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Breaking of Particle-Hole Symmetry by Landau Level Mixing in the $\nu = \frac{5}{2}$ Quantized Hall State

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We perform numerical studies to determine if the fractional quantum Hall state observed at filling $\nu = 5/2$ is the Moore-Read wavefunction or its particle hole conjugate, the so-called AntiPfaffian. Using a truncated Hilbert space approach we find that for realistic interactions, including Landau-level mixing, the ground state remains fully polarized and the AntiPfaffian is strongly favored.

Over the last twenty years one of the most intriguing puzzles in condensed matter physics has been the nature of an "even denominator" quantum Hall state observed[1] at filling fraction $\nu = 5/2$. Shortly after its discovery it was shown[2] that the 5/2 plateau disappears when a sufficiently strong in-plane magnetic field is applied to the 2-D electron layer. This observation was widely assumed to indicate a spin-singlet (or partially polarized) ground state, since increasing the in-plane field would force the spins to align and destroy such a ground state. However, numerical results by Morf[3] showed that in a relatively large finite size system, the polarized state is preferred over spin-singlets even in the absence of the Zeeman gap. There is now agreement among numerical calculations[3–5], using a variety of techniques and in different geometries, that the polarized ground state is adiabatically connected to a gapped phase, generally believed to be the Moore-Read[6] Pfaffian (Pf) state, but lies very close to a quantum phase transition to a compressible phase so that small changes in details, such as tilting the magnetic field, can push the system across the phase boundary as had been observed experimentally. Despite this convergence of views there remains a serious complication in comparing the Pfaffian state to the ground states found in numerical studies: It was recently realized[7] that the particle-hole conjugate of the Moore-Read Pfaffian state, called the AntiPfaffian (APf), is an equally valid candidate for systems which obey particle-hole symmetry; and no prior numerical study would have had the ability to distinguish between these two possibilities[8]. On the other hand, the actual experiments do not obey particle-hole symmetry and so the two candidates are inequivalent in experiments and, most likely, only one is realized. While the Pfaffian and the AntiPfaffian share many important properties, including non-Abelian statistics and their usefulness for quantum information processing[9], they represent different topological phases of matter. For example, they have different edge physics[7]. Determining which of these two states is actually realized in the physical system is now a rather crucial objective. This is the aim of the current paper.

In all previous numerical studies, calculations were performed in a Hilbert space restricted to a single Landau level (LL). Indeed, it is precisely this restriction that allows numerical calculations in systems of relatively large sizes (up to 22 electrons in some cases[5]). However, if the inter-particle interaction is two-body, such a restriction enforces a precise symmetry between particles and holes that is absent in the actual experiments, and this symmetry is broken once LL mixing is restored. While for most studies mixing makes only quantitative (albeit important) corrections, in the case of 5/2 it is crucial since it is the only factor that selects between Pfaffian and AntiPfaffian. Without consideration of LL mixing, the system is fine-tuned to a critical point between these phases[10]. Furthermore, single LL projection can only ever be quantitatively accurate to the extent that the Coulomb energy $E_c = e^2/\epsilon\ell_0$ is much smaller than the cyclotron energy $\hbar\omega_c$. Unfortunately, in actual quantum Hall experiments this is never so. In fact $E_c/\hbar\omega_c \gtrsim 1$ in all published experiments on 5/2. In the current paper we will set $E_c/\hbar\omega_c = 1.38$ as in Ref. 11.

The challenge of attacking this problem numerically is that without the projection to a single LL, the Hilbert space, even for a small system, is infinite. One approach to addressing this problem is to integrate out LL mixing terms perturbatively in $E_c/\hbar\omega_c$, leaving an effective single LL theory. This approach has recently been implemented to lowest order in Ref. 13. The single LL theory has been obtained, and it was tentatively concluded that at lowest order the LL mixing terms most likely favor AntiPfaffian over Pfaffian. While such an approach is well controlled, it also has obvious severe limitations: it is a perturbative expansion in a parameter which in the experiment is of order one. While in principle one could attempt to continue the expansion to higher orders hoping that the series converges quickly, even if one could perform the more complicated algebra, at higher orders one generates retarded interaction terms which then makes the resulting single LL analysis very difficult.

An alternate, seminumerical, organization of a perturbative expansion in LL mixing terms was developed in Ref. 12. We attempted a similar approach, hoping that terms of successively higher orders in $E_c/\hbar\omega_c$ would become rapidly less important. However, for $E_c/\hbar\omega_c \gtrsim 1$ corresponding to the experiments, we found that one would have to carry out this expansion to a higher order than feasible in order to obtain convergence. We have,

therefore, resorted to a different method of analysis.

The approach we take is non-perturbative and is similar in spirit to that of Ref. 14. We use a truncated Hilbert space method by keeping a limited number of LLs and allowing only a certain number of particle or hole excitations out of the valence LL, and performing exact diagonalizations on this restricted Hilbert space. One may view such an approach as variational in character, which can successively be improved by further expanding the Hilbert space. We note that matrix elements connecting the valence LL to increasingly high LLs drop very rapidly, so excluding high LLs is not expected to create substantial errors (see for example [12]).

Even given the Hilbert space truncation, it is still challenging to establish meaningful results from the limited size system. As such, our argument will proceed in three steps. (1) We show that the valence LL is polarized. This result was first established without LL mixing in Ref. [3], and is re-examined here for completeness as well as for ascertaining that LL mixing does not change this conclusion. This then allows us to concentrate on systems with a polarized valence LL. (2) We establish that excitations of electrons with opposite spin from that of the valence LL do not substantially effect the crucial physics. This allows us to further reduce the Hilbert space dimension considerably. (3) Finally, using our truncation method we can meaningfully address adequate system sizes and accurately determine the nature of the ground state.

We perform our calculations on the torus geometry at $\nu = 5/2$ where the Pfaffian and AntiPfaffian compete with each other directly (as compared to the sphere where, for a particular number of particles, the Pfaffian and AntiPfaffian do not occur at the same flux). Unless otherwise stated we will use a hexagonal unit cell. Following Haldane[15], we use two-dimensional conserved crystal momentum to classify the states. We consider two different classes of experimental samples where $\nu = 5/2$ has been observed. The first class, typical of earlier experiments[1, 2], include single heterointerfaces. In the current work we will focus on samples of this type using a Fang-Howard (FH) layer profile[16], with a layer width of $w = 0.65$ magnetic lengths[11]. The second class of samples is the somewhat wider (roughly 30 nm) symmetric quantum well (QW) typical of modern high-density ultra-high mobility experiments[17]. In this case, the LLL of the first excited subband may lie below the $2\downarrow$ LL of the lowest subband and hence should not be ignored[18]. We will return to the QW case before concluding.

Some of the Hilbert spaces which we examine are listed in Table I. The simplest of the Hilbert spaces are $\mathcal{H}_{p,\mathcal{N}}$ which describe $\mathcal{N}$ electrons filling half of the 1st spin down LL (where all other LLs are either completely filled or completely empty). This type of space, where all of the degrees of freedom are within one spin polarized LL, is typically the space used for study of the quantum Hall effect. Indeed, the trial wavefunctions we are interested in comparing to, the Pfaffian and the AntiPfaffian, are completely contained within this space. It is useful to define a normalized projection operator

$$\hat{P}_{p,\mathcal{N}}|\psi\rangle = P_{p,\mathcal{N}}|\psi\rangle \,/\, |\langle\psi|P_{p,\mathcal{N}}|\psi\rangle|^{1/2} \qquad (1)$$

where $P_{p,\mathcal{N}}$ is the usual projection to the Hilbert space $\mathcal{H}_{p,\mathcal{N}}$. Thus, $\hat{P}_{p,\mathcal{N}}|\psi\rangle$ is always a normalized wavefunction within the space $\mathcal{H}_{p,\mathcal{N}}$. We can further define the projected square overlap between two states ψ_1 and ψ_2 with the same total number of electrons N as $|\langle\psi_1|\hat{P}_{p,\mathcal{N}}\hat{P}_{p,\mathcal{N}}|\psi_2\rangle|^2$ where $\mathcal{N} = N \bmod N_\phi = N/5$.

We start by examining spin polarization of the valence

(a)	N_ϕ	N	$0\downarrow$+$0\uparrow$	$1\downarrow$+$1\uparrow$	$2\downarrow$+$2\uparrow$	$3\downarrow$+$3\uparrow$	d
$\mathcal{H}_{v,6}$	12	30	2̸4	6	0̸	0̸	6.7e2
$\mathcal{H}_{v,8}$	16	40	3̸2	8	0̸	0̸	2.6e4
$\mathcal{H}_{v,10}$	20	50	4̸0	10	0̸	0̸	1.2e6
$\mathcal{H}_{s,1}$	12	30	22-24	6-8	0̸	0̸	7.6e4
$\mathcal{H}_{s,2}$	12	30	23-24	5-7	0-1	0̸	2.5e4
$\mathcal{H}_{s,3}$	12	30	22-24	5-8	0-1	0̸	1.1e6
$\mathcal{H}_{s,4}$	12	30	22-24	4-8	0-2	0̸	6.0e6
$\mathcal{H}_{s,11}$	16	40	31-32	7-9	0-1	0̸	4.5e5
$\mathcal{H}_{s,12}$	16	40	30-32	7-10	0-1	0̸	3.3e7

(b)	N_ϕ	N	$0\downarrow$	$1\downarrow$	$2\downarrow$	$3\downarrow$	d	Pf	APf	$\langle$P$\|$A$\rangle^2$
$\mathcal{H}_{p,6}$	12	30	1̸2	6	0̸	0̸	1.4e1	.90	.90	.67
$\mathcal{H}_{p,8}$	16	40	1̸2	8	0̸	0̸	1.0e2	.53	.53	.016
$\mathcal{H}_{p,10}$	20	50	1̸2	10	0̸	0̸	9.2e2	.71	.71	.29
$\mathcal{H}_{p,12}$	24	60	1̸2	12	0̸	0̸	9.4e3	.56	.56	.059
$\mathcal{H}_{r,1}$	12	30	10-12	6-8	0̸	0̸	6.0e2	.94	.83	.67
$\mathcal{H}_{r,2}$	12	30	11-12	5-7	0-1	0̸	2.1e3	.79	.87	.67
$\mathcal{H}_{r,3}$	12	30	10-12	5-8	0-1	0̸	1.1e4	.80	.89	.67
$\mathcal{H}_{r,4}$	12	30	10-12	4-8	0-2	0̸	7.6e4	.83	.89	.67
$\mathcal{H}_{r,5}$	12	30	9-12	3-9	0-3	0̸	1.1e6	.82	.89	.67
$\mathcal{H}_{r,6}$	12	30	8-12	2-10	0-4	0̸	7.1e6	.82	.89	.67
$\mathcal{H}_{r,7}$	12	30	10-12	4-8	0-2	0-1	8.7e5	.81	.87	.67
$\mathcal{H}_{r,8}$	12	30	10-12	4-8	0-1	0-2	8.7e5	.79	.86	.67
$\mathcal{H}_{r,9}$	12	30	9-13	3-9	0-2	0-1	3.7e6	.82	.87	.67
$\mathcal{H}_{r,10}$	16	40	14-16	8-10	0̸	0̸	9.1e3	.63	.33	.016
$\mathcal{H}_{r,11}$	16	40	14-15	7-9	0-1	0̸	2.9e4	.36	.52	.016
$\mathcal{H}_{r,12}$	16	40	14-16	7-10	0-1	0̸	2.1e5	.34	.51	.016
$\mathcal{H}_{r,13}$	16	40	14-16	6-10	0-2	0̸	1.8e6	.37	.56	.016
$\mathcal{H}_{r,14}$	16	40	14-16	6-10	0-1	0-1	3.9e6	.36	.53	.016
$\mathcal{H}_{r,15}$	20	50	18-20	10-12	0̸	0̸	1.4e5	.40	.00	.29
$\mathcal{H}_{r,16}$	20	50	18-20	9-12	0-1	0̸	3.8e6	.01	.24	.29

TABLE I. Hilbert Spaces. N_ϕ is the flux and $N = (5/2)N_\phi$ is the total number of electrons. The next columns are the number of electrons allowed in each LL respectively (labelled with their spin). Entries with a slash through them are either empty or filled and frozen. Higher LLs are assumed empty. The dimensions of crystal momentum reduced Hilbert spaces, rounded to the nearest power of 10, are listed under "d". In (b) the LLL up spins are frozen and other up spin LL are empty. Columns 8 and 9 give the squared overlaps of the projected ground state with the Pfaffian and the AntiPfaffian respectively. The overlap between them is given in the last column. With sufficient LL mixing (i.e., any transitions allowed to LL2) in all cases the AntiPfaffian is favored. All overlaps increase as V_1 is increased slightly (see Figs 1, 2).

LL. First we restrict the Hilbert space to a single LL ($\mathcal{H}_{v,i}$ for $i = 6 - 10$) and, before doing exact diagonalization, we integrate out inter-LL transitions approximately at the RPA level[19], which modifies the inter-electron interactions. We find, in agreement with Ref. 3, that even in the absence of Zeeman energy, the ground state of the valence LL is fully polarized and gapped for $\mathcal{N} = 6 - 10$ electrons. Furthermore the signature crystal momentum of the Pfaffian state (and the AntiPfaffian) for both even and odd electrons is matched by the exact ground state. We find these results to be true for both FH and QW layer profiles

We reconsider the same problem including LL mixing with the truncated Hilbert space technique. Performing diagonalizations in Hilbert spaces $\mathcal{H}_{s,i}$ we now allow complete freedom within the valence LL, and we also allow a few holes in the 0th LL and a few electrons in the 2nd LL. We again find that the ground state of the valence LL is always fully polarized even in the absence of Zeeman splitting and the ground state momentum matches that of the Pfaffian and AntiPfaffian.

Concluding that the valence LL is polarized, we now turn to study the effect of the excitation of the spin up (the minority spin) electrons. Let us consider the ground states $\mathcal{H}_{r,i}$, which are exactly analogous to $\mathcal{H}_{s,i}$ except that the minority spin species have now been frozen (we do not allow any excitations of this species) although LL transitions for the majority spin are still allowed. We find, rather remarkably, that the projected squared overlap between the ground state in $\mathcal{H}_{r,i}$ and the ground state in $\mathcal{H}_{s,i}$ is .9893, .9984, and .9986 for i =2,3,4. This surprisingly shows that as the Hilbert space is expanded (for fixed number of electrons), the minority spin species becomes *less* important. For $i = 11$,12 we obtain .9864 and 0.9966 which shows that even for larger system, neglect of spin-reversed excitations remains extremely good. Considering the large Hilbert space and its moderate size even after projection to $\mathcal{H}_{p,8}$ (34 after all symmetries are removed) this result is highly significant. What this means is that, although the ground state wavefunction is dressed with virtual excitations to the other LLs, when it is projected back into a single LL, *the wavefunction is nearly independent of whether transitions of the minority spin species are allowed*. We note that this insensitivity to the presence of the minority spins seems to hold independent of our truncation scheme and details of the Hamiltonian, presumably, so long as we have a polarized and gapped ground state. The fraction of the wavefunction that survives projection is clearly reduced when the Hilbert space is expanded, but this is unimportant in determining the phase represented by the wavefunction.

The above result now allows us to completely freeze the minority spin species and study larger systems. We examined a number of different truncation combinations, some of which are shown in Table I.b. We find that as the Hilbert space is expanded, the spectrum rapidly converges. Indicating that only a few excitations out of the valence LL need be considered in order to capture the essential physics

We now turn to the main results of our work. For increasing system sizes, we consider the projected overlap of our exact diagonalizations with both the Pfaffian and the AntiPfaffian (see Table I.b). Note that for certain finite sized systems, there can be a substantial overlap between the Pfaffian and AntiPfaffian (see Table I.b), so that if the overlap of the ground state with one is large, the overlap with the other cannot be too small. Examining Table I.b, it is clear that the AntiPfaffian is favored over the Pfaffian, particularly for the larger Hilbert spaces. We find that the AntiPfaffian always has higher overlap except if transitions to LL2 are artificially forbidden ($\mathcal{H}_{r,i}$ for $i = 1, 11, 14$). As we look at larger systems, the contrast between Pfaffian and AntiPfaffian only improves. We have presented only a subset of our data, but the trends are not contradicted by any other cases we have looked at.

Examining the data more carefully makes the case even more compelling. For finite sized systems, the realistic Hamiltonian is clearly on the edge of a phase transition, in agreement with experiment[2] and prior numerical studies[3–5]. However, barring a level crossing transition, which does not occur here, phase boundaries are broadened in finite sized systems. In order to focus on the gapped phase, we add a small δV_1 (Haldane pseudopotential) interaction to the Hamiltonian. We define V_m to be the the energy of a pair of particles in a state of "relative angular momentum" m irrespective of what LL they occupy[15]. Defined this way, such a term does not break particle-hole symmetry. In Fig. 1, in a system with a very large Hilbert space, we see that adding only a small δV_1 greatly increases the projected overlap of the ground state with the AntiPfaffian trial state, but to a much lesser degree with the Pfaffian. Since for this size system, the overlap of the Pfaffian and AntiPfaffian is about 29%, much of the increase for the Pfaffian appears to be caused by this effect.

It is useful to examine also the torus with square unit cell geometry where additional information may be extracted (See Fig. 2). In contrast to the hexagonal unit cell, where there is a single three-fold degenerate ground state, for the square unit cell we find two low energy "ground" states at two different points in the Brillouin zone: one at the zone corner (ZC) and a doubly degenerate ground state at the zone boundary (ZB), as expected for either the Pfaffian or AntiPfaffian. In this case, however, the overlap between the Pfaffian and AntiPfaffian trial wavefunctions are 0.8% for ZC and 12% for ZB. Here, the contrast between Pfaffian and AntiPfaffian overlaps is even more apparent: examining the ZC we find a region of δV_1 where the overlap with the AntiPfaffian is very high, but the overlap with the Pfaffian is near zero. At the peaks in both figures, the AntiPfaf-

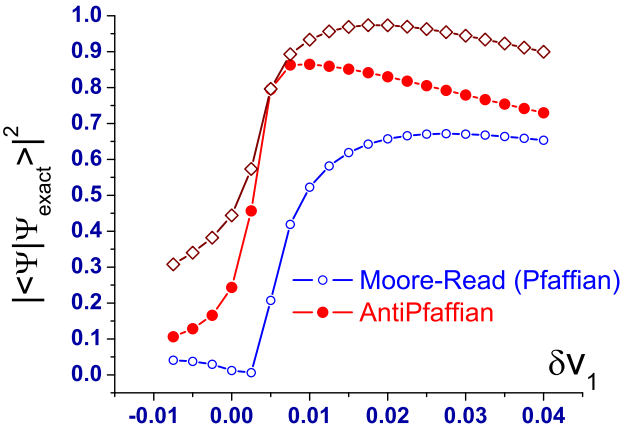

FIG. 1. (color online) The overlaps of the projected ground state with the MR Pfaffian and the AntiPfaffian for $\mathcal{H}_{r,15}$, $(N_\phi, N) = (20, 50)$. Varying V_1 slightly, the projected ground state obtains a large overlap with the APf, while the overlap with the Pf remains relatively small. A substantial part of the Pf overlap appears to be caused by the non-orthogonality of Pf with APf. Further increasing V_1, the system crosses over to a Composite Fermion (CF) Fermi-liquid[4], which in this case has the same crystal momentum. The top curve (also in Fig. 2 for the ZB case) is the projection of the ground state to the two-dimensional subspace spanned by the Pf and APf.

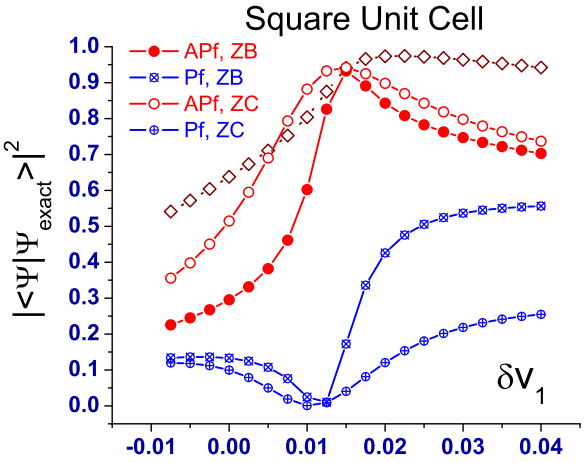

FIG. 2. (color online) Same as Fig. 1 but for a square periodic unit cell. ZC and ZB refer to the zone corner and boundary of the Brillouin zone. Note that for this geometry the overlap of the Pfaffian with the AntiPfaffian at the ZC is extremely small. A first order transition to the CF state occurs for $\delta V_1 > 0.04$. For negative δV_1 we expect a stripe-type order[4]. Here, as well as in Fig. 1, the completely symmetry reduced Hilbert space dimension within $\mathcal{H}_{p,10}$ is 263.

fian completely dominates while past the peaks both are present with the AntiPfaffian remianing dominant. However, such an admixture of Pf and APf will not occur in a thermodynamic system since they represent distinct phases.

We return now to the QW type samples. In the high density (very high mobility) cases, the LLL of the first excited subband state is about 30% of $\hbar\omega_c$ above the $n = 1$ LL. We find that in a 3-LL model the mixing is somewhat suppressed and the Pfaffian is preffered. However, adding the fourth ($n = 2$ lowest subband) LL changes it to the AntiPfaffian. We have tested convergence when more LLs are added. In particular, adding the fifth ($n = 1$, first excited subband) LL in a small, $N = 30$ and $N_\phi = 12$, system we have found that overlap changes are less than one quarter of a percent. While the sizes we can access in this case are more limited, the case for the AntiPfaffian remains relatively strong.

To conclude, we find the AntiPfaffian is strongly preferred. The large overlaps with the Pfaffian appear to be a finite size effect at least partially due to the relatively large overlap of the Pfaffian with the AntiPfaffian.

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