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Spin Order in Paired Quantum Hall States

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We consider quantum Hall states at even-denominator filling fractions, especially $\nu = 5/2$, in the limit of small Zeeman energy. Assuming that a paired quantum Hall state forms, we study spin ordering and its interplay with pairing. We give numerical evidence that at $\nu = 5/2$ an incompressible ground state will exhibit spontaneous ferromagnetism. The Ginzburg-Landau (GL) theory for the spin degrees of freedom of paired Hall states is a perturbed CP^2 model. We compute the coefficients in the GL theory by a BCS Stoner mean-field theory for coexisting order parameters, and show that even if repulsion is smaller than that required for a Stoner instability, ferromagnetic fluctuations can induce a partially or fully polarized superconducting state.

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Introduction.—The spin ordering of the observed quantized Hall plateau with $\sigma_{xy} = \frac{5}{2} \frac{e^2}{h}$ [1,2] has become a pressing issue due to its pertinence to the identification of this state of matter as a potential platform for topological quantum computation [3]. Experimental [4,5] and numerical studies [6] have not, thus far, settled the matter, although they are consistent with a fully spin-polarized Moore-Read (MR) Pfaffian ground state [7,8]. In this Letter, we revisit the spin-polarization of the ground state at $\nu = 5/2$ using (1) a variational Monte Carlo (VMC) comparison of the energies of polarized and unpolarized states, (2) a GL effective field theory, and (3) a Fermi liquid calculation of the magnetic instability of paired composite fermions. We find evidence that it is polarized even if the Zeeman energy vanishes. We give a simple physical picture of the energetics of various states, drawing on similarities with ferromagnetic superconductors.

For large enough Zeeman energy, the ground state must be fully polarized. However, the Zeeman energy in GaAs 2DEGs is small due to effective mass and g -factor renormalization. Thus, the system is near the limit of vanishing Zeeman energy, where the Hamiltonian is the full $SU(2)$ spin symmetry. At $\nu = 1$ and $\nu = 1/3$ in this limit, the spins order ferromagnetically, thereby spontaneously breaking this symmetry [9,10]. However at $\nu = 5/2$, an incompressible state is likely to exhibit pairing. It is thus natural to ask if similar spin-ordering physics occurs at $\nu = 5/2$, but from the perspective that the ground state is a spin-triplet paired state. Indeed, it is known [8,11] that both the fully polarized Pfaffian and the unpolarized (3, 3, 1) states belong to the same family of triplet paired states, for which the wave function is $\Psi = \Psi_{LJ} \Psi_{\vec{d}}$ with $\Psi_{LJ} = \prod_{j < k} (z_j - z_k)^m \prod_j e^{-|z_j|^2/4}$ and

$$\Psi_{\vec{d}} = \text{Pf} \left(\frac{\vec{d} \cdot (i\vec{\sigma}\sigma_2)_{\alpha\beta} |\alpha\rangle_j |\beta\rangle_k}{z_j - z_k} \right). \quad (1)$$

with $\alpha, \beta = \uparrow, \downarrow$. The complex unit vector \vec{d} above is

familiar from ^3He physics. For the fully polarized (along the \hat{z} direction) Pfaffian state, $\vec{d} = -(\hat{x} + i\hat{y})/\sqrt{2}$, so the spin part of the pair wave function is $|\chi_{jk}^s\rangle = |\uparrow\rangle_j |\uparrow\rangle_k$ which has $S_z = 1$. The (3, 3, 1) state corresponds to $\vec{d} = \hat{z}$, for which each pair has $S_z = 0$ and $|\chi_{jk}^s\rangle = |\uparrow\rangle_j |\downarrow\rangle_k + |\downarrow\rangle_j |\uparrow\rangle_k$ [11]. In the language of ^3He the (3, 3, 1) state is therefore a *unitary* triplet paired state, while the Pfaffian is a *nonunitary* triplet state [12]. With this insight, it was first observed by Ho [11] that one can obtain states in which the expectation value of the spin of a pair, $\vec{F} = i\vec{d} \times \vec{d}^*$ has any value $0 \leq |\vec{F}| \leq 1$. Indeed, one can check that $\vec{d} = \hat{z}(1 - F^2)^{1/4} e^{i\theta} - (\hat{x} + i\hat{y})(1 - \sqrt{1 - F^2})^{1/2}/\sqrt{2}$ gives a *partially* polarized state with polarization magnitude F . A state with a polarization axis different from \hat{z} can be obtained by rotating \vec{d} .

In this Letter, we analyze in several ways the energetics of spin for arbitrary triplet pairing, as well as the transitions between unpolarized and partially or fully polarized states. First, in a VMC calculation, we find that the energy of the polarized Pfaffian is lower than that of the unpolarized (3, 3, 1) state at $\nu = 5/2$. This suggests that if the ground state in the presence of Coulomb interaction is paired, it is fully or partially polarized. Second, we construct a Chern-Simons (CS) GL theory for spinful electrons [13], which we adapt to the case of a quantum Hall state of spin-1 bosons at even-denominator filling fraction. We thus derive an effective field theory for the dynamics of the vector \vec{d} , which turns out to be a perturbed CP^2 $NL\sigma M$ model analogous to the $O(3)$ $NL\sigma M$ of quantum Hall ferromagnets [9]. The $SU(3)$ symmetry of the CP^2 model is lowered to the physical $SU(2)$ symmetry by the Zeeman coupling $\tilde{g} = g\mu_B B$ which couples to the composite pair spin \vec{F} , and also by quadratic and quartic spin-spin interactions, c_2 and u . We analyze the resulting phase diagram as a function of \tilde{g} , c_2 , and u and conclude that, for $c_2 < 0$, as expected for a ferromagnetic pair-pair interaction, the system is either

partially or fully spin polarized. If u is sufficiently small (especially if negative), then the system is fully spin polarized. The unpolarized (3, 3, 1) state only occurs in the event of antiferromagnetic pair-pair interactions. Finally, we give a more microscopic derivation of the effective field theory, thereby obtaining values for c_2 and u , starting from a BCS Stoner mean-field picture of a triplet superconductor competing or cooperating with ferromagnetism. It is important to include the magnetization as an independent order parameter since the spins can order even if the composite fermions do not pair, as in the case of compressible states [14]. Since composite fermions have an enhanced effective mass, this is a strong possibility and, indeed, this ordering transition appears to have been observed in the compressible state at $\nu = 1/2$ [15]. Moreover, the interplay between these two orders has recently received attention in the context of ferromagnetic superconductors such as ZrZn_2 , UGe_2 , and URhGe [16–20], and because such interplay can result in a transition between a unitary and a nonunitary triplet state. Except at the ordering transition, the ferromagnetic order parameter can be integrated out, thereby leading to the GL theory mentioned in the previous paragraph and described below. However, the parameters \tilde{g} , c_2 , and u all receive important contributions from magnetic fluctuations, which we compute. Our most interesting conclusion from this analysis is that even if short-range repulsion is insufficient to trigger a Stoner instability, ferromagnetic fluctuations can drive a transition to a partially polarized nonunitary state once pairing is present.

Variational Monte Carlo calculation.—We can gain insight into which of the paired states (1) are favored by variationally comparing the energies of the (3, 3, 1) state and the Pfaffian. We have performed VMC on the sphere for up to 60 electrons in both states in the spirit of [21]. We have confirmed that at $\nu = 1/2$ the energy per particle of Coulomb interaction is $E_{\text{Pf}}/N = -0.457(2)$ in units of $e^2/\epsilon\ell_b$. However, we also find that the (3, 3, 1) state is slightly lower in energy $E_{331}/N = -0.4634(5)$. This is still higher than the composite Fermi sea (polarized or unpolarized [22]) in agreement with the absence of a plateau at $\nu = 1/2$ [14]. We analyze the $\nu = 5/2$ case in the spirit of [22] by mimicking the first Landau Level pseudopotentials of pure Coulomb interaction with an effective interaction in the lowest Landau Level, $V_{\text{eff}}(r) = (e^2/\epsilon)(1/r + a_1 e^{-\alpha_1 r^2} + a_2 r^2 e^{-\alpha_2 r^2})$. In this case, we find that the Pfaffian is lower in energy than the (3, 3, 1) state: $E_{\text{Pf}}/N = -0.361(5)$, and $E_{331}/N = -0.331(5)$. This is in agreement with the existing numerical evidence [6] that the ground state at $\nu = 5/2$ is spin polarized. To decide if the lowest energy paired state is fully or partially polarized, one would have to obtain the Coulomb energy of a partially polarized state, which is hard to do variationally, because no efficient algorithms for antisymmetrization exist.

CP^2 Ginzburg-Landau theory.—The calculation of the previous paragraph indicated that the ground state at $\nu = 5/2$ is polarized. We now try to understand this in the

context of a GL effective field theory. We begin with bosonic pairs with $e^* = 2$ at filling fraction $\nu_b = 1/8$. This corresponds to an electron filling fraction $\nu_e = 1/2$. (We ignore the filled $N = 0$ Landau level of the $\nu = 5/2 = 2 + 1/2$ state and focus on the partially filled $N = 1$ Landau level.) The basic field is a bosonic order parameter Ψ_i , $i = 0, \pm 1$ which is essentially \vec{d} : $\sqrt{\bar{\rho}/2}d_x = (\Psi_{-1} - \Psi_1)/\sqrt{2}$, $\sqrt{\bar{\rho}/2}d_y = (\Psi_1 + \Psi_{-1})/i\sqrt{2}$, $\sqrt{\bar{\rho}/2}d_z = \Psi_0$. Therefore the top and bottom components of Ψ_i represent Pfaffian states along the $S_z \pm 1$ direction while the middle component is a (3, 3, 1) state with $S_z = 0$.

$$\begin{aligned} \mathcal{L} = & \Psi_i^\dagger (\partial_0 - 2ia_0) \Psi_i + \frac{1}{2m^*} |(i\vec{\partial} + 2\mathbf{a} + 2\mathbf{A}_{\text{ex}})\Psi_i|^2 \\ & + \frac{1}{2} \nu (2\Psi_i^\dagger \Psi_i - \bar{\rho})^2 + \frac{1}{4\pi\alpha} \epsilon^{\mu\nu\lambda} a_\mu \partial_\nu a_\lambda \\ & + \frac{1}{2} \int d^2 r' (\rho(\mathbf{r}) - \bar{\rho}) V(\mathbf{r} - \mathbf{r}') (\rho(\mathbf{r}') - \bar{\rho}) \\ & + \frac{1}{2} g_{\text{eff}} \mu_B B \Psi_i^\dagger T_{ij}^z \Psi_j + c_2 (\Psi_i^\dagger \vec{T}_{ij} \Psi_j)^2 \\ & + u (\Psi_i^\dagger \vec{T}_{ij} \Psi_j)^4. \end{aligned} \quad (2)$$

In Eq. (2), m^* is the effective mass of a pair and at $\nu_e = 1/2$, $\alpha = 2$. The \vec{T}_{ij} s are the generators of the spin-1 representation of $SU(2)$. In addition to the familiar CS-GL and Coulomb interaction terms [23], the last line of (2) contains an effective Zeeman term $g_{\text{eff}} \mu_B$ for the pairs after the fermions are integrated out, as well as quadratic and quartic spin-spin interaction terms, c_2 and u respectively. These couplings can, in principle, be derived from the underlying composite fermion theory from which (2) emerges at length scales longer than the pair size. This is done in a simple model below. Coulomb exchange between the fermions induces a ferromagnetic interaction between pairs which competes with the fermion kinetic energy in a Stoner picture. If ferromagnetic exchange dominates, $c_2 < 0$, and a fully polarized Pfaffian or a partially polarized state becomes the ground state, but for now we consider both signs. Finally, in the description of spin-1 atoms in an optical trap (“spinor condensates”), the quartic coupling, u , would be negligible since the probability for 4 bosons to meet at a point is extremely small at low density [24]. In a system of weakly bound BCS-like pairs, however, such a term need not be small since the pair size is comparable to the spacing between pairs. This GL theory (2) is valid at energies below the pairing gap Δ_0 to neutral fermionic excitations. In this regime, the fermions may be integrated out so long as no vortices are present. When vortices are present, we must be more careful, since there will be fermionic zero modes which are crucial for the non-Abelian braiding statistics of vortices [25–29]).

When Ψ_i condenses, we can write it as $\Psi_i = \sqrt{\bar{\rho}/2} e^{2i\theta} \xi_i$ with $\bar{\xi}_i \xi_i = 1$. Since ξ_i , which transforms as a vector under spin rotations, is complex and of unit magnitude it takes values in the CP^2 model. Substituting

Ψ_i into (2) one can see that kinetic energy will be relieved if charge fluctuations $J_\mu^c = 2\partial_\mu\theta$ and spin fluctuation $J_\mu^s = \tilde{\xi}_i\partial_\mu\xi_i$ cancel. But because both currents are charged due to the CS gauge field, there is a Coulomb self-energy cost associated with both vortex and Skyrmion excitations. This energy cost favors large skyrmions and competes with the Zeeman energy, which favors small skyrmions. We follow the steps outlined in Kane and Lee [13,30], and obtain a perturbed CP^2 model for the ξ_i variables alone, which is a generalization of the perturbed $NL\sigma M$ of quantum Hall ferromagnets [9]:

$$\begin{aligned} \mathcal{L}_{\text{eff}} = & \rho\tilde{\xi}_i\partial_0\xi_i + \frac{1}{2}K(\partial_i\tilde{\xi}_i\partial_i\xi_i + (\tilde{\xi}_i\partial\xi_i)^2) + \mathcal{L}_{\text{Hopf}} \\ & + g_{\text{eff}}\mu_B B_{\tilde{\rho}}(|\xi_1|^2 - |\xi_{-1}|^2) + \tilde{c}_2(\tilde{\xi}_i\tilde{F}_{ij}\xi_j)^2 \\ & + \tilde{u}(\tilde{\xi}_i\tilde{F}_{ij}\xi_j)^4 + \frac{1}{8}\int d^2r' Q_{\text{Sk}}(\mathbf{r})V(\mathbf{r}-\mathbf{r}')Q_{\text{Sk}}(\mathbf{r}') \end{aligned} \quad (3)$$

In the above $\tilde{c}_2 = c_2\tilde{\rho}^2$ and $\tilde{u} = u\tilde{\rho}^4$, but for simplicity from now on we will omit the tildes. The CP^2 Skyrmion charge, $Q_{\text{Sk}} = (-i/2\pi)\epsilon^{\mu\nu}\partial_\mu\tilde{\xi}_i\partial_\nu\xi_i$, is equal to the vortex charge; it is 1/4 the electrical charge. Note that a Skyrmion texture in the magnetization vector $n_i = i\epsilon_{ijk}\xi_j \times \tilde{\xi}_k$ has CP^2 Skyrmion charge 2. The Hopf term in the first line of (3) gives the Abelian part of the Skyrmion statistics.

Phase diagram.—Let us consider the ground state of (3). The Hopf term is unimportant for energetics and so is the Coulomb energy of charged excitations. For $g = u = c_2 = 0$, the system is at a (multi)critical point controlled by the CP^2 model. At this critical point, the Pfaffian, the (3, 3, 1) state, and all states interpolating between them have the same energy. The phase diagram for $g = 0$, and general \tilde{c}_2 , \tilde{u} has the form depicted in Fig. 1. For $c_2, u > 0$ the system is in the (3, 3, 1) phase. For $\tilde{u} < 0$, there is a first-order phase transition at $\tilde{c}_2 = -\tilde{u} > 0$ from the (3, 3, 1) state to the fully polarized Pfaffian state. This is both a topological phase transition and a conventional ($\xi_y \rightarrow -\xi_y$) Z_2 symmetry-breaking transition. For $\tilde{u} > 0$, there is a second-order phase transition at $c_2 = 0$ from the (3, 3, 1) phase to a partially polarized (PP) state, which is a conventional Z_2 symmetry-breaking transition. In a wedge of the phase diagram between the lines $-\tilde{c}_2 = 2\tilde{u}$ and $\tilde{c}_2 = 0$ with $\tilde{u} > 0$, each pair has $F^2 = -\tilde{c}_2/2\tilde{u} \leq 1$. At $-\tilde{c}_2 = 2\tilde{u}$, $\tilde{u} > 0$ the system becomes fully polarized. This is a second-order phase transition at the mean-field level, but there is no symmetry distinction between the partially and fully polarized states. However, when we take into account the underlying fermions, there will be a topological phase transition between Abelian and non-Abelian states. In general, this transition will not occur at $-\tilde{c}_2 = 2\tilde{u}$ but, instead, before the system becomes fully polarized [28]. This will be discussed further elsewhere [31]. All of these phases have gapless spin excitations which are the Goldstone modes of spontaneously broken $SU(2)$. Finally,

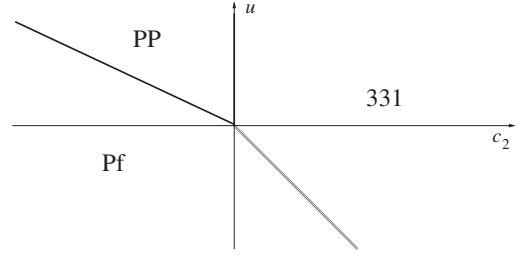


FIG. 1. Phase diagram for zero Zeeman coupling as a function of \tilde{c}_2 and \tilde{u} , as explained in the text.

turning on the $SU(2)$ symmetry-breaking perturbation g always induces nonzero magnetization. For $g > 2(c_2 + 2u)$, the system is fully polarized. We now turn to a more microscopic calculation of the parameters c_2 and u .

BCS Stoner calculation of c_2 , u .—Following Greiter *et al.* [8], by using flux attachment we can consider electrons at half filling as composite Fermions (CFs) which would be free if the CS gauge field is replaced by its mean-field value. The CFs would then form a Fermi sea [14]. Greiter *et al.* showed that gauge field fluctuations mediate an interaction between fermions which favors $p + ip$ superconductivity. However, in the absence of pairing, CF effective mass renormalization [14] and Coulomb repulsion would also favor ferromagnetism. Therefore, as a starting point, we assume the following BCS Stoner reduced Hamiltonian:

$$\begin{aligned} H = & \sum_k \frac{k^2}{2m^*} c_{k\alpha}^\dagger c_{k\alpha} + \vec{M} \cdot c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{k\beta} \\ & + \vec{\Delta}_k^* \cdot c_{k\alpha} (i\vec{\sigma}\sigma_2)_{\alpha\beta} c_{-k\beta} + \text{h.c.} \end{aligned} \quad (4)$$

For simplicity, we assume short-range repulsion $\vec{M} = U\sum_k c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{k\beta}$. The role played by the CS gauge field is apparent only through the interaction $V_{kk'} = \pi\vec{k} \times \vec{k}'/|\vec{k} \times \vec{k}'|^2$ which enters the self-consistency condition, $\vec{\Delta}_k = V_{kk'} \langle (i\vec{\sigma}\sigma_2)_{ab} c_{k'a} c_{-k'b} \rangle$. We note that Eq. (4) represents, in principle, a more general class of states than (1) since it is not assumed that $\vec{F} = \vec{M}$.

The spectrum of Bogoliubov–de Gennes quasiparticles resulting from (4) is

$$\begin{aligned} E_{k\pm}^2 = & \tilde{\epsilon}_k^2 + \Delta_k^2 + M^2 \\ & \pm \sqrt{|\vec{\Delta}_k^* \times \vec{\Delta}_k + 2i\tilde{\epsilon}_k\vec{M}_k|^2 + 4|\vec{M} \cdot \vec{\Delta}_k|^2}, \end{aligned} \quad (5)$$

where $\tilde{\epsilon}_k = \epsilon_k - \mu$ and we assume that $\vec{\Delta}_k$ has the chiral p -wave form [8] $\vec{\Delta}_k = \Delta_0\vec{d}(k_x + ik_y)/k_F$ if $k < k_F$ and $\vec{\Delta}_k = \Delta_0\vec{d}k_F/(k_x - ik_y)$, if $k > k_F$, where \vec{d} is a complex unit vector, as before. We integrate out the fermions to obtain the effective potential: $V_{\text{eff}} = \int_k \sum_{\sigma=\pm} (\tilde{\epsilon}_k - E_{k\sigma}) + \int_{kk'} \vec{\Delta}_k^* V_{k',k}^{-1} \vec{\Delta}_k + \frac{M^2}{2U}$. We take Δ_0 fixed and expand to fourth order in M , and $\vec{F} = i\vec{d} \times \vec{\Delta}_k^*$, thereby expanding about the (3, 3, 1) state. We obtain terms coupling the two order parameters:

$$\begin{aligned}
V_{\text{eff}} = & \alpha_2 F^2 + \alpha_4 F^4 + \gamma_1 \vec{F} \cdot \vec{M} + \gamma_3 F^2 \vec{F} \cdot \vec{M} \\
& + M_i R_{ij} M_j \vec{F} \cdot \vec{M} + \chi^{-1} M^2 + B_{ij} M_i M_j + u_a M^4 \\
& + u_b M^2 |\vec{d} \cdot \vec{M}|^2 + u_c |\vec{d} \cdot \vec{M}|^4, \quad (6)
\end{aligned}$$

where $\alpha_2 = m^* \pi \Delta_0^2$, $\alpha_4 = m^* \pi \Delta_0^2 / 6$, $\gamma_1 = 2m^* \pi \epsilon_F \eta^2$, $\gamma_3 = -2m^* \pi \epsilon_F \eta^2 / 7$, $u_m = 3m^* \pi / 2 \epsilon_F^2 \eta^2$, $u_{md} = 4m^* \pi / 3 \epsilon_F^2 \eta^2$, and $u_d = 8m^* \pi / 3 \epsilon_F^2 \eta^2$, with $\eta \equiv \Delta_0 / \epsilon_F$ assumed to be small but nonzero (the effective expansion parameter is M_0 / Δ_0). We also have $R_{ij} = r_m \delta_{ij} + r_d d_i d_j^*$ and $B_{ij} = B_d d_i d_j^* + B_F F_i F_j$, with $r_m = -8m^* \pi / \epsilon_F$, $r_d = -40m^* \pi / 7$, $A = 1/U - 4m^* \pi$, $B_d = (4m^* \pi (1 + F^2/3))$, and $B_F = 2m^* \pi / 3$. A similar result has been found in [20] in the limit that both Δ_0 and M are small (as opposed to our limit of small \vec{F} , \vec{M} but finite Δ_0).

The coupling between magnetism and superconductivity enhances the tendency to magnetism. $\chi^{-1} > 0$ would disfavor a magnetic moment in the absence of pairing; α_2 , $\alpha_4 > 0$ would favor unitary ground states. However, the coupling between magnetism and triplet superconductivity can lead to a nonzero moment and a nonunitary order parameter even when χ^{-1} , α_2 , $\alpha_4 > 0$. The condition is essentially that the smallest eigenvalue of the matrix $\partial^2 V_{\text{eff}} / \partial X_i \partial X_j$, with $X = (\vec{M}, \vec{F})$, become negative. This occurs when $\alpha_2 \chi^{-1} < \gamma_1^2 / 4$ or, equivalently, using the expressions after (6), $\frac{1}{U} - (4 + \eta^2) m^* \pi < 0$.

If we diagonalize the quadratic terms and integrate out the fields which correspond to the positive eigenvalues of $\partial^2 V_{\text{eff}} / \partial X_i \partial X_j$, we obtain an effective action of the form of (3) with c_2 and u given by

$$c_2 = \left(\frac{1}{U} - (4 + \eta^2) m^* \pi \right) \frac{\Delta_0^2}{2}, \quad u = \frac{3\pi m^* \epsilon_F^4}{2\Delta_0^2}. \quad (7)$$

As U is increased from zero, the system undergoes a second-order phase transition from the (3, 3, 1) state to a partially polarized state. The expressions (7) are only valid for small η , but for larger η a second transition will occur to the fully polarized Pfaffian state [31]. This is likely to be the physically relevant regime for the $\nu = 5/2$ state, where there is only one energy $e^2 / \epsilon \ell_0$, which sets the scale for both Δ_0 and ϵ_F .

Discussion.—From the results described above, we see that if the $\nu = 5/2$ quantum Hall state is a spin-triplet paired state, then it will be polarized in the limit of sufficiently strong ferromagnetic interactions. Whether or not this occurs and whether it is partially or fully polarized depends on the strength of the short-range repulsion relative to the effective fermion mass. Large repulsion would favor full polarization, while repulsion comparable to the effective mass would favor partial polarization even if lower than the Stoner critical value. The partially and fully polarized states could, in principle, be distinguished by NMR Knight shift measurements which probe the polarization directly. Experiments which are sensitive to the nature of quasiparticle excitations, either in the bulk or at the edge, such as resistively detected NMR or point contact

tunneling, respectively, could potentially distinguish these states. While we do believe our mean-field BCS Stoner model captures the essential physics, one should be careful before comparing with experiments, because we have not taken into account, for example, effective mass divergences at the Fermi surface, which are known to arise at $\nu = 1/2$ [14,32]. Another important issue concerns the identification of the excitations in the various partial and fully polarized states. One crucial question that begs an answer is the following: Do the excitations carry non-Abelian statistics? We discuss this elsewhere [31].

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 - [32] N. Read, Phys. Rev. B **58**, 16262 (1998), and references therein.