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Energetics of Pfaffian-AntiPfaffian Domains

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In several recent works it has been proposed that, due to disorder, the experimentally observed $\nu = 5/2$ quantum Hall state could be microscopically composed of domains of Pfaffian order along with domains of Anti-Pfaffian order. We numerically examine the energetics required for forming such domains and conclude that for the parameters appropriate for recent experiments, such domains would not occur.

Understanding the $\nu = 5/2$ fractional quantum Hall states has been an enduring challenge for the condensed matter community. Discovered experimentally[1] in 1987, the first compelling numerical work roughly a decade later[2] identified this state as being the Moore-Read[3], or "Pfaffian", phase of matter. Almost another decade later it was realized that the particle-hole conjugate of the Pfaffian, the so-called "AntiPfaffian", a different phase of matter, would fit the numerical data just as well[4,5]. Only very recently numerics have confirmed that the AntiPfaffian is likely to be energetically favorable over the Pfaffian for experiments in GaAs quantum wells[6–8].

This numerical conclusion has been cast into doubt by recent thermal transport experiments[9] which, at face value, do not match predictions for either the AntiPfaffian or the Pfaffian. This has raised the possibility[10–12] that the observed quantum Hall state at filling fraction $\nu = 5/2$ is microscopically composed of domains of Pfaffian order and domains of AntiPfaffian order, stabilized by disorder[11]. Such mixed domains could have quantized electrical conductivity, identical to what one would observe for either the Pfaffian or AntiPfaffian phase, but could have either unquantized thermal conduction (a so-called "thermal metal"[13]) or, possibly with fine tuning[11], could result in a number of novel phases of matter including the PH-Pfaffian[14,15], the $K = 8$ state, and the 113 state[10,11]. Although several alternative proposals[16–18] have been put forward to explain the experimental observations, the idea of multiple domains is certainly a compelling possibility.

In the current paper we numerically examine the energetics of the Pfaffian and AntiPfaffian. We derive the conditions that would result in domains in the physical system and compare them against what is known in the experiment. Our results strongly oppose the domain scenario.

The physical picture that could result in multiple domains is well described in Ref. 11. It is known that at $\nu = 5/2$, without Landau level mixing, the Pfaffian and AntiPfaffian are energetically equivalent. Landau level mixing weakly breaks this degeneracy. The question of whether Pfaffian or AntiPfaffian is favored was debated in the literature for most of a decade (See Ref. 6 and references therein for a review of this debate and why different groups obtained different results[19]). The debate is now resolved with the conclusion that Landau level mixing favors the AntiPfaffian[6–8] for GaAs quantum wells similar to those of the experiments[9]. However, the quasielectrons of the Pfaffian and quasielectrons of the AntiPfaffian need not have the same energy. If the quasielectrons of the AntiPfaffian cost more energy than those of the Pfaffian, then when the filling fraction is increased enough the Pfaffian will be favored. In the opposite case, due to the approximate particle-hole symmetry of the system the Pfaffian will have lower-energy quasiholes, and as a result will become favored when the filling fraction is lowered enough. Thus in either case, for a disordered system where the filling fraction is not uniform, one could obtain domains of Pfaffian and AntiPfaffian.

Our first objective is to determine at what filling fraction the transition occurs from AntiPfaffian to Pfaffian. To do this, we want to determine the energy of the quasiparticles of the Pfaffian versus the quasiparticles of the AntiPfaffian. Our result (see *Numerical-methods-1* section below) is that the quasielectrons of the Pfaffian have lower energy and the energy difference is approximately

$$E_{2qe} \approx 0.004 \tag{1}$$

where the energy here and elsewhere in the paper is given in natural units of $E_{interaction} = e^2/(\epsilon\ell)$ with ℓ the magnetic length. This is the energy difference in removing one flux from the system for the two different wavefunctions. This result has been obtained using DMRG techniques as explained in the methods section below. In the methods section we also discuss the result of trying to estimate this quantity using variational and exact diagonalization techniques on smaller system sizes.

The fact that the quasielectrons of the Pfaffian are lower energy tells us that the putative transition from AntiPfaffian to Pfaffian occurs at $\nu > 5/2$. Thus for all $\nu < 5/2$ we should have AntiPfaffian order with quasiholes.

We now want to compare this energy difference for quasielectrons to the energy difference between Pfaffian and AntiPfaffian at exactly $\nu = 5/2$ due to Landau level

mixing. Based on several recent works[6,8] (See *Numerical-methods-2* section below) we establish an energy difference per electron between Pfaffian and AntiPfaffian of

$$E_0 \approx .00066\kappa \tag{2}$$

where this energy is per electron in the valence Landau level and $\kappa = E_{interaction}/(\hbar\omega_c)$ (with ω_c the cyclotron frequency) is the Landau level mixing parameter which is approximately 1.6 in the experiments of Ref. 9.

We now balance the energies of the Pfaffian with quasielectrons to that of the AntiPfaffian with quasielectrons to find the critical filling fraction where the transition occurs. Recall that $\nu = n_e\phi_0/B$ with n_e the electron density and $\phi_0 = 2\pi\hbar/e$, and we will consider only electrons in the valence Landau level (so we are taking $\nu = 1/2 + \delta\nu$). The magnetic field is $B = \nu^{-1}n_e\phi_0$, and the missing flux density compared to $\nu = 1/2$ is $B_{1/2} - B = (2 - \nu^{-1})n_e\phi_0$. The energy difference per unit area between the quasielectrons of Pfaffian and AntiPfaffian is thus $E_{2qe}(2-\nu^{-1})n_e$ whereas the energy difference per unit area from Landau level mixing is $E_0 n_e$. Thus the total energy difference goes through zero at the critical filling ν_c such that $E_0 = E_{2qe}(2 - \nu_c^{-1})$, or

$$\nu_c^{-1} = 2 - E_0/E_{2qe} \ .$$

Plugging in numbers here gives us (at $\kappa = 1.6$ appropriate for the experiments)

$$\nu_c \approx 0.58$$

in the valence Landau level.

This critical value can be seen to be problematic for the interpretation of the experiment[9] as being made of domains of Pfaffian and AntiPfaffian stabilized by the long wavelength disorder which is expected to be in the experimental system. In short, it requires an unreasonably large change in local filling fraction to putatively stabilize the Pfaffian. In the experiment, the quantum Hall plateau extends only between filling fractions $\nu \approx 0.48 - 0.51$ within the valence Landau level. Further, between $\nu = 0.5$ and $\nu_c = 0.58$ there are several other phases of matter observed, including reentrant incompressible (presumed bubble) phases and compressible phases.

Let us discuss the microscopic picture in a bit more detail. In a model with long range disorder, the system will break up into compressible and incompressible strips situated around the electrons' equi-density contours (which are in turn determined by the equi-potential contours of the disorder). Typically only a single such contour can percolate across the system, as regions of higher (lower) density are confined around local minima (maxima) of the disorder. When this contour has filling fraction $\nu = 0.48 - 0.51$ within the valence Landau level, the percolating state is incompressible, giving rise to a quantized Hall plateau. However, for filling fractions outside of the plateau, we should conclude that the phase at the percolating contour is compressible. Since ν_c is *far* outside of the plateau, we should assume that compressible regions (as well as possibly other states of matter) must intervene between AntiPfaffian order and any Pfaffian order, should the latter exist. At least in this picture of long range disorder (precisely the picture used to justify the domain scenario) it then seems impossible to construct an electrically incompressible phase of matter based on domains of Pfaffian and AntiPfaffian. Since our best estimate of ν_c is almost an order of magnitude further away from the center of the plateau than the half-width of the plateau itself, our conclusion should be very robust to any minor modification of assumptions (such as changes in methods of extrapolating to large system size, *etc*; see numerical methods sections).

For a hypothetical system where Landau level mixing (and therefore E_0) is much smaller, one could imagine a situation where the energetics of mixed domains is more viable. If there were a case where Pfaffian domains are possible, a more accurate accounting of the full energy budget would also include the energy costs associated with the tension of the domain wall itself. This would set a minimum size of Pfaffian domains within the AntiPfaffian background. Using DMRG we have estimated the domain wall tension to be on the order of $0.0010 - 0.0024\, e^2/\epsilon\ell^2$. In the case of the experiments of Ref. 9, this tension, not previously considered, makes the idea of mixed domains even less favorable. The detailed energetics of domain walls are discussed in the Supplmemental material to this paper.[20] Another possibility for mixed domain physics would be if it turns out that there is a phase transition at finite κ between AntiPfaffian and Pfaffian ground states, as has been suggested in Ref. 21. However, we have not seen any numerical evidence supporting this scenario.

To summarize the result of our paper: We find that for typical high mobility samples similar to that of Ref. 9, the picture of mixed domains of Pfaffian and AntiPfaffian proposed by Refs. 10–12 is not viable.

Numerical Methods 1: Quasielectron vs Quasihole Energy. Our numerical method is based on DMRG on an infinite cylinder geometry. We first generate Pfaffian and AntiPfaffian matrix product state (MPS) wavefunctions by using DMRG on the half-filled $N = 1$ LL, for several values of the cylinder circumference L and MPS bond dimension χ (larger χ being more accurate). By seeding the DMRG with product states with different "root configurations," we are able to obtain all the distinct topologically degenerate ground states of both the Pf and APf phases. To determine the quasielectron, quasihole, and domain wall energies, we use these different ground states as semi-infinite left / right boundary conditions in a *finite* DMRG variational optimization on a number N_s of orbitals, as described in Ref. 22. By choosing different topological sectors a, b for the left / right boundary condition, we form an interface between two distinct topological sectors, which traps an anyon c in the fusion outcome $N_{a\bar{b}}^c$. For example, using sector $a = \sigma^+$ (root

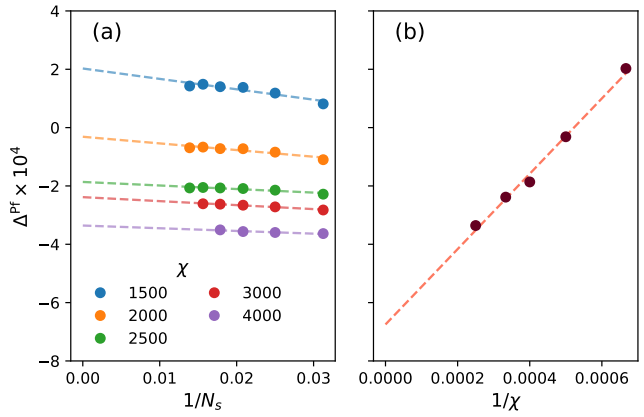

Figure 1. Example of extrapolation of DMRG results in the two cutoffs N_s and χ. (a) Extrapolation in the size of the interface region N_s. (b) The $N_s \to \infty$ values are extrapolated in the bond dimension χ. The data is for the Pfaffian wavefunction at $L = 26\ell$.

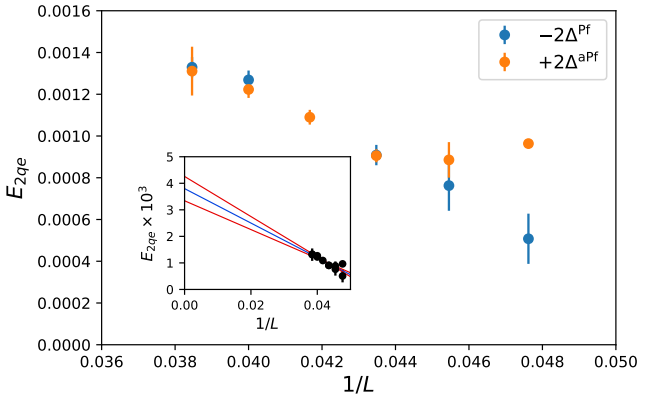

Figure 2. DMRG results after extrapolation in the cutoffs. $\Delta \equiv E_{+e/4} - E_{-e/4} - \frac{1}{2}E(1)$, for both Pfaffian and AntiPfaffian, plotted vs the inverse cylinder circumference $1/L$ (in units of ℓ). We find $\Delta^{\rm Pf} < 0$ (i.e. the Pfaffian has lower-energy quasielectrons) and the PH relation $\Delta^{\rm Pf} + \Delta^{\rm APf} = 0$ is obeyed quite accurately for $L \geq 23\ell$. Inset: $1/L$ extrapolation of the data (outer lines indicate the uncertainty of the fit).

$\cdots 0101 \cdots$, where 0 and 1 denote empty and occupied Landau orbitals in the initial product state) on the left and sector $b = \mathbb{1}$ (root $\cdots 0110 \cdots$) on the right gives the $+e/4$ quasielectron σ^+. Exchanging left and right gives the $-e/4$ quasihole. From this we obtain the energies $E^{\alpha}_{\pm e/4}$, with $\alpha =$ Pf or APf, relative to that of the vacuum. We calculate the energies for multiple values of the cutoffs $32 \leq N_s \leq 80$ and $1500 \leq \chi \leq 4000$ and extrapolate both to infinity, as shown in Fig. 1.

The quantity of interest is $E_{2qe} = 2(E^{\rm APf}_{+e/4} - E^{\rm Pf}_{+e/4})$, but it is convenient to define $\Delta^{\alpha} \equiv E^{\alpha}_{+e/4} - E^{\alpha}_{-e/4} - \frac{1}{2}E(1)$, where $E(1)$ is the energy of a filled $N = 1$ LL. These satisfy $\Delta^{\rm APf} - \Delta^{\rm Pf} = E_{2qe}$ and $\Delta^{\rm Pf} + \Delta^{\rm APf} = 0$ due to particle-hole symmetry; the latter provides a numerical consistency check. The extrapolated values of Δ^{α} are shown as a function of cylinder circumference $21\ell \leq L \leq 26\ell$ in Fig. 2. At the available sizes we find $E_{2qe} \simeq 0.001$. While the value appears to drift with L, a linear extrapolation in $1/L$ (likely an overestimate) yields $E_{2qe} \simeq 0.004$, which is the result we use in Eq. 1. Note that other reasonable extrapolations could easily have given a much lower value (whereas a much larger value appears very unlikely). A smaller estimate of E_{2qe} would only give a *larger* value of ν_c making our conclusion even stronger. The Pfaffian-AntiPfaffian domain wall tension can similarly be computed by forming an interface between their respective vacuum sectors.

To support our results we also use the exact Pfaffian and AntiPfaffian wavefunctions on finite systems to obtain variational estimates of quasielectron and quasihole energies at a total flux that is displaced by $\pm\phi_0$ away from $\nu = 5/2$. We generate the Pfaffian by an ultra-short-range 3-body repulsive potential $H_{\rm Pf}$. For our purposes it is more convenient to generate the AntiPfaffian by a potential that is the particle-hole conjugate of the $H_{\rm Pf}$, rather than taking particle-hole conjugates of a series of wave functions. For odd number N of electrons, we find an equal number $(N+1)/2$ of degenerate states for quasielectrons and quasiholes. Particle-hole conjugation in finite-sized systems at these fillings changes the electron number by 1. As a result, for even electrons, the number of degenerate quasiholes of the Pfaffian exceed those of the AntiPfaffian quasielectrons by 1. All the sizes presented in Fig. 3 involve quasielectrons and are unrelated by particle-hole conjugation. The quasielectrons of the Pfaffian (as well as the quasiholes of the Antipfaffian) are generated by their respective Hamiltonians and are not degenerate at these fillings. In these cases we find the lowest variational energy of the second Landau level Coulomb interactions among the lowest $(N+1)/2$ model states (typically the first, occasionally the second if the lowest two are close in energy). In cases where we have degeneracies we find the optimum state of quasielectrons by diagonalizing the Coulomb potential in the subspace of the degenarate manifold of model states. We take the lowest energy states of the multiplets (corresponding to the quasielectrons maximally spaced from each other). Since we are limited to smaller sizes it is harder to draw definitive conclusions. It is clear from the data that the extrapolation is likely to have a substantial uncertainty. However, we use these as guides to estimate bounds on the energy. From the data shown in Fig. 3 the extrapolation of the value of E_{2qe} is somewhere between 0.0025 and 0.0062, which is highly consistent with our DMRG value. The lower bound makes ν_c larger than the DMRG's. Even if we take the higher number seriously, this only reduces ν_c to .54, which is still far outside the experimentally observed plateau.

To avoid getting too close to phase boundaries across which a transition to a crystalline phase may occur, we

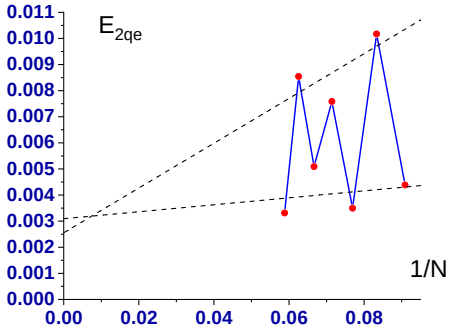

Figure 3. Quasielectron energy difference between Pfaffian and AntiPfaffian as a function of system size. The numerical method is variational and exact diagonalization (See text). The upper points are for even numbers of electrons and the lower points are for odd. The fact that the two linear extrapolations do not intersect at $1/N = 0$ suggests that we cannot completely trust the extrapolation. Here, $N = 11, 12, 13, 14, 15, 16, 17$ on a hexagonal torus.

have altered the Coulomb interaction by a small amount. For all sizes above $N = 12$, as in our DMRG calculation, we have added 0.0325 to the v_1 pseudopotential. For our largest size $N = 17$ system that we have studied by exact calculations, the first two pseudopotentials of the Coulomb repulsion for electrons in the second Landau Level are $v_1 = 0.4246310$ and $v_3 = 0.3306233$ (only odd relative angular momenta are relevant since the valence electrons are believed to be fully spin-polarized). For smaller sizes we have instead made a smaller change of 0.0225. This compensates for the fact that smaller sizes have larger v_1 and thus avoids a transition to the composite Fermi liquid phase.

Numerical Methods 2: Pfaffian-AntiPfaffian Splitting. We start by examining the iDMRG results from Ref. 8. The first key result (Fig. 7 of that work) is that the energy splitting between Pf and APf is very nearly linear in Landau level mixing up to at least $\kappa = 1.38$. The magnitude of the splitting in that plot is roughly .00047 κ. However, upon increasing the number of Landau levels included in the calculation, the spitting increases (Fig. 9 of that work). The authors of that work warn us not to take this result to be too precise quantitatively, but nonetheless we are able to trust the trends. We then examine the diagonalization results of Ref. 6. Here the splitting is calculated to first order in κ. However, given the linearity with κ obtained in Ref. 8, this appears to be sufficient. From the the inset to Fig. 1 in Ref. 6, extrapolated to large system size, we obtain the stated energy splitting .00066κ that we use in Eq. 2. Note that there may be some uncertainty in this number given that we are extrapolating to large κ and large system size. However, as mentioned in the main text, even a very substantial change in this number would not change the final conclusion of our paper.

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[1] R. Willett, J. P. Eisenstein, H. L. Störmer, D. C. Tsui, A. C. Gossard, and J. H. English, Phys. Rev. Lett. **59**, 1776 (1987).
[2] R. H. Morf, Phys. Rev. Lett. **80**, 1505 (1998).
[3] G. Moore and N. Read, Nuclear Physics B **360**, 362 (1991).
[4] S.-S. Lee, S. Ryu, C. Nayak, and M. P. A. Fisher, Phys. Rev. Lett. **99**, 236807 (2007).
[5] M. Levin, B. I. Halperin, and B. Rosenow, Phys. Rev. Lett. **99**, 236806 (2007).
[6] E. H. Rezayi, Phys. Rev. Lett. **119**, 026801 (2017).
[7] E. H. Rezayi and S. H. Simon, Phys. Rev. Lett. **106**, 116801 (2011).
[8] M. P. Zaletel, R. S. K. Mong, F. Pollmann, and E. H. Rezayi, Phys. Rev. B **91**, 045115 (2015).
[9] M. Banerjee, M. Heiblum, V. Umansky, D. E. Feldman, Y. Oreg, and A. Stern, Nature **559**, 205 (2018).
[10] D. F. Mross, Y. Oreg, A. Stern, G. Margalit, and M. Heiblum, Phys. Rev. Lett. **121**, 026801 (2018).
[11] C. Wang, A. Vishwanath, and B. I. Halperin, Phys. Rev. B **98**, 045112 (2018).
[12] B. Lian and J. Wang, Phys. Rev. B **97**, 165124 (2018).
[13] J. T. Chalker, N. Read, V. Kagalovsky, B. Horovitz, Y. Avishai, and A. W. W. Ludwig, Phys. Rev. B **65**, 012506 (2001).
[14] D. T. Son, Phys. Rev. X **5**, 031027 (2015).
[15] L. Fidkowski, X. Chen, and A. Vishwanath, Phys. Rev. X **3**, 041016 (2013).
[16] S. H. Simon, Phys. Rev. B **97**, 121406 (2018).
[17] K. K. W. Ma and D. E. Feldman, Phys. Rev. B **99**, 085309 (2019).
[18] S. H. Simon and B. Rosenow, arXiv:1906.05294 (2019).
[19] In short, references such as K. Pakrouski et al, Phys. Rev. X 5, 021004 (2015) treated an incomplete Hamiltonian. It was later found in Ref. 6 that if one includes only the first five 3-body pseudopotentials the Pfaffian is favored, but when one includes more 3-body pseudopotentials, the AntiPfaffian is favored agreeing with Hilbert-space truncation methods[7] and DMRG[8].
[20] Supplementary material to this paper.
[21] N. Samkharadze, D. Ro, L. N. Pfeiffer, K. W. West, and G. A. Csáthy, Phys. Rev. B **96**, 085105 (2017).

[22] M. P. Zaletel, R. S. K. Mong, and F. Pollmann, Phys. Rev. Lett. **110**, 236801 (2013).