

# Spin instabilities and quantum phase transitions in integral and fractional quantum Hall states

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The spin excitations of quantum Hall states at filling factors  $\nu=2$  and  $\frac{4}{3}$  are investigated numerically in the systems with comparable cyclotron ( $\hbar\omega_c$ ) and Zeeman ( $E_Z$ ) gaps. The relevant quasiparticles and their interactions are studied, including spin wave and skyrmion bound states. For  $\nu=2$ , a spin instability at a finite value of  $\varepsilon=\hbar\omega_c-E_Z$  leads to an abrupt paramagnetic to ferromagnetic transition, in agreement with the mean-field approximation. However, for  $\nu=\frac{4}{3}$  a new quantum phase transition is found in finite-size droplets that involves a gradual change from para- to ferromagnetic occupancy.

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The elementary excitations of a two-dimensional electron gas (2DEG) with energy quantized into Landau levels (LL's) by a high magnetic field  $B$  have been extensively studied for decades. The charge excitations govern transport, including the integral and fractional quantum Hall effects (IQHE and FQHE).<sup>1</sup> The spin excitations appear in the context of spin waves (SW's),<sup>2</sup> spin instabilities, related quantum phase transitions (QPT's),<sup>3,4</sup> and skyrmions.<sup>5,6</sup>

In this Rapid Communication we study spin excitations of IQH and FQH systems with densities  $\varrho$  corresponding to the filling factors  $\nu=2\pi\varrho\lambda^2\approx 2$  and  $\frac{4}{3}$  (here,  $\lambda=\sqrt{\hbar c/eB}$  is the magnetic length). The cyclotron ( $\hbar\omega_c$ ) and Zeeman ( $E_Z$ ) splittings are assumed comparable and much larger than the Coulomb energy  $E_C=e^2/\lambda$ . In this situation, the spin excitations couple two partially filled LL's with different orbital indices,  $n=0$  and 1. These LL's, denoted by  $|0\uparrow\rangle$  and  $|1\downarrow\rangle$ , are separated by a small gap  $\varepsilon=\hbar\omega_c-E_Z\ll E_C$  from each other and by large gaps  $\sim\hbar\omega_c\gg E_C$  from the lower, filled  $|0\downarrow\rangle$  LL and from the higher, empty LL's, as shown schematically in Fig. 1(c).

For the  $\nu=2$  ground state (GS), it is well known<sup>3</sup> that a spin-flip instability occurs at a finite gap  $\varepsilon$  and wave vector  $k$ . In the mean-field approximation (MFA), this instability signals an abrupt, interaction-induced QPT from paramagnetic ( $P$ ;  $|0\downarrow\rangle$  and  $|0\uparrow\rangle$  filled) to ferromagnetic ( $F$ ;  $|0\downarrow\rangle$  and  $|1\downarrow\rangle$  filled) occupancy. Our numerical results confirm the validity of the MFA for  $\nu=2$ . However, for  $\nu=\frac{4}{3}$  they predict a new and unexpected  $P\rightarrow F$  QPT that occurs through a series of intermediate GS's with increasing number of spin flips as  $\varepsilon$  is decreased from  $\varepsilon_P$  to  $\varepsilon_F$  (the lower and upper boundaries of  $\varepsilon$  for the  $P$  and  $F$  occupancies, respectively). Since the transition range  $\Delta\varepsilon=\varepsilon_P-\varepsilon_F$  scales with the inverse system size, the gradual  $P\rightarrow F$  QPT should be experimentally observed only in finite FQH droplets.<sup>7</sup>

The model is the same as that used earlier,<sup>6,8</sup> except that now the spin excitations connect two different LL's. The electrons are confined to a spherical surface<sup>9</sup> of radius  $R$ . The radial magnetic field  $B$  is due to a monopole of strength  $2Q$ , defined in units of the flux quantum  $\phi_0=hc/e$  so that  $4\pi R^2B=2Q\phi_0$  and  $R^2=Q\lambda^2$ . The single-electron states are labeled by angular momentum  $l=Q+n$  and its projection  $m$ .

Only the partially filled  $|0\uparrow\rangle$  and  $|1\downarrow\rangle$  LL's (labeled by pseudospin  $s=\uparrow$  and  $\downarrow$ ) are included in the calculation, and

the filled, rigid  $|0\downarrow\rangle$  LL enters through the exchange energy  $\Sigma_{10}$ . The ratio  $\varepsilon/E_C$  is taken as an arbitrary parameter. Although we do not discuss the effect of the finite width  $w$  of a realistic 2DEG (Ref. 6) and only present the results obtained using the pseudopotential  $V(\mathcal{R})$  (interaction energy as a function of relative pair angular momentum<sup>10</sup>) for  $w=0$ , shown in Fig. 1(a), we have checked that our conclusions remain valid for  $w\leq 5\lambda$ .

The Hamiltonian  $H$  for electrons confined to the  $|0\uparrow\rangle$  and  $|1\downarrow\rangle$  LL's contains the single-particle term  $(\varepsilon-\Sigma_{10})$  and the intra- and inter-LL two-body interaction matrix elements  $\langle m_1s, m_2s' | V | m_3s', m_4s \rangle$  calculated for the Coulomb potential  $V(r)=e^2/r$  and connected with pseudopotentials  $V_{ss'}(\mathcal{R})$  shown in Fig. 1(a) through the Clebsch-Gordan coefficients (on a sphere,  $\mathcal{R}=2l-L$  where  $L=I_1+I_2$  is pair angular momentum).

Hamiltonian  $H$  is diagonalized in the basis of  $N$ -electron Slater determinants  $|m_1s_1 \cdots m_Ns_N\rangle$ . This allows automatic resolution of the projection of pseudospin ( $S_z=\Sigma s_i$ ) and of angular momentum ( $L_z=\Sigma m_i$ ). The quantum number  $K=\frac{1}{2}N+S_z$  measures the number of reversed spins relative to the paramagnetic configuration. The length of angular momentum ( $L$ ) is resolved numerically in the diagonalization of each  $(S_z, L_z)$  Hilbert subspace. The length of pseudospin is not a good quantum number because of the pseudospin-asymmetric interactions. The results obtained on Haldane sphere are easily converted to the planar geometry, where  $L$  and  $L_z$  are appropriately<sup>11</sup> replaced by the total and center-of-mass angular momentum projections,  $M$  and  $M_{CM}$ .

Let us begin with the discussion of the IQH regime. Figure 2 presents the spin-excitation spectra for  $N=14$ , at the filling factors equal to or different by one flux from  $\nu=2$ . Only the lowest state is shown for each  $K$  and  $L$ . The energy  $E$  is measured from the lowest paramagnetic state (at  $E=E_0$ ) and excludes the inter-LL gap  $\varepsilon$ . Symbols  $e^*$  and  $h$  denote reversed-spin electrons (particles in the  $|1\downarrow\rangle$  LL) and holes (vacancies in the  $|0\uparrow\rangle$  LL) created in the "vacuum" state (completely filled  $|0\uparrow\rangle$  LL).

The excitation spectrum of the "vacuum" state is shown in Fig. 2(b). The  $K=1$  band is a SW; in a finite system it has  $L=1$  to  $N$ , as follows from addition of the  $e^*$  and  $h$  angular momenta,  $l_{e^*}=Q+1$  and  $l_h=Q$ . In an infinite system, the

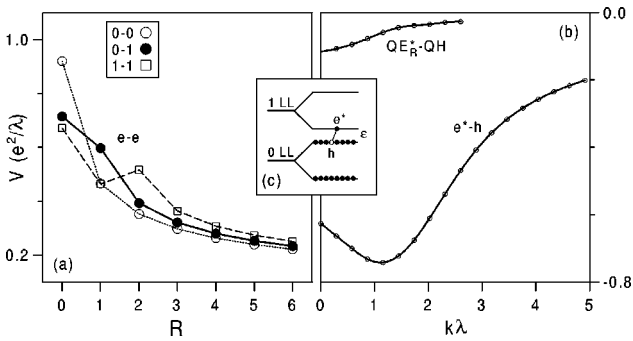


FIG. 1. The Coulomb pseudopotentials  $V$  for the pair of (a) electrons in the  $n=0$  and  $1$  LL's, and (b) reversed-spin electron ( $e^*$ ) or quasielectron ( $QE_{e^*}$ ) in the  $n=1$  LL and hole ( $h$ ) or quasihole ( $QH$ ) in the  $n=0$  LL. (c) Schematic of the LL structure at  $\nu=2$ , with the  $h$  and  $e^*$  quasiparticles.

continuous SW dispersion is given by<sup>2</sup>  $E_{SW}(k) = E_0 + \frac{1}{2}E_C \sqrt{\pi/2} \{1 - \exp(-\kappa^2) [(1+2\kappa^2)I_0(\kappa^2) - 2\kappa^2 I_1(\kappa^2)]\}$ , where  $\kappa = \frac{1}{2}k\lambda$ ,  $I_0$  and  $I_1$  are the modified Bessel functions, and  $k=L/R$ .  $E_{SW}(k)$  starts at  $E=E_0$  for  $k=0$  and has a minimum at  $k \approx 1.19\lambda^{-1}$  and  $E \approx E_0 - 0.147 E_C$ . The vanishing of SW energy at  $k=0$  is the result of exact cancellation of the sum of  $e^*$  and  $h$  exchange self-energies,  $-\Sigma_{10} + \Sigma_{00}$ , by the  $e^*-h$  attraction  $V_{e^*h}$  at  $k=0$ ; the entire  $e^*-h$  pseudopotential is shown in Fig. 1(b).

The energy spectra corresponding to consecutive spin flips ( $K=2,3,\dots$ ) at  $\nu=2$  all contain low-energy bands at  $L \geq K$ . For each  $K$ , the GS's (open circles) have  $L=K$  and their energies fall on a nearly straight line,  $E(K)$ . These GS's are therefore denoted by  $\mathcal{W}_K = K \times SW$  and interpreted as containing  $K$  SW's with parallel angular momenta each of length  $L=1$ , similar to the  $L=K$  SW condensates at  $\nu=1$ .<sup>6</sup> The new feature at  $\nu=2$  is the SW-SW attraction (due to a finite dipole moment of an inter-LL SW) giving rise to a negative slope of  $E(K)$ .

Let us now turn to Figs. 2(a) and 2(c) showing spin excitation spectra in the presence of an  $e^*$  or  $h$ . The series of GS's for  $K \geq 1$  (open circles) are charged bound states, similar to the skyrmions and anti-skyrmions at  $\nu=1$ . Their angular momenta result from a simple vector addition of  $l_{e^*}$  and  $l_h$ . For  $\mathcal{S}_K^- = K \times SW + e^*$  and  $\mathcal{S}_K^+ = K \times SW + h$  we get  $L = (l_{e^*})^{K+1} \oplus (l_h)^K = Q+1$  and  $L = (l_{e^*})^K \oplus (l_h)^{K+1} = |Q$

$-2K|$ , respectively. In both cases, finite  $L \propto Q$  means massive LL degeneracy, as expected for charged particles in a magnetic field.

Let us check if the negative SW energy at  $k \approx 1.19\lambda^{-1}$  or the SW-SW attraction causes instability of the  $\nu=2$  GS towards the formation of one or more SW's when  $\varepsilon$  is decreased. The single-SW instability has been ruled out by Giuliani and Quinn<sup>3</sup> who showed that it is pre-empted by a direct transition to the ferromagnetic GS. The critical value of  $\varepsilon$  for this  $P \rightarrow F$  QPT is expressed through the involved self-energies,  $\varepsilon_0 = \Sigma_{10} + \frac{1}{2}(\Sigma_{11} - \Sigma_{00}) = \frac{3}{8}\sqrt{\pi/2}E_C \approx 0.47E_C$ , and it is larger than  $E_0 - E_{SW}$ . Since the energy per spin flip,  $[E(K) - E_0]/K$ , is smaller for the SW condensates and skyrmions than for a single SW, we still need to check for a possible  $\text{vac} \rightarrow \mathcal{W}_K$ ,  $e^* \rightarrow \mathcal{S}_K^-$ , or  $h \rightarrow \mathcal{S}_K^+$  instability. Figure 3(a) shows that despite evident SW-SW, SW- $e^*$ , and SW- $h$  attraction ( $\delta E = E - E_0 + K\varepsilon_0$  is the energy to create  $K$  SW's in "vacuum" or in the presence of an  $e^*$  or  $h$ ), the  $\mathcal{W}_K$  and  $\mathcal{S}_K^\pm$  energies are all positive at  $\varepsilon = \varepsilon_0$ . This precludes spin instability at  $\nu=2$  other than the direct  $P \rightarrow F$  transition (skipping the states with intermediate spin).

To translate our finite-size spectra to the case of an infinite 2DEG, in Fig. 3(b) we have plotted the energies of the SW condensate calculated for different electron numbers,  $N \leq 14$ . Clearly, all data fall on the same curve when  $\delta E/\sqrt{N}$  is plotted as a function of "relative" spin polarization,  $\zeta = K/N$ . This resembles the insensitivity to  $N$  of the  $\delta E(\zeta)$  curves for the SW condensates at  $\nu=1$ , except that now  $\delta E \propto N^{1/2}$  (rather than  $\propto N^0$ ).

The data of Fig. 3 allow calculation of the SW binding energies,  $U_K = [E(K-1) - E_0] + [E_{SW} - E_0] - [E(K) - E_0]$ , for the  $\mathcal{W}_K$  and  $\mathcal{S}_K^\pm$  states. Because of the SW-SW attraction, all these energies increase in a similar way as a function of  $K$ , in contrast to  $\nu=1$  where  $U_K$  decreased for skyrmions and vanished for the SW condensate.

Let us now turn to the FQH regime. At  $\nu=4/3$ , which occurs for  $2Q=3(N-1)$ , and for sufficiently large  $\varepsilon$ , the  $N$  electrons in the  $|0\uparrow\rangle$  LL form the Laughlin  $\nu=\frac{1}{3}$  state. These electrons, each with angular momentum  $l=Q$ , can be converted into an equal number of composite fermions (CF's) (Ref. 12) each with effective angular momentum  $l^* = l - (N-1)$ , exactly filling their effective LL. The elementary

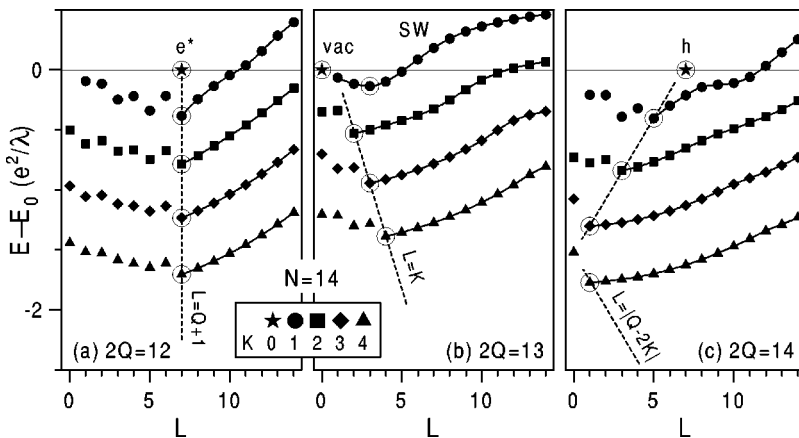


FIG. 2. The excitation energy spectra of 14 electrons in the  $|0\uparrow\rangle$  and  $|1\downarrow\rangle$  LL's calculated on a sphere for  $2Q=12$  (a), 13 (b), and 14 (c), corresponding to filling factors  $\nu \approx 2$ . The lowest  $|0\downarrow\rangle$  LL is filled.  $E_0$  is the energy of the lowest paramagnetic ( $K=0$ ) state, and dashed lines mark the lowest states for different values of  $K$ .

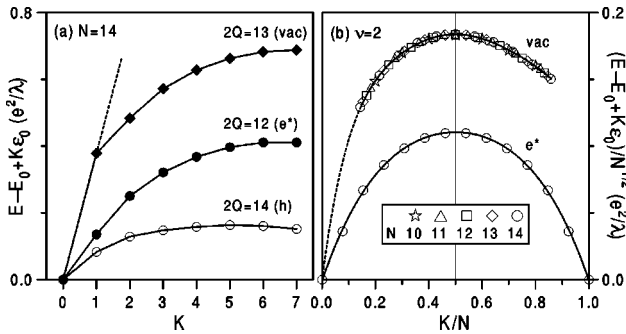


FIG. 3. (a) The energy of skyrmions, anti-skyrmions, and spin-wave condensates of Fig. 2, plotted as a function of  $K$ . Setting  $\epsilon = \epsilon_0$  ensures degeneracy of para- and ferromagnetic ( $K=0$  and  $N$ ) configurations. (b) The energy of spin-wave condensates for  $N=10$  to 14 (rescaled by  $\sqrt{N}$ ) as a function of  $\zeta = K/N$ . The skyrmion curve is shown for comparison.

charge excitations of the  $\nu = \frac{1}{3}$  state are two types of Laughlin quasiparticles (QP's), quasielectrons (QE's) and quasiholes (QH's), corresponding to an excess particle in an (empty) excited CF LL, or a hole in the (filled) lowest CF LL, respectively.

The reversed-spin quasielectrons ( $QE_R$ 's) (Refs. 8 and 13) do not occur at  $\nu = \frac{4}{3}$  because of the electrons completely filling the  $|0\downarrow\rangle$  LL. This causes a difference between the SW's at  $\nu = \frac{4}{3}$  and  $\frac{1}{3}$ , similar to that between  $\nu=2$  and 1. At  $\nu = \frac{1}{3}$  the SW consisted of a QH and a  $QE_R$ , and at  $\nu = \frac{4}{3}$  it is formed by a QH and a different reversed-spin QP that we will denote by  $QE_R^*$ .

The  $QE_R^*$  has the same electric charge of  $-\frac{1}{3}e$  as QE or  $QE_R$  but it belongs to an excited electron LL,  $|1\downarrow\rangle$ . Similar to the case for QH, QE, and  $QE_R$ , the existence and stability of the  $QE_R^*$  depend on the validity of the CF transformation for the underlying system of  $N-1$  electrons in the  $|0\uparrow\rangle$  LL and one electron in the  $|1\downarrow\rangle$  LL. This requires Laughlin correlations between the  $|1\downarrow\rangle$  electron and the  $|0\uparrow\rangle$  electrons, i.e., the occurrence of a Jastrow prefactor,  $\prod_{ij}(z_i^{(0)} - z_j^{(1)})^\mu$ , in the many-body wave function, with  $\mu=2$  for  $\nu = (1 + \mu)^{-1} = \frac{1}{3}$ . Such correlations result from short-range  $e-e$  repulsion, and the criterion is<sup>14,15</sup> that the pseudopotential  $V$  must decrease more quickly than linearly as a function of the average square  $e-e$  separation  $\langle r^2 \rangle$ . On a plane (or on a

sphere for  $\langle r^2 \rangle \ll R^2$ , i.e., for  $R \ll Q$ ) this is equivalent to a superlinear decrease of  $V$  as a function of  $R$ .

It is clear from Fig. 1(a) that the Coulomb inter-LL pseudopotential  $V_{01}(R)$  is a short-range repulsion for  $R \geq R_0 = 1$ . This implies the Jastrow prefactors with  $\mu > R_0 = 2, 3, \dots$  in the  $|0\uparrow\rangle^{N-1} \oplus |1\downarrow\rangle$  wave function, if only  $\nu \leq (1 + \mu)^{-1}$ . In particular, this establishes the  $QE_R^*$  as a stable reversed-spin QP of the  $\nu = \frac{4}{3}$  state, in analogy to the reversed-spin electron,  $e^*$ , at  $\nu=2$ . The angular momentum of  $QE_R^*$  on a sphere can be obtained in the two-component CF picture<sup>16</sup> appropriate for  $\nu = \frac{1}{3}$ , i.e., with both 0-0 and 0-1 Laughlin correlations modeled by attachment of two flux quanta to each electron. The resulting CF angular momenta are  $l_{QH} = Q^*$  and  $l_{QE} = l_{QE_R^*} = Q^* + 1$ , where  $Q^* = Q - (N-1)$ .

The excitation spectra at filling factors equal to or different by one flux from  $\nu = \frac{4}{3}$  are displayed in Fig. 4.  $N=8$  in each frame, and the values of  $2Q$  are 20, 21, and 22, corresponding to the following GS's at  $K=0$ : (a) QE at  $L=4$ , (b) "vacuum" (filled CF LL) with  $L=0$ , and (c) QH at  $L=4$ . The low-energy charge excitations for  $2Q=21$  form the magnetoroton (QE+QH) band. The low-energy spin excitations with  $K=1$  are the following: (a)  $QE_R^*$  at  $L = l_{QE_R^*} = 4$  for  $2Q=20$ , (b) the SW ( $QE_R^* + QH$ ) band with  $L$  going from 1 to  $N=8$ , as follows from vector addition of  $l_{QH}$  and  $l_{QE_R^*}$ , for  $2Q=21$ , and (c) a band of  $QE_R^* + QH_2$  states with a bound GS denoted as  $QE_R^*QH_2$  for  $2Q=22$ .

To draw analogy with Fig. 2, QE corresponds to an electron in the  $|1\uparrow\rangle$  LL (not shown because of high energy),  $QE_R^*$  to  $e^*$ , QH to  $h$ , and  $QE_R^*QH_2$  to  $S_1^+$ . The latter state is the only "skyrmion" at  $\nu = \frac{4}{3}$ . The  $S_K^-$  states with  $K \geq 1$  and  $L = Q^* + 1$  or the  $S_K^+$  states with  $K \geq 2$  and  $L = |Q^* - 2K|$  do not occur because of the weakened Coulomb repulsion at short range in the excited LL. As shown in Fig. 1(a), the linear behavior of  $V_{11}(R)$  between  $R=1$  and 5 prevents Laughlin correlations for two or more electrons in the  $n=1$  LL. This invalidates the CF model and causes breakup of  $QE_R^*$ 's when two of them approach each other (at this point, pairing of electrons in the  $n=1$  LL occurs.<sup>15,17</sup>) For the same reason, no  $\mathcal{W}_K$  states at  $L=K$  appear in Fig. 4(b) for  $K > 1$ .

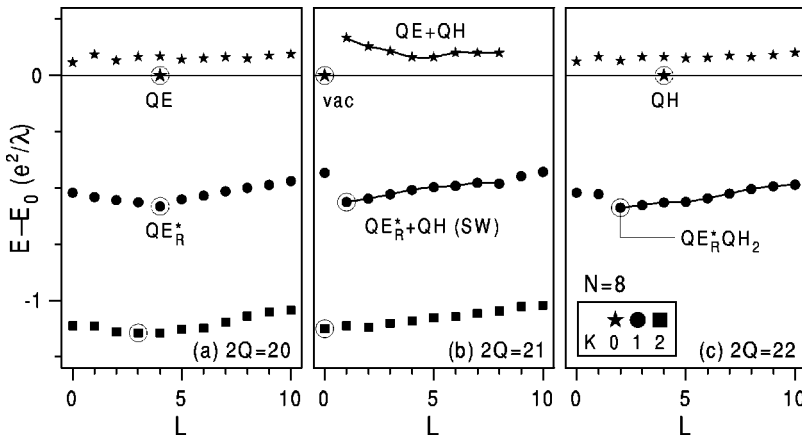


FIG. 4. Same as Fig. 2, but for  $N=8$  electrons and for the monopole strengths  $2Q=20$  (a), 21 (b), and 22 (c), corresponding to the filling factors  $\nu \approx \frac{4}{3}$ .

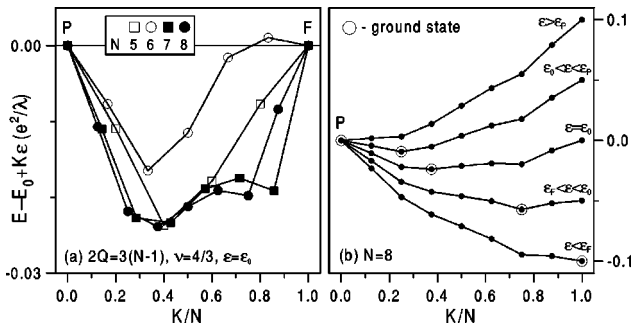


FIG. 5. (a) Same as Fig. 3(b), but for the filling factor  $\nu = \frac{4}{3}$ . (b) Data for  $N=8$  plotted for different values of  $\varepsilon$ .

Even more significant in Fig. 4 than the absence of  $S_K^\pm$  and  $W_K$  states is the large and negative SW energy  $E_{\text{SW}}^*(k)$  at  $\nu = \frac{4}{3}$ . This is in striking contrast to the  $\nu=2$  case, and it is explained as follows. The SW energy is the sum of the  $QE_R^*$  and QH self-energies and the  $QE_R^*$ -QH attraction. Of these three terms, only the  $QE_R^*$  self-energy,  $-\sum_{10} = -\frac{1}{2}\sqrt{\pi/2}E_C$ , is the same at  $\nu=2$  and  $\frac{4}{3}$ , while the QH self-energy  $\sum_{00}^*$  and the  $QE_R^*$ -QH pseudopotential  $V_{QE_R^*QH}(k)$  are both reduced (because of only partial filling of the  $|0\rangle$  LL and the fractional QP charge, respectively). As a result, the large and negative  $-\sum_{10}$  term becomes dominant in  $E_{\text{SW}}^*(k)$ . Note that even without knowing analytic expressions for  $\sum_{00}^*$  or  $V_{QE_R^*QH}(k)$ , the fact that  $V_{QE_R^*QH}(\infty) = 0$  allows the estimate of  $V_{QE_R^*QH}(k)$ , as shown in Fig. 1(b), and of  $\sum_{00}^* \approx 0.17 E_C$ . Note that  $V_{QE_R^*QH}(0) \approx -0.11 E_C \approx \frac{1}{6} V_{e^*h}(0)$  and  $\sum_{00}^* \approx \frac{1}{7} \sum_{00}$ .

The dependence of the GS energy on  $\zeta = K/N$  for  $\nu = \frac{4}{3}$  is shown in Fig. 5(a). As in Fig. 3,  $\varepsilon$  is set to the value  $\varepsilon_0$  for which the  $P$  and  $F$  configurations (at  $\zeta=0$  and 1) are degenerate.

Clearly, (almost) all energies at  $0 < \zeta < 1$  are negative. This effect does not depend on  $N$ ; on the contrary, all data points for moderate values of  $\zeta$  seem to fall on the same curve, characteristic of an infinite (planar) system. Negative excitation energies imply that the paramagnetic Laughlin  $\nu = \frac{4}{3}$  state is unstable toward flipping of only a fraction  $\zeta < 1$  of spins when  $\varepsilon$  is decreased. This is illustrated in Fig. 5(b) where we display the data for  $N=8$  corresponding to five different values of  $\varepsilon$ . The gradual decrease of  $\varepsilon$  from  $\varepsilon_P$  to  $\varepsilon_F$  drives the system through entire series of GS's (open circles) with fractional values of  $\zeta$ . This sequence of GS's are distinctly different from the abrupt  $P \rightarrow F$  QPT found at  $\nu=2$ , and they are not expected in the MFA.

We do not know the scaling of energies in Fig. 5(a) with  $N$  for large systems, but expect it to be sublinear. This implies collapse of the transition range  $\Delta\varepsilon$  for  $N \rightarrow \infty$ , and precludes detection of the gradual  $P \rightarrow F$  QPT in an infinite 2DEG. However, this QPT could still be observed in finite-size FQH droplets,<sup>7</sup> where  $\Delta\varepsilon$  remains finite.

In conclusion, our numerical study of small systems at  $\nu = 2$  serves as a test of the MFA which predicts an abrupt interaction-induced  $P \rightarrow F$  QPT associated with the spin-flip instability. This test should also be applicable to a similar instability and QPT which occurs for a bilayer<sup>18</sup> (where  $\hbar\omega_c$  is replaced by the symmetric-antisymmetric splitting  $\Delta_{\text{SAS}}$ ). For the fractional  $\nu = \frac{4}{3}$  state the series of spin-flip GS's between the para- and ferromagnetic states is a prediction that is susceptible to experimental observation.

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