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# Composite fermion pairing induced by Landau level mixing

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Pairing of composite fermions provides a possible mechanism for fractional quantum Hall effect at even denominator fractions and is believed to serve as a platform for realizing quasiparticles with non-Abelian braiding statistics. We present results from fixed-phase diffusion Monte Carlo calculations which predict that substantial Landau level mixing can induce a pairing of composite fermions at filling factors  $\nu = 1/2$  and  $\nu = 1/4$  in the  $l = -3$  relative angular momentum channel, thereby destabilizing the composite-fermion Fermi seas to produce non-Abelian fractional quantum Hall states.

The recent observation by Wang *et al.* [1, 2] of fractional quantum Hall effect (FQHE) at filling factor  $\nu = 3/4$  has come as a surprise, because a priori one would have expected a composite-fermion (CF) Fermi sea here [3–5], where composite fermions are bound states of electrons and an even number of quantized vortices [6–8]. The half-filled Landau level (LL) state at  $\nu = 1/2$  is known to be a Fermi sea of composite fermions with two quantized vortices bound to them. A Fermi sea of composite fermions carrying four vortices has also been confirmed unambiguously at  $\nu = 1/4$  through commensurability oscillations [9]. This implies, by particle-hole (PH) symmetry, a CF Fermi sea (CFFS) also at  $\nu = 1 - 1/4 = 3/4$ . Further support to a CFFS at these fractions comes from the observation of FQHE at several fractions belonging to the sequences  $\nu = s/(4s \pm 1)$  and  $\nu = 1 - s/(4s \pm 1)$  [10–12], which are integer quantum Hall states of composite fermions carrying four vortices; these terminate into CFFSs at  $\nu = 1/4$  and  $\nu = 3/4$  in the limit  $s \rightarrow \infty$ .

FQHE at an even denominator fraction was first observed at  $\nu = 5/2$  [13, 14], which corresponds to half filling in the second LL. It has been proposed that FQHE here arises from a pairing of composite fermions [15–18], which is modeled in terms of the Moore-Read Pfaffian (MR-Pf) wave function [15] representing a chiral  $p$ -wave pairing of composite fermions. (Even denominator FQHE in the  $\mathcal{N} = 1$  LL of bilayer graphene is analogous to the  $5/2$  state in GaAs quantum wells (QWs) [19–22].) Why is there a difference between the physics at half filling in the lowest and the second LLs? For this purpose one must consider the CF-CF interaction, which derives from the electron-electron interaction. Extensive comparisons with exact diagonalization studies as well as experiments have shown that the model of non-interacting composite fermions is qualitatively valid when the short-range part of the interelectron interaction is dominant, which is the case in the lowest LL (LLL) [8]. The short range part of the electron-electron interaction is weaker in the second LL (as measured by the Haldane pseudopo-

tentials [23]), rendering the interaction between composite fermions slightly attractive, and thereby causing a pairing instability of the CFFS [24]. The excitations of this state are predicted, akin to the Abrikosov vortices in a two-dimensional chiral  $p$ -wave superconductor, to be realizations of particles obeying non-Abelian braid statistics [15, 18, 25–27].

What can weaken the short range part of the interelectron interaction in the LLL? One possibility is finite QW width. There is indeed evidence for FQHE at  $\nu = 1/4$  in very wide QWs [28–31]. Ref. [32] has proposed that the modification of the interaction due to QW width makes the CFFS unstable to an  $f$ -wave pairing. However, the  $3/4$  FQHE has been observed in rather narrow QWs (width of only 20 nm [1]), which sit comfortably in the CFFS region of the phase diagram evaluated in Ref. [32].

With the QW width ruled out as a relevant factor, one is left with LL mixing (LLM) as the possible cause for FQHE at  $\nu = 3/4$ . The FQHE at  $\nu = 3/4$  has been observed in hole-type samples [1], which, because of the larger hole mass, and hence smaller cyclotron energy, have much stronger LLM than electron-type samples. Indeed, the LLM parameter is  $\kappa \simeq 10$  and 14 for the two samples of Ref. [1], where  $\kappa = (e^2/\epsilon\ell)/(\hbar\omega_c)$  is the ratio of the Coulomb energy to the cyclotron energy (here  $\epsilon$  is the dielectric constant of the semiconductor,  $\ell = \sqrt{\hbar c/eB}$  is the magnetic length, and  $\hbar\omega_c = \hbar eB/m_b c$  is the cyclotron energy of particles with band mass  $m_b$ ).

It is clear that LLM will screen the short range part of the interelectron interaction. Can it induce pairing of composite fermions? The answer to this question relies on the ability to calculate accurately small energy differences in the presence of significant LLM. Below we consider quantitatively the possibility of CF pairing driven by LLM at filling factors  $\nu = 1/2$  and  $\nu = 1/4$ . (For technical reasons stated below, the state at  $\nu = 3/4$  is not amenable to our calculation.) For  $\kappa \rightarrow 0$ , one can employ a perturbative approach [33–41], wherein LLM enters through a renormalization of the two-body interaction, while also introducing three and higher body in-

interactions. Given that large  $\kappa$  values are of interest, we instead use a fixed-phase diffusion Monte Carlo method (FPDMC) [42–44], which provides a non-perturbative treatment of LLM. While this method has its own approximations (mentioned below), it provides strict variational upper bounds for the energies of various states, and has given a fairly reasonable account of experiments on spin transitions [45] and the competition between the FQHE and the crystal phase [46–48]. Our calculations suggest that the 1/2 and 1/4 CFFSs are unstable to pairing in the presence of substantial LLM. At both of these filling factors, we find that the most favored pairing channel for composite fermions is  $l = -3$ , which belongs in the same phase as the anti-Pfaffian (APf) state.

We note here that LLM has been considered previously in the context of the 5/2 state. Here, the MR-Pf is energetically equivalent to, although topologically distinct from, its hole partner called the APf [49, 50] in the absence of LLM. Much theoretical work has investigated how LLM will break the tie between the two [36, 37, 40, 51–55]. In contrast to the situation at  $\nu = 5/2$ , where both the MR-Pf and the APf states are present even in the absence of LLM, the present work asks if LLM can induce pairing, and hence FQHE, where none was present in the absence of LLM.

We begin by enumerating all of the candidate states that we study in this article. For the incompressible states, we consider the MR-Pf state, its generalizations [18], and several Jain parton states [56], all of which are non-Abelian. For all the calculations we will be employing the spherical geometry [23] which has  $N$  electrons on the surface of a sphere moving under the influence of a radial magnetic field produced by a magnetic monopole of strength  $Q$  at the center, which emanates a total flux of  $2Q\phi_0$ , with  $\phi_0 = hc/e$  defining the flux quantum. The state with  $n$  filled LLs is denoted by  $\Phi_n$  (with  $\Phi_{-n} = [\Phi_n]^* \equiv \Phi_{\bar{n}}$ ) in what follows, with  $\Phi_1 = \prod_{j < k} (u_j v_k - v_j u_k)$ , where  $u_i = \cos(\theta_i/2)e^{i\phi_i/2}$  and  $v_i = \sin(\theta_i/2)e^{-i\phi_i/2}$  are the spinor coordinates of the  $i^{\text{th}}$  electron with  $\theta_i$  and  $\phi_i$  being its polar and azimuthal angles on the sphere. The states occur at  $2Q = \nu^{-1}N - \mathcal{S}$  where the shift  $\mathcal{S}$  is one of the topological properties of a FQHE state [57]. Here are the explicit states:

(i) The CFFS of composite fermions carrying  $2p$  vortices is given by  $\Psi^{\text{CFFS}} = \mathcal{P}_{\text{LLL}} \Phi^{\text{eFS}} \Phi_1^{2p}$ , where  $\Phi^{\text{eFS}}$  is the electron-Fermi sea wave function in the spherical geometry at zero flux, and  $\mathcal{P}_{\text{LLL}}$  refers to projection into the LLL, for which we use the Jain Kamilla (JK) method described in Refs. [58, 59]. We also consider the unprojected CFFS, labeled as unproj-CFFS. We shall consider only filled shell states [60, 61] that occur for particle numbers  $N = 4, 9, 16, 25$ .

(ii) For wave functions for the CF pairs in relative angular momentum  $l$  we follow Ref. [18]. For positive  $l$ , we

write

$$\Psi_{\nu=1/2p}^{\text{Pf}_l} = \text{Pf} \left[ \frac{(u_i^* v_j^* - v_i^* u_j^*)^{(l-1)}}{(u_i v_j - v_i u_j)} \right] \Phi_1^{2p}, \quad (1)$$

whereas for negative  $l$ , we have

$$\Psi_{\nu=1/2p}^{\text{Pf}_{-|l|}} = \text{Pf} \left[ \frac{(u_i v_j - v_i u_j)^{(|l|-1)}}{(u_i^* v_j^* - v_i^* u_j^*)} \right] \Phi_1^{2p}. \quad (2)$$

Here  $\text{Pf}[M_{i,j}] \sim \mathcal{A}(M_{1,2} M_{3,4} \cdots M_{N-1,N})$ , where  $N$  is even,  $M_{ij}$  is an antisymmetric matrix and  $\mathcal{A}$  represents antisymmetrization.  $\Psi^{\text{Pf}_1}$  represents the MR-Pf wave function which occurs at shift  $\mathcal{S} = 2p + 1$ .  $\Psi^{\text{Pf}_{-1}}$  represents the PH-symmetric (PHS)-Pf wave function [62–65], and occurs at the same shift  $\mathcal{S} = 2p - 1$  as the PHS-Pf proposed by Son [66].  $\Psi^{\text{Pf}_{-3}}$  occurs at the same shift  $\mathcal{S} = 2p - 3$  as the APf. Another paired state with shift  $\mathcal{S} = 2p - 3$ , lying in the APf phase, is given by [67]:

$$\Psi_{\nu=1/2p}^{\text{Pf}'_{-3}} = \text{Pf} \left[ \frac{(u_i v_j - v_i u_j)}{(u_i^* v_j^* - v_i^* u_j^*)^2} \right] \Phi_1^{2p}. \quad (3)$$

We will use the unprojected wave functions to fix the phase, except for  $\Psi^{\text{Pf}_1}$  which already resides in the LLL.

(iii) The unprojected Jain 221 parton wave function [56] at  $\nu = 1/2$  is given by  $\Psi_{1/2}^{\text{unproj-221}} = \Phi_2^2 \Phi_1$ . This is a non-Abelian state [68] representing an  $f$ -wave pairing of composite fermions [32, 64]. It is the exact ground state for a short-range Hamiltonian [69, 70] and is possibly relevant for 1/2 FQHE in  $\mathcal{N} = 3$  LL of monolayer graphene [71]. We do not consider the LLL-projected 221 state as that requires the construction of this state in the Fock space, which can be accomplished only for very small systems. For  $\nu = 1/4$ , the closely related 22111 parton state can be conveniently projected into the LLL as  $\Psi_{1/4}^{22111} \equiv [\mathcal{P}_{\text{LLL}} \Phi_2 \Phi_1^2] / \Phi_1 = [\Psi_{2/5}]^2 / \Phi_1$ , which can be evaluated for fairly large systems by the standard projection methods [58, 59].

(iv) The unprojected  $\bar{2}2111$  parton state [64] at  $\nu = 1/2$  is given by  $\Psi_{1/2}^{\text{unproj-}\bar{2}2111} = \Phi_2^2 \Phi_1^3$ . This state has the same shift  $\mathcal{S}$  as the APf, and its low-lying entanglement spectrum is identical to that of the APf for small systems [64]. These features suggest that the  $\Psi_{1/2}^{\text{unproj-}\bar{2}2111}$  lies in the same phase as the APf. The state can be projected into the LLL as  $\Psi_{1/2}^{\bar{2}2111} \equiv [\mathcal{P}_{\text{LLL}} \Phi_2 \Phi_1^2] / \Phi_1 = [\Psi_{2/3}]^2 / \Phi_1$ , which can be explicitly performed for fairly large systems by the JK projection with the reverse-vortex attachment [72, 73]. The unprojected and projected  $\bar{2}211111$  parton states for  $\nu = 1/4$ , which lie in the same universality class as the APf, can be constructed similarly:  $\Psi_{1/4}^{\text{unproj-}\bar{2}211111} = \Phi_2^2 \Phi_1^5$  and  $\Psi_{1/4}^{\bar{2}211111} \equiv [\mathcal{P}_{\text{LLL}} \Phi_2 \Phi_1^2] / \Phi_1 = [\Psi_{2/3}]^2 \Phi_1$ .

The APf wave function at  $\nu = 1/2$  is obtained from the MR-Pf wave function by performing PH transformation,

and the APf wave function at  $\nu = 1/4$  can be accessed by multiplying it by  $\Phi_1^2$ . We do not consider the APf state because no convenient wave function is known for it (it must be constructed by an explicit PH transformation in the Fock space representation) and also because previous work has shown that at  $\nu = 1/2$  the energies of the MR-Pf and the APf wave functions remain very close even with LLM [54].

The above “trial” wave functions are used to fix the “phase” in the FPDMC calculation that incorporates LLM. The basic outline is as follows (see Ref. [42] and the supplemental material (SM) [74] for more details). Given a trial wave function  $\Psi(\mathcal{R})$  where  $\{\mathcal{R}\}$  collectively denotes the positions of all particles, we first write  $\Psi(\mathcal{R}) = \Phi(\mathcal{R})e^{i\varphi(\mathcal{R})}$  where  $\Phi(\mathcal{R}) = |\Psi(\mathcal{R})|$  is non-negative, and  $\varphi(\mathcal{R})$  is the phase of the wave function. The variational energy of the system of interacting electrons in a magnetic field described by the vector potential  $\mathbf{A}$  is given by  $\langle \Psi(\mathcal{R}) | H | \Psi(\mathcal{R}) \rangle = \langle \Phi(\mathcal{R}) | H_R | \Phi(\mathcal{R}) \rangle$  with  $H_R = \sum_{j=1}^N [\mathbf{p}_j^2 + [\hbar \nabla_j \varphi(\mathcal{R}) + (e/c) \mathbf{A}(\mathbf{r}_j)]^2] / 2m_b + V_{\text{Coulomb}}(\mathcal{R})$ . We now assume that the phase  $\varphi(\mathcal{R})$  remains fixed. The lowest energy in this phase sector is obtained by varying  $\Phi(\mathcal{R})$ . The energy minimization is accomplished by applying the standard DMC method [75, 76] to the imaginary time Schrödinger equation  $-\hbar \frac{\partial}{\partial \tau} \Phi(\mathcal{R}, \tau) = [H_R(\mathcal{R}) - E_T] \Phi(\mathcal{R}, \tau)$ , where the fixed phase appears effectively through a vector potential. Details of the FPDMC method, as well as its application to the spherical geometry, are given in Refs. [42–46]. The principal shortcoming of this method is that the accuracy of the energy depends on the choice of the phase. Previous studies [45, 46, 77] have indicated that the phase of an accurate LLL wave function remains a reasonably good approximation even in the presence of LLM. Here we also use “unprojected” wave functions (which are not confined to the LLL) to fix the phase. Even though the wave function is modified in the FPDMC process, we will continue to label it by the initial trial wave function.

We will assume that the state is fully spin-polarized, as expected at high magnetic fields. We will not include corrections due to finite QW thickness and consider a purely two-dimensional system. Our results are thus applicable to narrow QWs. All energies below are quoted in units of  $e^2/\epsilon\ell$ .

Fig. 1 presents the energies of the CFFS and the Pf<sub>-3</sub> states for  $\nu = 1/4$  as a function of  $1/N$  for several values of  $\kappa$  (for all extrapolations see the SM [74]). The energies include the contribution  $-N^2/(2\sqrt{Q}) e^2/(\epsilon\ell)$  from electron-background and background-background interaction, assuming a uniform neutralizing background charge. Because of the shift, the electron density has an  $N$  dependence, which causes a dominant correction to the energy; we multiply the raw energy of the system by  $\sqrt{2Q\nu/N}$  to compensate for the finite-size effect [78]. This leads to better fits by linear regression in  $1/N$  and reduces the error in the thermodynamic limit. The un-

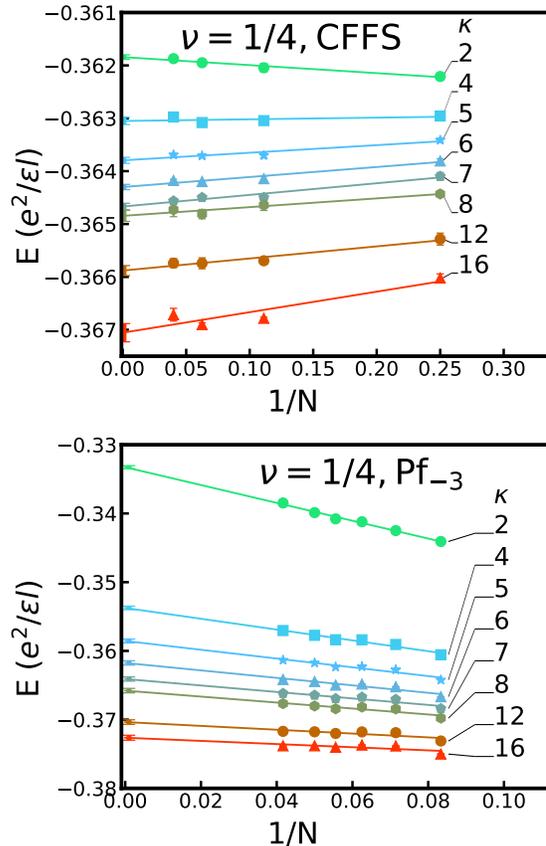


FIG. 1. The energies of the CFFS and the Pf<sub>-3</sub> states for  $\nu = 1/4$  (bottom) as a function of  $1/N$  for several different values of the LL mixing parameter  $\kappa$  (labeled on plots). The thermodynamic values of energies, whose uncertainties are labeled near the vertical axes, are obtained by linear regression. Extrapolations for all candidate states are shown in the SM [74].

certainty in the thermodynamic limit originates primarily from the deviation of the finite-size energy from the fitted line. The thermodynamic energies of various states as a function of  $\kappa$  are plotted in Fig. 2. In the absence of LLM ( $\kappa = 0$ ), the CFFS has significantly lower energy than the paired states, consistent with experiments that have confirmed the CFFS here [3, 5, 79] and earlier numerical studies [80]. Our most important finding is that at both  $\nu = 1/2$  and  $\nu = 1/4$  the CFFS is unstable to pairing as  $\kappa$  is increased. Further, at both of these filling factors, there is a level crossing into the  $l = -3$  paired state at  $\kappa \approx 6 - 7$ . This state has a very high energy at small  $\kappa$  (as is the case for all states that are not LLL projected), but its energy comes down rapidly with LLM. As shown in the SM [74], even at large LLM, the pair-correlation function of the  $l = -3$  paired states show oscillations that decay with distance and converge to the density, as anticipated for gapped liquid states [61, 81].

As mentioned earlier, LLM weakens the short-distance repulsion between the electrons and may thus induce a

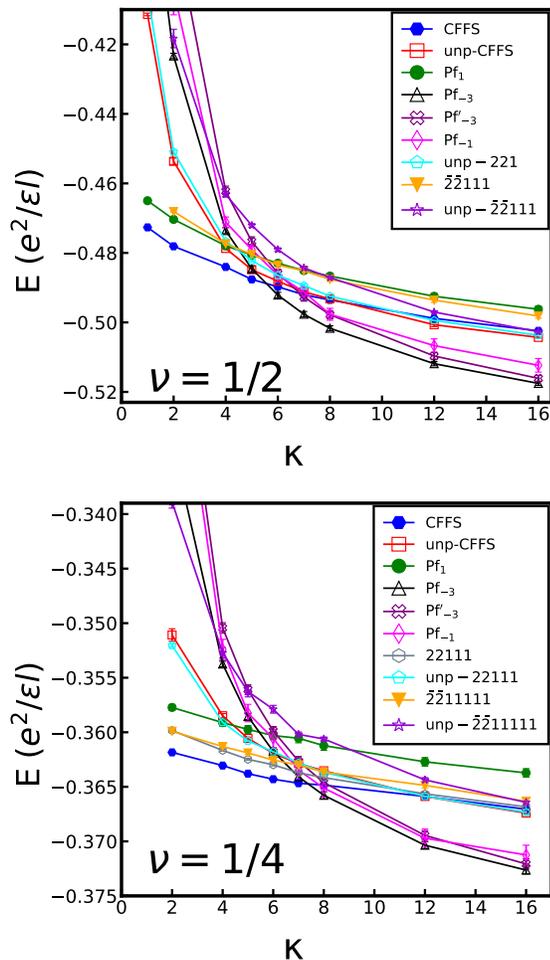


FIG. 2. This figure shows the thermodynamic energies as a function of the LL mixing parameter  $\kappa$  when the phase sector is fixed using various trial states shown on the figures. For small  $\kappa$  the lowest energy is obtained in the CFFS phase sector, but for large  $\kappa$  the state derived from the  $l = -3$  paired state wins at both  $\nu = 1/2$  and  $\nu = 1/4$ .

weak residual attractive interaction between CFs leading to their pairing. We do not have a simple qualitative argument for why pairing in the  $l = -3$  channel is preferred over other pairing channels. Only detailed calculations, like the ones presented here, can help identify the optimal pairing channel, as is also the case for the extensively studied CF pairing at  $\nu = 5/2$  (see SM for further discussion [74]); of course, the decisive verification will come only from experiments.

The results are sensitive to the trial wave function used to fix the phase even within the same topological sector. For example, the energies starting from the projected and unprojected 22111 or CFFS states are significantly different for small  $\kappa$ , although they tend to be similar for large  $\kappa$ . That implies that the precise value of  $\kappa$  where the phase transition takes place from the CFFS to the paired state is only approximate. Finite width corrections are

also likely to affect the transition. These points notwithstanding, our calculations make what we believe to be a plausible case that a transition will take place as a function of  $\kappa$  into a paired state. We note here that FQHE at  $\nu = 1/2$  has been observed in wide QWs [31, 82–86]; some calculations have suggested a two-component Abelian Halperin-331 state [87–89] while others the MR-Pf or the APf [90, 91]. In contrast, for our current problem where we are considering the role of LLM at zero width, the MR-Pf ( $\text{Pf}_1$ ) is not competitive for any  $\kappa$ .

The topological properties of  $\Psi^{\text{Pf}_{-3}}$ , which is in the same phase as the APf, have been enumerated in earlier articles [49, 50]. All candidate states support quasiparticles with fractional charge  $e/4p$ . The APf state supports an upstream neutral mode, which is experimentally measurable [92]; this can distinguish it from the MR-Pf and  $221^{2p+1}$  states (with the caveat that edge reconstruction can produce upstream neutral modes in these states as well). A decisive measurement would be the thermal Hall conductance [93], which is given by  $c[\pi^2 k_B^2 / (3h)]T$ , where the chiral central charge is  $c = 1 + l/2$  for the state with CF pairing in the relative angular momentum  $l$  channel.

Unfortunately, the above calculation cannot be performed directly at  $\nu = 3/4$ , because the hole conjugates of the unprojected wave functions are not defined, and even for the LLL projected states the hole conjugates can be constructed only for very small systems, as this requires working with their explicit Fock space representations. Nonetheless, our results support the idea that LLM is responsible for a paired FQHE here. Ref. [54] found that even though the energies of the MR-Pf and APf wave functions vary substantially with  $\kappa$ , they remain surprisingly close, and the same is true of the gaps of the  $1/3$  and  $2/3$  FQHE states. It is therefore a plausible first guess that the  $3/4$  FQHE state stabilized in Ref. [1] may be in the same universality class as the hole partner of the  $l = -3$  paired state.

We have not considered the possibility of the crystal state in our calculations. Previous theoretical (see [46] and references therein), as well as experimental studies (see [94] and references therein), have indicated that sufficient LLM can also stabilize the crystal phase. At what  $\kappa$  the crystal phase appears at  $\nu = 1/4$  and  $\nu = 1/2$  is left for a future study.

Before ending, we note that values of  $\kappa > 7$  at  $\nu = 1/2$  have been achieved in hole-type GaAs QWs as well as AlAs QWs [47, 94–97]. No evidence has yet been seen for FQHE at  $\nu = 1/2$  or  $\nu = 1/4$  in narrow QWs. It may be that our calculation underestimates the critical  $\kappa$  for pairing instability. It is also possible that better quality samples would be needed for the observation of these states; after all, FQHE at  $\nu = 3/4$  has also revealed itself only in the highest quality samples that have become available recently [12].

In summary, we have found theoretically that LLM can cause a pairing of composite fermions to produce

non-Abelian FQHE states. Specifically, we predict that the CFFSs at  $\nu = 1/2$  and  $\nu = 1/4$  will transition, with increasing LL mixing, into  $l = -3$  paired states of composite fermions carrying two and four vortices, respectively. We further speculate that the observed FQHE at  $\nu = 3/4$  is the hole partner of the latter. We hope that our work will motivate further study of the even denominator states in the LLL in the presence of high LLM.

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