1, 2, and 3-body effective interactions for electrons in the 1LL. However, the one-body potentials, by translational symmetry, are independent of orbital index. Since they only serve to modify the chemical potential, they will also 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, 21, 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 2-dimensional Hilbert space spanned by the doublet, which separates the Pf and the aPf components without mixing in any other state of the \( H_1 \). Fig. 1 shows the difference in the ground state energy difference \( E_{\text{Pf}} - E_{\text{aPf}} = \Delta_0 \) as a function of the number of LLs included in the sum of Eq. 2. As observed in the 3-LL model, the aPf is favored unless only the lowest 2 LLs are kept. The inset shows \( \Delta_0 \) for odd sizes divided by the number of electrons plotted vs \( 1/N_e \).

2-body and 3-body pseudo-potentials.- A very practical way of presenting the electronic interaction potential for quantum Hall states is to express them in terms of the energy (or pseudo-potential) for \( n \)-electrons in a state of fixed relative angular momentum. It was first introduced by Haldane[28] for the 2-body case and later extended to the \( n \)-body case by Simon et. al.[29]. Fig. 2 gives the values of the 3-body pseudo-potentials \( V_M \) (in units of \( \varepsilon k \)), in an ascending order. The first 5 are labeled by their relative angular momenta \( M \). The inset gives the results of Sodemann and MacDonald, who crucially calculated \( V_0 \). In both cases the most important pseudo-potentials 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 $M=9$ 3-body pseudo-potential. 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 counterparts. Table II is the same as Table I but for 2-body pseudo-potentials, which are only available for the ground state reverts to the aPf vs. $\kappa$ in each case. The sudden bends and kinks in the gaps result from level crossings of the lowest excited state.

In the remainder of this letter the effective Hamiltonian for the infinite system (see Table II) will be used. While the first five pseudo-potentials (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[32] and Laughlin[41] respectively. It is:

\[
H(M=9) = -0.0088\langle 0,3\rangle\langle 0,3\rangle + 0.0033\langle 3,1\rangle\langle 3,1\rangle + 0.0007 \left[ \langle 0,3\rangle\langle 3,1\rangle + \langle 3,1\rangle\langle 0,3\rangle \right],
\]

where the states $|l,m\rangle$ have relative angular momentum $M = 2l + 3m$. The relevant pseudo-potentials 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 eigenvalues and eigenvectors will have a non-linear dependence on $\kappa$. However, the linear regime will suffice for our conclusions.

The majority of numerical calculations on the 5/2 state have been carried out in the spherical geometry[28]. Because of the different shifts for Pf and aPf on the sphere, P-H symmetry is not applicable. Comparing the Pf with aPf(solid) and Pf(dashed) vs. $\kappa$. The inset is the respective energy gap (in units of $\varepsilon\kappa$) vs. $\kappa$ in each case. The sudden bends and kinks in the gaps result from level crossings of the lowest excited state.
includes any meaningful energetic comparison between Pf and aPf.

As in the Pakrouski et al. paper, we compare overlaps and gaps between the ground and the first excited state. As noted by these authors, the gap in the spectrum tracks the respective overlaps and may provide another diagnostic tool. Fig. 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 \( V_9 \) pseudo-potential 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 \( \Delta_0 \) 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. While the effect of a finite thickness of the 2-D layer has been ignored here, it seems unlikely that it could have a qualitative effect on the properties of the ground state.

The linear dependence on \( V_9 \) is also seen on the sphere for both gaps and overlaps (Fig. 5). The trend of the gaps, shown in the inset, track those of the corresponding overlaps. The Pf and the aPf have opposing dependence on \( V_9 \). It is difficult to pin-point the transition point with any accuracy here, but it is somewhere between the crossing points of overlaps and the gaps. This is just a finite-size effect due to the size mismatch between the Pf and aPf, which prevents the two states from competing

**Discussion.**– Entanglement properties rather than high overlaps are a better indicator of which topological phase of matter a particular state may belong to. These have already been reported for the aPf ground state of the for the same ground state.

Since there is no shift on the torus, comparison of the two states is straightforward. Fig. 5 shows the overlaps as a function of \( \kappa \) for a series of \( \delta V_9 \) values. The dependence on \( V_9 \) for each \( \kappa \) is also linear (not shown). In contrast to the sphere results for small \( \kappa \), there is opposing dependence of the overlaps on \( \kappa \), with the aPf increasing and Pf decreasing. Increasing \( \delta V_9 \) past 0.008 reverses the trends and the overlap with the Pf increases with \( \kappa \).

**FIG. 4.** (Color online) Plot of the aPf-Pf energy difference for \( N_e = 15 \) as a function of \( \delta V_9 \). 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.** (Color online) Plot of overlaps and respective gaps (inset in units of \( \varepsilon \) ) vs. \( \delta V_9 \) of the aPf \((N_e = 14)\) and the Pf \((N_e = 16)\) on the sphere for \( \kappa = 0.1 \).

**FIG. 6.** (Color online) Plot of overlaps for the aPf (solid) and the Pf (dashed) as a function of \( \kappa \) for a sequence of \( \delta V_9 \) values in increments of 0.001. The top and bottom curves are for \( \delta V_9 = 0 \). The second top (and bottom) are for 0.001, etc. The system undergoes a phase transition at \( \delta V_9 \approx 0.008 \).
Coulomb potential, both on the cylinder\cite{22} and on the sphere\cite{27}. However, very high overlaps can be reached (97\%, $\kappa = 2.1$ for $N_c = 14$ on the sphere and 96\%, $\kappa = 1.5$ for $N_c = 16$ on the hexagonal torus) by adiabatically varying the effective Hamiltonian to include only three ($V_3$, $V_6$, and $V_9$) of the 3-body pseudo-potentials and the Bishara-Nayak 2-body pseudo-potentials used by Woj's et. al. This can be done without encountering a phase transition. While these parameters may seem unjustified or unphysical they do establish 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 parameters. The only exception is when just the lowest two LLs are kept, then the Pf is preferred. A reversal to the Pf at very large sizes cannot be ruled out by the present study. However, the aPf ground state appears to be robust, particularly on the torus, making such a reversal unlikely.

I thank Jainendra Jain, Thierry Jolicoeur, Kyril Pakrouski, and Mike Peterson for discussions and correspondence. I also thank Thierry Jolicoeur, Roger Mong, Zlatko Papic, Steve Simon, and Mike Zaletel for comments and suggestions and particularly Mike Zaletel for encouraging me to resolve the discrepancy between the two approaches. This work is supported by DOE Grant de-sc0002140.

---

1. X.-G. Wen, International Journal of Modern Physics B 06, 1711 (1992)
2. H. L. Tsui, D. C. Stormer and A. C. Gossard, Phys. Rev. Lett. 48, 1559 (1982).
3. R. B. Laughlin, Phys. Rev. Lett. 50, 1395 (1983).
4. R. Willett, J. P. Eisenstein, H. L. Störmer, D. C. Tsui, A. C. Gossard, and J. H. English, Phys. Rev. Lett. 59, 1766 (1987).
5. W. Pan, J.-S. Xia, V. Shvarts, D. E. Adams, H. L. Stormer, D. C. Tsui, L. N. Pfeiffer, K. W. Baldwin, and K. W. West, Phys. Rev. Lett. 83, 3530 (1999).
6. J. S. Xia, W. Pan, C. L. Vicente, E. D. Adams, N. S. Sullivan, H. L. Stormer, D. C. Tsui, L. N. Pfeiffer, K. W. Baldwin, and K. W. West, Phys. Rev. Lett. 93, 176802 (2004).
7. G. Moore and N. Read, Nuclear Physics B 360, 362 (1991).
8. N. Read and D. Green, Phys. Rev. B 61, 10267 (2000).
9. J. K. Jain, Phys. Rev. Lett. 63, 199 (1989).
10. C. Nayak and F. Wilczek, Nuclear Physics B 417, 359 (1994).
11. N. Read and E. Rezayi, Phys. Rev. B 54, 16864 (1996).
12. N. Read, Phys. Rev. B 79, 045308 (2009).
13. A. Kitaev, Annals of Physics 321, 2 (2006) January Special Issue.
14. C. Nayak, S. H. Simon, A. Stern, M. Freedman, and S. Das Sarma, Rev. Mod. Phys. 80, 1083 (2008).
15. R. H. Morf, Phys. Rev. Lett. 80, 1505 (1998).
16. E. H. Rezayi and F. D. M. Haldane, Phys. Rev. Lett. 84, 4685 (2000).
17. X. Wan, Z.-X. Hu, E. H. Rezayi, and K. Yang, Phys. Rev. B 77, 165316 (2008).
18. J. Zhao, D. N. Sheng, and F. D. M. Haldane, Phys. Rev. B 83, 51515 (2011).
19. M. Levin, B. I. Halperin, and B. Rosenow, Phys. Rev. Lett. 99, 236806 (2007).
20. S.-S. Lee, S. Ryu, C. Nayak, and M. P. A. Fisher, Phys. Rev. Lett. 99, 236807 (2007).
21. E. H. Rezayi and S. H. Simon, Phys. Rev. Lett. 106, 116801 (2011).
22. M. P. Zaletel, R. S. K. Mong, F. Pollmann, and E. H. Rezayi, Phys. Rev. B 91, 045115 (2015).
23. M. P. Zaletel, R. S. K. Mong, and F. Pollmann, Phys. Rev. Lett. 110, 236801 (2013).
24. M. P. Zaletel and R. S. K. Mong, Phys. Rev. B 86, 245305 (2012).
25. B. Estienne, Z. Papić, N. Regnault, and B. A. Bernevig, Phys. Rev. B 87, 161112 (2013).
26. A. Wójcik, C. Tóke, and J. K. Jain, Phys. Rev. Lett. 105, 096802 (2010).
27. K. Pakrouski, M. R. Peterson, T. Jolicoeur, V. W. Scarola, C. Nayak, and M. Troyer, Phys. Rev. X 5, 021004 (2015).
28. F. D. M. Haldane, Phys. Rev. Lett. 51, 605 (1983).
29. S. H. Simon, E. H. Rezayi, and N. R. Cooper, Phys. Rev. B 75, 195306 (2007).
30. S. H. Simon and E. H. Rezayi, Phys. Rev. B 87, 155426 (2013).
31. M. R. Peterson and C. Nayak, Phys. Rev. B 87, 245129 (2013).
32. L. Sodemann and A. H. MacDonald, Phys. Rev. B 87, 245425 (2013).
33. The shift $S$ is defined by the flux-charge equation $N_\phi = v_\phi^2 - N_e - S$, where $v_\phi$ is the filling factor of the valence electrons. On the sphere S=3 and -1 for the Pf and aPf respectively.
34. Z. Papić, F. D. M. Haldane, and E. H. Rezayi, Phys. Rev. Lett. 109, 266806 (2012).
35. M. Tinkham, Group Theory and Quantum Mechanics (McGraw-Hill Book Company, New York, 1964).
36. J. P. Eisenstein, L. N. Pfeiffer, and K. W. West, ArXiv e-prints (2017), arXiv:1701.0463 [cond-mat.mes-hall].
37. L. Tiemann, G. Gamez, N. Kumada, and K. Muraki, Science 335, 328 (2012).
38. A. E. Feiguin, E. Rezayi, K. Yang, C. Nayak, and S. Das Sarma, Phys. Rev. B 79, 115322 (2009).
39. L. D. Landau and E. M. Lifshitz, Quantum Mechanics (Pergamon Press, Oxford, 1977).
40. It can be seen that finite-size effects become larger as $M$ is increased. For larger $M$s the average relative distance between the particles increases and may become comparable to the linear dimension of the system. As a result the $M = 12$ may be off by 15-20% of its infinite-size value.
41. R. B. Laughlin, Phys. Rev. B 27, 3383 (1983).