Spin Instabilities and Quantum Phase Transitions in Integral and Fractional Quantum Hall States

Arkadiusz Wójs¹,² and John J. Quinn¹

¹Department of Physics, University of Tennessee, Knoxville, Tennessee 37996, USA
²Institute of Physics, Wroclaw University of Technology, Wroclaw 50-370, Poland

The inter-Landau-level spin excitations of quantum Hall states at filling factors $\nu = 2$ and $\frac{1}{2}$ are investigated by exact numerical diagonalization for the situation in which the cyclotron ($\hbar \omega_c$) and Zeeman ($E_Z$) splittings are comparable. The relevant quasiparticles and their interactions are studied, including stable 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 $\nu = \frac{1}{2}$ a new and unexpected quantum phase transition is found which involves a gradual change from paramagnetic to ferromagnetic occupancy of the partially filled Landau level as $\varepsilon$ is decreased.

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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) [1]. The spin excitations appear in the context of spin waves (SW’s) [2], spin instabilities and related quantum phase transitions (QPT’s) [3], and skyrmions [3,4].

In this letter we study spin excitations of IQH and FQH systems with densities $\rho$ corresponding to the filling factors $\nu = 2\pi \rho \lambda^2 \approx 2$ and $\frac{1}{2}$ (here, $\lambda = \sqrt{hc/eB}$ is the magnetic length). The cyclotron ($\hbar \omega_c$) and Zeeman ($E_Z$) splittings are assumed comparable and much larger than the Coulomb energy $E_C = \varepsilon^2/\lambda$. 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 [3] 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 $\nu = \frac{1}{2}$ they predict a new and unexpected P→F QPT that occurs through a series of intermediate GS’s involving 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).

The model is the same as that used earlier [6,7], except that now the spin excitations connect two different LL’s. The electrons are confined to a spherical surface 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 $4\pi R^2 B = 2Q\phi_0$ 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 $\Sigma_{0\downarrow}$. 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 [8] and only present the results obtained using the pseudopotential $V(R)$ (interaction energy as a function of relative pair angular momentum $\lambda$) 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 $\langle m_1s, m_2s' | V | m_1s', m_4s \rangle$ calculated for the Coulomb potential $V(r) = \varepsilon^2/r$ and connected with pseudopotentials $V_{\lambda \phi}(R)$ shown in Fig. 1(a) through the Clebsch–Gordan coefficients (on a sphere, $R = 2l - L$ where $L = I_1 + I_2$ is pair angular momentum).
Hamiltonian $H$ is diagonalized in the basis of $N$-electron Slater determinants $|m_1s_1 \ldots m_N s_N\rangle$. This allows automatic resolution of the projection of pseudospin ($S_z = \sum s_i$) and of angular momentum ($L_z = \sum m_i$). 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 approximately 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. Fig. 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 ($E = E_0$) 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 continuous SW dispersion is given by $E_{SW}(k) = E_0 + \frac{\hbar^2}{2m_e}C \sqrt{\pi/2} \{1 - \exp(-\kappa^2)\} \{1 + 2\kappa^2\} I_0(\kappa^2) - 2\kappa^2 I_1(\kappa^2)\}$, where $\kappa = \frac{\hbar k}{L/R}$. $E_{SW}(k)$ starts at $E = E_0$ for $k = 0$ and has a minimum at $k \approx 1.19\hbar^{-1}$ and $E \approx E_0 - 0.147 Ec$. 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. 2(b).

The energy spectra corresponding to consecutive spin flips ($K = 2, 3, \ldots$) 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 $W_K = K \times SW$ and interpreted as containing $K$ SW's with parallel angular momenta each of length $L = 1$, similar to the $L = K$ SW condensates at $\nu = 1$. 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 Fig. 2(a) and (b) 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 simple vector addition of $l_e$ and $l_h$. For $S_K = K \times SW + e^*$ and $S_K^+ = K \times SW + h$ we get $L = (l_e) + 1 \# K = Q + 1$ and $L = (l_e) + (l_h)^{K+1} = |Q - 2K|$, 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 who showed that it is preempted 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, $\varepsilon_0 = \frac{1}{2} (\Sigma_{10} - \Sigma_{00}) = \frac{\hbar}{2} \sqrt{\frac{\pi}{2}} Ec \approx 0.47 Ec$, 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 $\text{vac} \rightarrow W_K, e^* \rightarrow S_K^+$, or $h \rightarrow S_K^+$ instability. Fig. 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 $W_K$ and $S_K^+$ 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 allows calculation of the SW binding energies, $U_K = |E(K - 1) - E_0| + |E_{SW} - E_0| - |E(K) - E_0|$, for the $W_K$ and $S_K$ 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 $\nu = \frac{4}{3}$, 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) \([1]\) each with effective angular momentum \( l' = l - (N - 1) \), exactly filling their effective LL. The elementary charge excitations of the \( \nu = \frac{1}{3} \) state are two types of Laughlin quasiparticles (QP's), quasi-electrons (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) \([2]\) do not occur at \( \nu = \frac{1}{3} \) 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 \( \nu = \frac{1}{3} \) 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 QE, 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 \(|0\downarrow\rangle\) 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 \([3,4]\) 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. 3(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 \( \mu > R_0 = 2, 3, \ldots \) 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 \( \nu = \frac{1}{3} \) 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 \([13]\) 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 \( l_{QE} = l_{QE^*} = Q^* + 1 \), where \( Q^* = Q - (N - 1) \).

The excitation spectra at filling factors equal to or different by one flux from \( \nu = \frac{1}{3} \) 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* states with a bound GS denoted as QE'RQH* for \( 2Q = 22 \).

To draw analog with Fig. 3, 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'RQH* to \( S^+ \). The latter state is the only “skyrmion” at \( \nu = \frac{1}{3} \). The \( S^+ \) 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. 4(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 break-up of QE'R's when two of them approach each other (at this point, pairing of electrons in the \( n = 1 \) LL occurs \([5,6]\) ). For the same reason, no \( W_K \) states at \( L = K \) appear in Fig. 4(b) for \( K > 1 \).

Even more significant in Fig. 3 than the absence of \( S^+_K \) and \( W_K \) states is the large and negative SW energy \( E_{SW}(k) \) at \( \nu = \frac{1}{3} \). 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 QEQH$^*_R$ QH attraction. Of these three terms, only the QEQH$^*_R$ self-energy, $-\Sigma_{10} = -\frac{1}{2}\sqrt{\pi/2} E_C$, is the same as $\nu = 2$ and $\frac{1}{3}$, while the QH self-energy $\Sigma_{00}$ and the QEQH pseudopotential $V_{QEH}(k)$ are both reduced (because of only partial filling of the $|0\uparrow\rangle$ LL and the fractional QP charge, respectively). As a result, the large and negative $-\Sigma_{10}$ term becomes dominant in $E_{SW}^*(k)$. Note that even without knowing analytic expressions for $\Sigma_{00}$ or $V_{QEH}(k)$, the fact that $V_{QEH}(\infty) = 0$ allows the estimate of $V_{QEH}(k)$, as shown in Fig. 3(b), and of $\Sigma_{00} \approx 0.17 E_C$. Note that $V_{QEH}(0) \approx -0.11 E_C \approx \frac{1}{6} V_{FQH}(0)$ and $\Sigma_{00} \approx \frac{7}{5} \Sigma_{00}$. The dependence of the GS energy on $\zeta = K/N$ for $\nu = \frac{1}{3}$ is shown in Fig. 3(a). As in Fig. 3(b), $\zeta$ is set to the value $\zeta_0$ 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 $\nu = \frac{3}{4}$ state is unstable toward flipping of only a fraction $\zeta < 1$ of spins when $\varepsilon$ is decreased. This is illustrated in Fig. 3(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 novel 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.

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 [7] (where $\hbar \omega_c$ is replaced by the symmetric-antisymmetric splitting $\Delta_{SAS}$). For the fractional $\nu = \frac{1}{3}$ state the series of spin-flip GS’s between the para- and ferromagnetic states is a novel prediction that is susceptible to experimental observation.

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