Skyrme crystal or Skyrme liquid?

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We address the quantum melting phase transition of the Skyrme crystal. Based on generic sum rules for two-dimensional, isotropic electron quantum liquids in the lowest Landau level, we propose analytic expressions for the pair distribution functions of spin-polarized and spin-unpolarized liquid phases at filling factors $2/3 \leq \nu \leq 1$. From the pair distribution functions we calculate the energy of such liquid phases and compare with the energy of the solid phase. The comparison suggests that the quantum melting phase transition may lie much closer to $\nu = 1$ than ever expected.

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Whether or not a solid phase composed of skyrmions exists near filling factor $\nu = 1$ poses, probably, one of the most fascinating problems in recent history of the quantum Hall effect. This phase, known as Skyrme crystal, is, nowadays, the target of a number of experiments based on various techniques which, in the past, have borne out the existence of the skyrmions themselves. To date, however, little experimental evidence of the existence of the Skyrme crystal has been provided. Bayot et al. have reported a peak in the specific heat at very low temperatures which may be attributed to a phase transition from a finite-temperature liquid phase into a solid phase at zero temperature. The spin polarization measured by Barret et al. seems to be consistent, at least in the range of filling factors $1 - \nu \approx 0.2$, with that calculated by Brey et al. for a proposed solid phase. This apparent consistency neither guarantees that a zero-temperature liquid phase exists out of that range nor, most importantly, rules out its existence close to $\nu = 1$; for an alternative proposal of an unpolarized or partially polarized quantum liquid is not available to compare with.

If a solid phase really exists at zero temperature, the following question needs to be answered: What is the filling factor at which quantum fluctuations turn the solid into a liquid? Filling factors $\nu = 2/3$ and $\nu = 4/3$ set the lower and upper melting transition limits, respectively. (We will focus on $\nu < 1$ since the physics for $\nu > 1$ is similar due to particle-hole symmetry.) For large enough Zeeman energy per electron, $g \mu_B B/2$, the $\nu = 2/3$ state is a spin-polarized liquid. More precisely, it is a $\nu = 1/3$ Laughlin state of holes. For $g \mu_B B/2 = 0$ there has been mounting numerical and experimental evidence of a spin-unpolarized liquid ground state. To zero in on the actual location of the melting transition one can try to estimate the energy scale of the quantum fluctuations associated to the phonon modes in the classical solid phase and compare it with some relevant energy scale, typically, set by the Coulomb interaction.

This is a very crude approximation; moreover, it does not provide any information about the liquid phase. Another approach, used in Wigner crystal studies and which we explore in this Letter, is to offer an alternative description of the ground state in terms of a quantum liquid, obtain its energy, and compare it with that of the solid phase.

After Laughlin’s proposal of a wave function for the main filling factors $\nu = 1/M$ (where $M$ is an odd integer $\geq 3$), many other wave functions have been proposed for other filling factors with notorious success. For many purposes, however, a many-body wave function contains redundant information which can be compacted in a more advantageous way. In this spirit we note that the ground state energy per particle, $E/N \equiv \epsilon$, for an infinite, neutral, and isotropic liquid state can be obtained from the pair distribution function $g(r)$:

$$
\epsilon = \frac{\nu}{2} \int_0^\infty dr \left[ g(r) - 1 \right] V(r),
$$

where $V(r)$ is the interaction potential. In general, $g(r)$ can only be obtained from the wave function using the plasma analogy. On occasions, however, one can find an analytic approximation for $g(r)$ based on the fact that it must fulfill generic sum rules. In addition to these sum rules and in order to get the desired accuracy, one must provide microscopic information specific to the quantum liquid state. This information is essential, but, as shown below, can be obtained from simple considerations which do not necessarily involve the wave function. Here we find $g(r)$ and calculate the energy of spin-polarized and spin-unpolarized quantum liquid phases in the range of filling factors between $\nu = 2/3$ and $\nu = 1$. Exact diagonalizations for $\nu = 2/3$, where we certainly expect liquid phases, and $\nu = 4/5$ allow us to confirm the reliability of this procedure. Figure shows the energy per particle of both liquid phases compared to that of the solid phase proposed by Brey et al. in a mean-field approximation. Our results confirm the existence of liquid...
phase ground states at $\nu = 2/3$ and also at $\nu = 4/5$ \[1\]. Most importantly, our results suggest that, even without considering partial polarization of the liquid phase, the quantum melting phase transition takes place very close to $\nu = 1$. In fact, it seems to occur near the transition point that separates the square Skyrme lattice from the triangular one \[3\].

\[\text{FIG. 1. Energy per particle in the Hartree-Fock approximation of the solid phase or Skyrme crystal (dots) and of the polarized (stars) and unpolarized (solid line) liquid phases proposed in the text. For completeness, the values obtained from the exact diagonalizations are presented by circles for both polarized and unpolarized phases. The results for the polarized liquid phase include a Zeeman energy shift of } g \mu_B B/2 = -0.0075 e^2/\ell \text{ and all the energies are referred to } -\frac{1}{\mu_0} \sqrt{\pi/2}.\]

Following early work by Girvin \[10\], we start by noting that the pair distribution function of a liquid state in the lowest Landau level (LLL) can be expanded in terms of wave functions for relative states of two particles. Girvin noticed that it is convenient to recast this expansion in terms of the pair distribution function for the $\nu = 1$ liquid plus a perturbative series. When the liquid is fully polarized

\[g(r) = 1 - e^{-r^2/2} + e^{-r^2/4} \sum_{m=1}^{\infty} c_m \frac{2}{m!} \left( \frac{r^2}{4} \right)^m, \]

where the prime denotes a sum restricted to odd values of $m$. The generalized $g(r)$ for fully spin-unpolarized states (i.e., with equal density of spin-up and spin-down electrons)

\[g(r) = \frac{1}{2} [g_{\uparrow\uparrow}(r) + g_{\downarrow\downarrow}(r)],\]

is divided into a contribution coming from equal spin electrons, $g_{\uparrow\uparrow}(r) \equiv g_{\uparrow\uparrow}(r)$, and a contribution from opposite spin electrons, $g_{\downarrow\uparrow}(r) \equiv g_{\downarrow\uparrow}(r)$. It is natural to expand $g_{\uparrow\uparrow}(r)$ in a way similar to that in \[9\]. It is also convenient to make a similar expansion for $g_{\uparrow\downarrow}(r)$, except for the fact that the sum runs now over all possible non-negative integer values of $m$:

\[g_{\uparrow\downarrow}(r) = 1 - e^{-r^2/2} + e^{-r^2/4} \sum_{m=0}^{\infty} \tilde{c}_m \frac{2}{m!} \left( \frac{r^2}{4} \right)^m. \]

If, for all $m$, $c_m \to 0$ and $\tilde{c}_m \to 0$, one recovers the partial distribution functions $g_{\uparrow\uparrow}(r)/2$ and $g_{\uparrow\downarrow}(r)/2$ of the $\nu = 1$ liquid ferromagnet with minimum polarization in the direction of the field ($S_z = 0$). Note that, in general, not any set of coefficients $c_m$ and $\tilde{c}_m$ represents a good liquid. First of all, at any filling factor, $c_m \to 0$ and $\tilde{c}_m \to 0$ for $m \to \infty$ since $g(r) \to 1$ for $r \to \infty$. Secondly, the pair distribution function must satisfy certain sum rules which establish relations between the coefficients. Finally, these coefficients must be consistent with the microscopic information one must provide.

**Spin-polarized liquids.** When one applies the charge neutrality, perfect screening, and compressibility sum rules \[10\] to the expression \[4\], one obtains the following set of equations:

\[\sum_{m=1}^{\infty} \tilde{c}_m = (1 - \nu^{-1})/4\]

\[\sum_{m=1}^{\infty} (m+1) \tilde{c}_m = (1 - \nu^{-1})/8\]

\[\sum_{m=1}^{\infty} (m+1)(m+2) \tilde{c}_m = (1 - \nu^{-1})^2/8.\]

The charge neutrality and perfect screening sum rules can actually be derived exactly from general considerations applicable to any isotropic liquid state in the LLL \[13\]. In short, they come about due to the fact that the number of particles and the total angular momentum are good quantum numbers for the Hamiltonian. The compressibility sum rule can only be invoked as it is if there is a classical plasma analog similar to that for the Laughlin states \[8\]. For the filling factors considered below this analog exists \[13\].

Now, in order to incorporate the microscopic information related to the short-distance behavior into the pair distribution function, we first express it in a more orthodox way \[12\]:

\[g(r) = \frac{1}{\nu^2} e^{-r^2/2} \sum_{m \neq 0}^{\infty} \langle n_m n_0 \rangle \frac{r^{2m}}{2m m!}. \]

A series expansion of \[8\] allows us to relate the coefficients $c_m$ to the correlation factors $\langle n_m n_0 \rangle \equiv \langle c_m^\dagger c_m c_0^\dagger c_0 \rangle$ which we try to calculate in what follows. The particle-hole symmetry dual filling factors of $\nu = 1/M$, $\nu = 1 - 1/M$, lie in the range we want to explore here and we assume a Laughlin state of holes at these filling factors.
There are no simple wave functions representing these liquids, but the same particle-hole symmetry allows us to write
\[ \langle n_m n_0 \rangle = 1 - \langle h_m^\dagger h_m \rangle - \langle h_m^\dagger h_0 \rangle + \langle h_m h_m h_0^\dagger h_0 \rangle \] (9)
where the \( h_m^\dagger \) and \( h_m \) represent creation and annihilation operators of holes. For the proposed Laughlin states
\[ \langle h_m^\dagger h_m h_0^\dagger h_0 \rangle = 0, \quad m \leq M - 1 \] (10)
which gives \( \langle n_m n_0 \rangle = 2 \nu - 1 \) for \( m \leq M - 1 \). With this result we find \( c_m = -(1 - \nu)^2 \) for odd \( m \leq M - 2 \) and, with Eqs. (3), (5), and (7), we calculate the next three coefficients, setting the rest to zero. In Table I we present the energy calculated from the analytic \( g(r) \) so obtained for \( \nu = 2/3 \) and \( \nu = 4/5 \) along with that obtained from exact numerical diagonalizations on the spherical geometry for the same filling factors. The perfect agreement between these two values confirms the existence of a Laughlin liquid state of holes at those filling factors and, moreover, confirms the reliability of the analytic pair distribution functions. We calculate now the energy of Laughlin liquids at any filling factor beyond \( \nu = 4/5 \) within the set \( \nu = 1 - 1/M \) (stars in Fig. 1). As \( \nu \to 1 \), numerics cannot be employed as a test of accuracy. However, all the coefficients must vanish in this limit and we expect the expansion (3) to get even more reliable. In fact, our results are consistent with the known behavior \( \epsilon(\nu = 1) = d \epsilon(\nu)/d\nu|_{\nu=1} = -\frac{1}{2} \sqrt{\pi/2} \) and with the expected fact that the triangular Skyrme crystal (the two closest points to \( \nu = 1 \) in the solid phase) has lower energy than the Laughlin-like liquid states near \( \nu = 1 \). Figure 1 also shows that the polarized liquid phase beats the solid phase at \( \nu = 2/3 \), but not at \( \nu = 4/5 \), in agreement with Ref. [3].

**Spin-unpolarized liquids.** The two first previously mentioned sum rules can also be invoked for the pair distribution function (3) of a two-component liquid. We obtain three sets of equations:
\[ \sum_{m=0}^{\infty} c_m = (1 - 2 \nu^{-1})/4, \quad \sum_{m=0}^{\infty} \tilde{c}_m = 1/4, \] (11)
\[ \sum_{m=0}^{\infty} (m + 1)(c_m + \tilde{c}_m) = (1 - \nu^{-1})/4, \] (12)
where we implicitly consider \( c_m = 0 \) for \( m = 0, 2, 4, 6, \ldots \)
The first two equations refer to \( g_{\uparrow\uparrow} \) and \( g_{\uparrow\downarrow} \), separately. They result again from generic considerations which take into account the fact that the number of particles for each component (spin orientation) is a good quantum number. These two can be combined into a single one since the energy of the unpolarized phase depends only on \( g_{\uparrow\uparrow} + g_{\uparrow\downarrow} \), i.e., on \( c_m + \tilde{c}_m \). The compressibility sum rule has not been invoked this time for we are not aware of any two-species plasma analog for the filling factors considered above. Its existence cannot be discarded though.

Next, we provide the microscopic details of the unpolarized liquid states we propose. An expansion like (8) including the spin degree of freedom allows us again to relate the coefficients \( c_m \) and \( \tilde{c}_m \) to the correlation factors \( \langle n_m n_0 \rangle \equiv \langle n_m n_0 \rangle \) and \( \langle n_m n_0 \rangle \equiv \langle n_m n_0 \rangle \). The duality between \( \nu \) and \( 1 - \nu \) in previous section allowed us to propose sensible liquid ground state wave functions at filling factors \( \nu = 1 - 1/M \), but, here, the spin degree of freedom breaks such a duality. However, note that one can always find an appropriate hard-core interaction model for which the polarized ground state satisfies Eq. (10), whether or not its wave function is explicitly known. Similarly, the hard-core interaction model \( V_0 \gg V_1 > V_2 > V_3 = 0 \) guarantees that the unpolarized ground state satisfies \( \langle n_{0\uparrow} n_{0\downarrow} \rangle = \langle n_{0\uparrow} n_{0\uparrow} \rangle = 0 \) for \( \nu \leq 1 \). It also guarantees the upper limit
\[ \langle n_1 n_0 \rangle = 2\langle n_{1\uparrow} n_{0\uparrow} \rangle + 2\langle n_{1\uparrow} n_{0\downarrow} \rangle \leq (2\nu - 1), \] (13)
which, as follows from previous arguments, is the value associated to the fully polarized state at filling factors \( 2/3 \leq \nu \leq 1 \) for any \( S_z \). The inequality reflects the freedom for a pair of particles to occupy states with even relative angular momenta. We propose the following factorization: \( \langle n_1 n_0 \rangle = f(\nu)(2\nu - 1) \) with \( f(\nu) \leq 1 \). In general, \( f(\nu) = \alpha + (1 - \alpha)\nu \) since we do not expect terms proportional to \( \nu^3 \) or higher to be relevant in a density-density correlation function and the condition \( f(\nu = 1) = 1 \) must be fulfilled. Thus we set \( \tilde{c}_0 = 0 \) and \( c_1 + \tilde{c}_1 = 2(1 - \alpha)(1 - \nu^{-1}) - 2\alpha(1 - \nu^{-1})^2 \) and, using Eqs. (11) and (12), we can calculate \( \tilde{c}_2 \) and \( c_3 + \tilde{c}_3 \). We specifically set \( \alpha = 25/8 - 2\sqrt{2} \) which builds a \( g(r) \) from which we reproduce the expected behavior of the energy for a very dilute state of skyrmions at vanishing Zeeman coupling, \( \frac{d\epsilon(\nu)}{d\nu}|_{\nu=1} = -\frac{1}{4} \sqrt{\pi/2} \). Moreover, this choice of \( \alpha \) is also consistent with our best numerical estimate of \( \langle n_1 n_0 \rangle \) for \( \nu = 2/3 \). As Table I shows, the energy obtained from the analytical expression of \( g(r) \) for \( \nu = 2/3 \) and \( \nu = 4/5 \) and the exact results for the real Coulomb interaction are remarkably close. The solid phase energy (see Fig. 1) lies clearly above the exact and estimated values, which proves the existence of unpolarized liquid phases at these filling factors. (Note that the energy of the polarized phases are always above the corresponding ones of the unpolarized phases, but a partially polarized liquid at \( \nu = 4/5 \) is possible and might have lower energy for the value of the Zeeman coupling considered). One can interpret these unpolarized states as \( \nu = 1/3 \) and \( \nu = 1/5 \) hole liquid states, with each hole being “accompanied” by one and two spin flips (i.e., spin waves), respectively. Although we cannot present a rigorous argument, it is tempting to interpret this hole-spin waves association as a skyrmion, and call these states Skyrme liquids.

In order to address the quantum melting phase transition we need the energy at any filling factor \( 2/3 \leq \nu \leq 1 \):
\[ \epsilon = -\frac{\nu}{2} \sqrt{\frac{\pi}{2}} \left[ 1 - \frac{1}{2}(1 - \nu^{-1}) + \left( \frac{25\sqrt{2}}{64} - \frac{1}{2}(1 - \nu^{-1})^2 \right) \right]. \]

(14)

Although, as required, this expression reproduces known results fairly well, we have to stress that \textit{its derivative is continuous as a function of} \( \nu \). In other words, it does not capture the expected gaps in the chemical potential at the main filling fractions. Experimentally, however, only the gap at \( \nu = 2/3 \) is clearly visible for fully-polarized phases. Towards \( \nu = 1 \) the gaps at \( \nu = 5/7 \) and \( \nu = 4/5 \) are the next in importance, but they barely show up in the longitudinal or Hall resistivities even at the lowest temperatures. In addition, the gaps are smaller in unpolarized phases \[ [2] \] so we expect the analytical expression \[ [2] \] to capture the overall behavior of the real \( \epsilon(\nu) \) of a spin-unpolarized liquid, particularly close to \( \nu = 1 \). Before drawing conclusions about the quantum melting phase transition from Fig. 1 one should keep in mind that quantum fluctuations have not been considered in the solid phase calculation and that they are bound to lower the energy of this phase. The magnitude of this correction has been carefully estimated for the Wigner crystal \[ [6] \] and it is not unreasonable to expect an energy shift of the same order of magnitude for the Skyrme crystal. Borrowing the results from Ref. \[ [6] \] we estimate the shift to be \(-0.001e^2/\ell \) for \( \nu = 4/5 \), decreasing in absolute value as \( \nu \to 1 \). In our favor we must also say that partially polarized liquid phases, which have not been considered here, are expected to lower the ground state energy for typical values of the Zeeman energy. All considered, our results seem to place the quantum melting phase transition very close to \( \nu = 1 \). As expected, the triangular Skyrme crystal dominates sufficiently close to \( \nu = 1 \), but the transition point to the square lattice \( (\nu \approx 0.96) \) lies near the one where the unpolarized liquid phase begins to take over \( (\nu \approx 0.92) \).

There are still many open questions regarding the nature of the zero-temperature melting phase transition over which this work does not shed any light. Disorder, for instance, plays a major role in this matter and has not been considered. Still, our results cast a caveat in what refers to the range of existence of the square-lattice Skyrme crystal and, in addition, provide an alternative description for the electronic ground states in the range of filling factors \( 2/3 \leq \nu \leq 1 \).

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\begin{tabular}{|c|c|c|c|c|c|}
\hline
\( \nu \) & \( N = 4 \) & \( N = 6 \) & \( N = 8 \) & \( N = 10 \) & \( N = 12 \) & \( N \to \infty \) \\
\hline
2/3 (P) & -0.5501 & -0.5396 & -0.5341 & -0.5310 & -0.5289 & -0.518 \\
2/3 (U) & -0.6010 & -0.5744 & -0.5618 & -0.5518 & -0.5545 & -0.527 \\
4/5 (P) & -0.5804 & -0.5649 & -0.5607 & -0.552 & -0.552 \\
4/5 (U) & -0.6580 & -0.6069 & -0.5923 & -0.56(7) & -0.566 \\
\hline
\end{tabular}

\begin{table}
\centering
\caption{Energy per particle (in units of \( e^2/\ell \)) obtained from exact diagonalizations on a sphere for finite number of particles, \( N \), at filling factors \( \nu = 2/3 \) and \( \nu = 4/5 \) (when possible, values for \( N > 12 \) have been obtained, but are not shown here). The spin-polarized and spin-unpolarized calculations are denoted by P and U, respectively. We also include the thermodynamic value obtained from a 1/\( N \) quadratic extrapolation and the energy obtained from the pair distribution functions described in the text. The last digit of the extrapolated value for \( \nu = 4/5 \) (U) cannot be taken at face value due to the small number of points available for the extrapolation.}
\end{table}