Shape Deformation driven Structural Transitions in Quantum Hall Skyrmions

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The Quantum Hall ground state away from $\nu = 1$ can be described by a collection of interacting skyrmions. We show within the context of a nonlinear sigma model, that the classical ground state away from $\nu = 1$ is a skyrmion crystal with a generalized Néel order. We show that as a function of filling $\nu$, the skyrmion crystal undergoes a triangle → square → triangle transition at zero temperature. We argue that this structural transition, driven by a change in the shape of the individual skyrmions, is stable to thermal and quantum fluctuations and may be probed experimentally.

Within a variational scheme, we show that at values of $\nu$ significantly greater than 1/2, recent OPNMR [4] and optical magneto-absorption [5] experiments observe a sharp fall in the spin polarization as the filling factor is changed from $\nu = 0$ to $\nu = 1$ and more. In this paper, we calculate the $T = 0$ classical phase diagram of a system of interacting skyrmions using an effective classical O(3) nonlinear sigma model (NLSM).

The low energy excitations about the ferromagnetic $\nu = 1$ ground state in GaAs heterostructures are extended objects called skyrmions with spin significantly greater than 1. Recent theoretical work [9] have analysed the crystalline state of skyrmions in two dimensions ? Specific heat measurements [7] on GaAs heterojunctions at $\nu = 0.77$, show a sharp peak at a temperature $T_c \approx 30$mK. It has been suggested [6] that this anomaly may be associated with the freezing of skyrmions into a crystal lattice. Previous theoretical work [8,9] have analysed the crystalline state of skyrmions. Using a mean-field analysis of electrons confined to the lowest Landau level, Fertig et. al. [8] claim that at $T = 0$, the skyrmions form a square lattice with a Néel orientation ordering. On the other hand, by a mapping onto an effective nonlinear sigma model, Green et. al. [9] conclude that the skyrmions form a triangular lattice with a generalized Néel ordering.

In this paper, we calculate the $T = 0$ classical phase diagram of a system of interacting skyrmions using an effective classical O(3) nonlinear sigma model (NLSM). Within a variational scheme, we show that at values of $\nu$ sufficiently away from 1, the ground state is a triangular lattice of skyrmions with a three sublattice generalized Néel orientation order. As we approach $\nu = 1$, we find a structural transition to the square lattice with Néel orientation order. This structural transition is accompanied by a change in the shape of the individual skyrmions and a jump in the spin polarization. In the dilute limit, $\nu \rightarrow 1$, we find a reentrant triangular phase which is different from the previously encountered triangular phase! We also provide arguments for the stability of these phases to thermal and quantum fluctuations.

The energy functional Eq. (1) has been expressed in dimensionless variables, with all energies in units of the cyclotron energy $\hbar \omega_c$, $\omega_c = eB/m^*c$ ($m^*$ is the electron band mass) and all lengths in units of the magnetic length $l_c$, $2\pi^2 l_c^2 = \hbar c/eB$. The parameters in the energy functional are $\gamma = e^*/(16\sqrt{2}\pi)$, $g^* = g \mu_B B/\hbar \omega_c$ and $e^* = (e^2/\hbar l_c)(1/\hbar \omega_c)$ ($K$ is the dielectric constant of GaAs).

$$E[\bar{w}, w] = E_0[\bar{w}, w] + E_Z[\bar{w}, w] + E_{\text{coul}}[\bar{w}, w].$$  \hfill (1)

The first term on the right

$$E_0[\bar{w}, w] = \gamma \int_{\bar{z},\bar{z}'} \frac{1}{(1 + \bar{w}w)^2} (\partial_z \bar{w} \partial_z w + \partial_{\bar{z}} \bar{w} \partial_{\bar{z}} w)$$  \hfill (2)

describes spin exchange. The Zeeman coupling of the spins to the external magnetic field $B$ is given by

$$E_Z[\bar{w}, w] = \frac{g^*}{2\pi} \int_{\bar{z},z} \frac{\bar{w}w}{(1 + \bar{w}w)}$$  \hfill (3)

while the charged quasiparticles interact via a long-range coulomb interaction,

$$E_{\text{coul}}[\bar{w}, w] = \frac{e^*}{2} \int_{\bar{z},z} \int_{\bar{z}',z'} \frac{q(\bar{z}, z) q(\bar{z}', z')}{|\bar{z} - z'|}.$$  \hfill (4)
In the absence of Coulomb and Zeeman interactions, any (anti)meromorphic function \( w(z) \) is a solution of the resulting Euler Lagrange equations \([3]\). The topological charge is simply \( Q = \sum n_i \), where \( i \) runs over the poles of \( w \) and \( n_i \) is the degree of the \( i^{th} \) pole. The one skyrmion solution given by

\[
w(\tilde{z}, \zeta) = \frac{\lambda e^{i\Omega}}{z - \xi},
\]

clearly has a \( Q = 1 \). The spin and charge distributions are centred at \( \xi \) and fall off as power laws with a scale set by \( \lambda \). The \( XY \) component of the spin at \( \mathbf{x} \) is oriented at an angle \( \Omega \) to the position vector \( \mathbf{x} \). The \( Z \) component of the spin \( S_Z \), however, diverges logarithmically.

In the presence of the Zeeman and Coulomb interactions, Eq. (8) is no longer the minimum energy solution. These terms destroy scale invariance, and generate a ‘size’ for the optimal skyrmion, leading to a finite \( S_Z \). It is natural to try the following variational form for the single skyrmion solution which minimises Eq. (1):

\[
w(\tilde{z}, \zeta) = \frac{\lambda e^{i\Omega}}{z - \xi}e^{-\kappa|z - \xi|}.
\]

With \( \lambda \) and \( \kappa \) as variational parameters, we have checked that the lowest energy single skyrmion solution has a \( \kappa > 0 \). The topological charge remains 1, since the configuration in Eq. (8) can be smoothly deformed to the configuration in Eq. (6).

A system of \( N \) identical \( Q = 1 \) skyrmions centred at \( \{\xi_i\} \) with orientations \( \{\Omega_i\} \), can now be parametrized by

\[
w(\tilde{z}, \zeta) = \sum_{i=0}^{N} \frac{\lambda e^{i\Omega_i}}{z - \xi_i}e^{-\kappa|z - \xi_i|}.
\]

The topological charge \( Q = N \), however we observe that even for \( \kappa = 0 \), the spin \( S_Z \) is finite. This illustrates the fact that the \( Z \) component of the total spin of overlapping skyrmions is not the sum of the individual spins. Our crystalline ansatz corresponds to placing the \( \{\xi_i\} \) on a triangular or a square lattice. We have studied both the ferro-oriented \( \{\Omega_i = 0, \forall i\} \) and generalized Néel oriented \( \{\Omega_i\} \) configurations. We find that the ferro-oriented configurations always have a higher energy and so shall ignore them for the rest of this paper. Since the square lattice is bipartite, the Néel configuration is characterised by \( \Omega_1 = 0 \) for the \( A \) sublattice and \( \Omega_2 = \pi \) for the \( B \) sublattice. Likewise, for the tripartite triangular lattice, the generalized Néel ordering is obtained by assigning \( \Omega_1 = 0, 2\pi/3, 4\pi/3 \) to the \( A, B \) and \( C \) sublattices respectively. These orientation assignments emerge naturally in the \( \kappa = 0 \) limit of Eq. (6), when it reduces to an elliptic function. The sum of the residues of an elliptic function in the unit cell should equal zero. In the present context this is precisely the generalized Néel condition that the sum of the orientations of all the skyrmions in a unit cell is zero (mod \( 2\pi \)).

To find the classical ground states, we numerically compute the energy (accurate to 1 part in \( 10^6 \)) using our crystalline ansatz and minimize with respect to the variational parameters \( \kappa \) and \( \lambda \) for a given crystalline ansatz. We have chosen typical values of the carrier concentration \( n = 1.5 \times 10^{11} \) cm\(^{-2}\) and magnetic fields \( B = 6 - 10 \) Tesla and have varied \( \nu \) by tilting the magnetic field with respect to the normal keeping its magnitude fixed. The lattice spacing \( a \) for a given lattice type is fixed by the value of \( \nu \) (e.g., for a square lattice, \( a = \sqrt{2\pi/(1 - \nu)} \)).

To highlight the role of the ‘size’ parameter \( \kappa \), we refer to Fig. 1, a plot of \( E(\kappa) \), the energy of the Néel triangular lattice minimized with respect to \( \lambda \), as a function of \( \kappa \) for three different values of \( \nu \). As \( \nu \to 1 \), the lattice gets very dilute, and the energy \( E(\kappa) \) attains its minimum at a value of \( \kappa \) close to the single skyrmion value. Next consider the dense region when \( \kappa^{-1} > a \) (strongly overlapping skyrmions). The nonadditivity of spins in this region, implies that \( E_Z \) is insensitive to \( \kappa \). The self-part of \( E_{\text{coul}} \) and \( E_0 \) however, increase linearly with increasing \( \kappa \) (for small \( \kappa \)) as in Fig. 1. Keeping a fixed, a further increase in \( \kappa \) will separate the skyrmions from each other, giving rise to another minimum at the single skyrmion value of \( \kappa \). These minima become degenerate at \( \nu \approx 1.05 \). A further decrease in \( \nu \) makes the energy of the second minimum lower. This suggests that there are two different triangular crystals associated with \( \kappa = 0 \) (“fat” skyrmions) and \( \kappa > 0 \) (“thin” skyrmions). For the square lattice, the “thin” skyrmion solutions have lower energy throughout the \( \nu \) range of physical interest.

Figure 2 shows the minimised energies of the Néel square and the Néel triangular crystals as a function of \( \nu \). When \( \nu \) is away from 1, a triangular lattice with \( \kappa = 0 \) (\( \Delta_1 \) phase) has the lowest energy. The smaller Zeeman energy of the competing square lattice with \( \kappa > 0 \) is off-
set by $E_0$ and $E_{\text{coul}}$. As $\nu$ approaches 1, $E_{\text{coul}}$ decreases, resulting in a weak first-order transition (slope discontinuity) to a square lattice with $\kappa > 0$ at $|\nu - 1| \approx 0.05$ (for $B = 7$ T). Thus the structural transition between the $\Delta_1$ and the square phase is accompanied by a change in the size of the individual skyrmions. In the region of parameter space which favours the square phase, the $\kappa > 0$ triangular lattice loses out on a higher $E_0$ and $E_2$. As $|\nu - 1|$ gets very close to zero, the difference in energy between these two lattices vanishes. In the limit of extreme dilution, $\nu \to 1$, the energy of the $N$-skyrmion configuration can be evaluated as an expansion in $(\kappa a)^{-1}$,

$$E_N = N E_1 + e^4 \sum_{i>j} \frac{1}{|x_i - x_j|} + O \left( \frac{1}{\kappa a} \right),$$

where $E_1$ is the single skyrmion energy and the coulomb interaction is between point charges. To leading order, $E_N$ is clearly minimised by placing the charges on a triangular lattice ($\Delta_2$ phase), however it could have any orientational order. Higher order terms favour a Néel orientation. Thus a second structural transformation should occur between the square Néel lattice and a triangular Néel lattice with $\kappa > 0$ ($\Delta_2$ phase) via a weak first order phase transition as $\nu$ approaches 1.

In the vicinity of the $\Delta_1$-square transition, we find that $\kappa^{-1} \sim a$. A simple scaling argument shows that the shape stiffness of a single skyrmion is of the same order as the elastic stiffness of the crystal in the neighbourhood of the transition. The single skyrmion energy is of the form

$$E_1 = \gamma c_1 + \frac{g^* c_2 R^2}{2} + \frac{e^* c_3}{R}$$

where $R$ sets the scale for the size of the skyrmion and $c_1, c_2$ and $c_3$ are constants of $O(1)$. At $R \sim a$, the shape stiffness, $\partial^2 E_1/\partial R^2|_{R=R_1}$ (where $R_1$ minimises $E_1$) is comparable to the elastic stiffness of the crystal $\sim e^2/Ka^3$. The novel feature of this structural transition is that it is caused by the shape deformability of the “atoms”, revealing a richer physics than that of Wigner crystallisation.

A computation of the spin polarization of the skyrmion crystals at $T = 0$ (Fig. 3), agrees well with the experimental data of $\nu$ obtained at 1.5K. Since the spin polarization is a measure of the size $R$ of the individual skyrmions, this indicates that $R$ does not change significantly over this temperature range. An interesting feature is that the $\Delta_1$ ($\kappa = 0$) to square ($\kappa > 0$) structural transition is accompanied by a discontinuity of about 5-10% in the spin polarization, and so may be probed by accurate spin polarization measurements. Since thermal fluctuations and the presence of quenched disorder smear out this discontinuity, it may be necessary to go to very low temperatures to see this effect.

![Fig. 2 Energy density (in units of meV/ $l_0^2$) as a function of $\nu$ for the triangular ($\Delta_1$) and square crystals at $B = 7$ T.](image)

![Fig. 3 Spin polarization as a function of $\nu$ at $B = 7$ T for the square and triangular lattices compared to the experimental points taken from Ref. [4]. The structural transition predicted by our theory is accompanied by a discontinuity in the spin polarization at $\nu \approx 0.95$, as seen from the dashed curve.](image)

How ‘good’ is our classical variational ansatz Eq. [9]? A more general ansatz for the individual skyrmions would involve deviations of the shape from circular symmetry, and giving each skyrmion an arbitrary topological charge $Q$. It is easy to see that both these generalisations lead to an increased energy, in the region where the skyrmions do not overlap.

How do quantum and thermal fluctuations affect the classical $T = 0$ phase diagram presented above? The qualitative features of the phase diagram in the $T - \nu$ plane (Fig. 4) may be glimpsed from general arguments. Moving away from $\nu = 1$ along the $T = 0$ axis, reduces the lattice spacing, and shrinks the skyrmion size (due to coulomb repulsion). At a critical lattice spacing, zero-point fluctuations would melt the crystal. Quantum
melting in a strong magnetic field would ensue when the magnetic length \( l_c \sim \alpha a \), where \( \alpha \sim 0.1 - 0.2 \). This corresponds to an energy scale of \( (\hbar/0.1a)^2 m \), where \( m \) is the mass of the skyrmion. At the melting transition, this should compare with the coulomb energy \( e^2/a \).

We estimate the quantum melting transition (QM) to occur at \( \nu \sim 0.8 \). This melting into a quantum oriented liquid (QL) is most likely continuous with an intermediate quantum hexatic phase. Beyond this of course, the description in terms of skyrmions breaks down as \( \nu \) approaches the next quantum hall plateau, e.g. 2/3. In addition, we encounter a new quantum orientation disorder transition (QOD) in the limit of extreme dilution. The oriented (Néel) crystal is characterised by power-law correlations in the sublattice orientation. Quantum fluctuations would destroy this order when the fluctuations in the orientation become of the order of 2\( \pi \), i.e. when \( h^2/2I \sim J(a) \), where \( I \) is the moment of inertia of the skyrmion and \( J(a) \) is the energy cost in changing the orientation (and is a decreasing function of \( a \)). This leads to a quantum disoriented crystal in the dilute limit via a Kosterlitz - Thouless transition.

An increase in temperature, \( T \), would result in an oriented crystal with quasi-long range order in position and orientation. The advantage that the square phase had over the \( \Delta_2 \) phase at \( T = 0 \) now diminishes, since the renormalized \( \gamma \) gets weaker and the coulomb interaction remains relatively unaffected. Thus at higher temperatures, the square phase disappears, giving rise to an isostructural (first-order) phase boundary, where the two triangular Néel phases, \( \Delta_1 \) and \( \Delta_2 \) meet. This first-order line terminates on a continuous melting curve (a Wigner crystal estimate \[9\] gives \( T_m \sim \sqrt{1 - \nu} \) which occurs via a defect mediated mechanism (KTNHY \[12\]). In this case a hexatic phase (H) intervenes between the solid and the classical liquid (CL) phase. Indeed there has been a recent suggestion \[13\] that the presence of an isostructural critical point might reveal a hexatic phase in the vicinity.

The application of hydrostatic pressure constitutes an additional ‘field variable’ \[14\]. Pressure induces wavefunction overlap which leads to a reduction in \( g \), thus reducing the Zeeman contribution. We find that when \( g \rightarrow 0 \), the square Néel phase ceases to be a ground state.

As in the case of the Wigner crystal at \( \nu \sim 0.2 \) \[15\], we expect that disorder in the GaAs will not destroy the (quasi)-long range crystalline order of the skyrmions. However, the weak first-order structural transitions reported above, will be rendered continuous. We note that length scales \( a \) and \( \kappa^{-1} \) are both around \( 10^4 \) times larger than the GaAs lattice spacing, making the substrate essentially a continuum. Sliding of the skyrmion crystal would however be prevented by pinning to the ever present disorder in GaAs.

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![Fig. 4 Conjectured Phase diagram as a function of filling \( \nu \) and temperature. The solid and the dashed lines represent first-order and continuous boundaries respectively. The various phases shown are defined in the text.](image-url)