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. As a function of filling factor ν and Landé factor g, the Skyrmion crystal undergoes a triangle $\rightarrow$ square $\rightarrow$ triangle transition at zero temperature. We argue that this structural transition is driven by a change in the shape of the individual Skyrmions and may be probed experimentally. Quantum fluctuations lead to an orientationally disordered phase at low Skyrmion densities. [S0031-9007(97)04457-8]

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Following a recent suggestion [1–3], there has been growing experimental evidence [4–6] that the charged quasiparticle excitations about the $\nu = 1$ quantum Hall state in GaAs heterostructures are extended objects called Skyrmions with spin significantly greater than $1/2$. Recent nuclear magnetic resonance [4] and optical magnetoabsorption [5] experiments observe a sharp fall in the spin polarization as the filling factor is changed from $\nu = 1$, consistent with the existence of Skyrmions.

What is the ground state of a system of interacting 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 [7] that this anomaly may be associated with the freezing of Skyrmions into a crystal lattice. Previous theoretical work [8,9] has analyzed 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 study the $T = 0$ phase diagram of a system of interacting Skyrmions in the ν-g plane, using an effective classical $O(3)$ nonlinear sigma model (NLSM). The Landé g factor can be tuned by the application of hydrostatic pressure [10]. For a fixed nonzero g, the ground state at high Skyrmion density is a triangular lattice with a three sublattice generalized Néel orientation order. A decrease in the density (as ν approaches 1), leads to a structural transition to a 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. This sequence of transitions occurs both at low g ($g = 0.1g_0$) and at $g = g_0$, where g_0 is the zero pressure value of the Landé g factor. The phase boundary however moves farther away from $\nu = 1$ as g increases. The effect of quantum fluctuations leads to melting of the solid at high Skyrmion densities and orientational disordering at low densities. We conjecture a qualitative form of the phase diagram in the ν-T plane.

Before describing our work in detail, we demarcate the precise regime of validity of NLSM for the description of charged excitations of the quantum Hall system near $\nu = 1$. It has been shown [11] that single Skyrmion properties computed from the NLSM approaches that obtained from electron Hartree-Fock and exact diagonalization (within the lowest Landau level approximation) when spin is large. The differences in energy of a single Skyrmion computed within these three schemes is negligible when the spin is $\gtrsim 10$, while it is about 5% when the spin is ~ 4. At $g = 0.1g_0$, the spin of the Skyrmions is >10 for all values of ν considered. We emphasize that at these values of g, the NLSM provides a *quantitatively accurate* description. At $g = 1$, the spin is significantly less than 10, and so the precise position of the transitions may be inaccurate. However we believe that the qualitative scenario described above will continue to hold.

The low energy, long wavelength excitations about the ferromagnetic $\nu = 1$ ground state in GaAs hetrostructures are described by an NLSM [1,2], in terms of a unit vector field that represents the local spin polarization. Neutral excitations correspond to spin waves, while charged excitations correspond to defect configurations (Skyrmions) with topological charge Q [the electronic charge density is equal to the topological charge density $4\pi q(\mathbf{x}) = \mathbf{n} \cdot (\partial_x \mathbf{n} \times \partial_y \mathbf{n})$ in the long wavelength limit [1]]. The topological charge $Q = \int q(\mathbf{x})\, d^2x$ is always an integer and counts the number of times the spin configuration $\mathbf{n}(\mathbf{x})$ wraps around the unit sphere.

For convenience we work in a notation where the unit vector field $\mathbf{n}(x, y)$ is replaced by a complex field $w(z \equiv x + iy, \bar{z} \equiv x - iy)$, obtained by the stereographic projection of the unit sphere onto the complex plane. Thus

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$w = \cot(\frac{\theta}{2})e^{i\phi}$, where θ and ϕ are the polar angles of the unit vector $\mathbf{n}$. For static, classical spin configurations, the energy functional [2] may be written as

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

The first term on the right,

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

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

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

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

$$E_{\text{coul}}[\bar{w}, w] = \frac{e^*}{2} \int_{\bar{z},z} \int_{\bar{z}',z'} \frac{q(\bar{z}, z)q(\bar{z}', z')}{|z - z'|}\,. \quad (4)$$

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, $2\pi l_c^2 = hc/eB$. The parameters in the energy functional are $\gamma = e^*/16\sqrt{2\pi}$, $g^* = g\mu_B B/\hbar\omega_c$, and $e^* = (e^2/Kl_c)\,(1/\hbar\omega_c)$ (K is the dielectric constant of GaAs).

In the absence of Coulomb and Zeeman interactions, any (anti)meromorphic function $w(z)$ is a solution of the resulting Euler Lagrange equations [12]. The topological charge is simply $Q = \sum_i n_i$, where i runs over the poles of w and n_i is the degree of the ith pole. The one Skyrmion solution given by

$$w_0(\bar{z}, z; \Omega, \xi) = \frac{\lambda_0 e^{i\Omega}}{z - \xi}\,, \quad (5)$$

clearly has a $Q = 1$. The spin and charge distributions are centered at ξ and fall off as power laws with a scale set by λ_0. The XY component of the spin at $\mathbf{x}$ is oriented at an angle Ω 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. (5) 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. The most general variational ansatz which leads to circularly symmetric spin and charge densities can be written as [13]

$$w(\bar{z}, z; \Omega, \xi) = \frac{e^{i\Omega}}{z - \xi}\, e^{-\kappa|z-\xi|}[\lambda_0 + F(|z - \xi|)]\,. \quad (6)$$

An exact asymptotic analysis [13] of the solution w shows that $F(r) \to 0$ as $r \to 0$ and ∞. Since F is a smooth function, the configuration in Eq. (6) can be smoothly deformed to the configuration in Eq. (5) and so the topological charge remains 1. We expand F in a complete set of functions, $F(r) = e^{-(br)^2/2} \sum_{n=1}^{\infty} \lambda_n (br)^{2n}/\sqrt{2n!}$, where b is a suitably chosen scale parameter. Minimization of the energy with respect to the set $\{\kappa, \lambda_0, \{\lambda_n\}\}$, would lead to the exact solution. In practice, however, we find that including more than the first five parameters $(\kappa, \lambda_0 \ldots \lambda_3)$ changes the minimized energy by less than 0.1%. With just two parameters κ and λ_0, the error in the energy is typically around 1%, and at worst 3%.

A system of N identical $Q = 1$ Skyrmions centered at $\{\xi_I\}$ with orientations $\{\Omega_I\}$, can now be parametrized by

$$w(\bar{z}, z) = \sum_{I=1}^{N} w(\bar{z}, z; \Omega_I, \xi_I)\,. \quad (7)$$

Our crystalline ansatz corresponds to placing the $\{\xi_I\}$ on a triangular or a square lattice. This leads to spin and charge densities commensurate with the crystal symmetry [14]. We have studied both the ferro-oriented ($\Omega_I = 0, \forall I$) and generalized Néel oriented configurations. Since the square lattice is bipartite, the Néel configuration is characterized by $\Omega_I = 0$ for the A sublattice and $\Omega_I = \pi$ for the B sublattice. Likewise, for the tripartite triangular lattice, the generalized Néel ordering is obtained by assigning $\Omega_I = 0$, $2\pi/3$, and $4\pi/3$ to the A, B, and C sublattices, respectively.

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, for a given lattice and orientational ordering. As for the one Skyrmion case, retaining only two parameters, κ and λ_0, leads to energies accurate to better than 3%. We have calculated the phase diagram using this two parameter ansatz. The existence of the structural transition discussed in the introduction has also been verified using the more accurate five parameter ansatz.

We have chosen typical values of the carrier concentration ($n = 1.5 \times 10^{11}$ cm^{-2}) and the magnetic field ($B =$ 10 T) and have varied ν 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 ν (e.g., for a square lattice, $a \equiv \sqrt{2\pi/|1 - \nu|}$).

Figure 1 shows the percentage difference in the minimized energies of the Néel square and the Néel triangular crystals as a function of ν for $g = g_0$ and $0.1g_0$ (the ferro-oriented crystals have much higher energies in this region). When ν is away from 1, a triangular lattice (Δ_1 phase) has the lowest energy. The smaller Zeeman energy of the competing square lattice is offset by E_0 and E_{coul}. As ν approaches 1, E_{coul} decreases, resulting in a weak first-order transition (slope discontinuity) to a square lattice. The structural transition between the Δ_1 and the square phase is accompanied by a jump in the size of the individual Skyrmions.

As $|\nu - 1|$ gets very close to zero, the energy of the ferro-oriented triangular lattice becomes comparable to

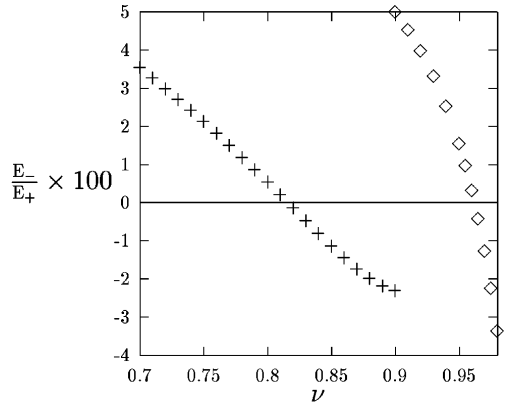

FIG. 1. Percentage difference of the energy densities of the triangular (E_{Δ_1}) and square ($E_\square$) crystals at $B = 10$ T as a function of ν. $E_\pm \equiv E_\square \pm E_{\Delta_1}$. The symbols correspond to $\diamond$: $g = 0.1g_0$; $+$: $g = g_0$.

the Néel-oriented lattices. For $g = g_0$, the ferrotriangular lattice becomes the ground state when $|\nu - 1| < 0.025$. For $g = 0.1g_0$, the square Néel lattice remains the ground state until at least $|\nu - 1| = 0.005$. In the limit of extreme dilution, $\nu \to 1$, the energy of the N-Skyrmion configuration can be evaluated as an expansion in $(\kappa a)^{-1}$,

$$E_N = NE_1 + e^* \sum_{i>j} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} + \mathcal{O}\left(\frac{1}{\kappa a}\right), \quad (8)$$

where E_1 is the single Skyrmion energy and the Coulomb interaction is between point charges. To leading order, E_N is clearly minimized by placing the charges on a triangular lattice (Δ_2 phase); however, it could have any orientational order. Higher order contributions favor the ferro-orientational ordering [15], consistent with our numerical calculations. Thus a second structural transformation occurs between the square Néel lattice and a triangular ferrolattice (Δ_2 phase) via a weak first-order phase transition as ν approaches 1. Note that the Δ_1-square structural transition moves towards $\nu = 1$ as g decreases. Indeed at $g = 0$ the Δ_1 phase always has the lowest energy.

In the vicinity of the Δ_1-square transition, we find that the size of the Skyrmions $\sim a$. 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 neighborhood of the transition. The single Skyrmion energy is of the form

$$E_1 = \gamma c_1 + \frac{g^* c_2 R^2}{2} + \frac{e^* c_3}{R}, \quad (9)$$

where R sets the scale for the size of the Skyrmion and c_1, c_2, and c_3 are ~ 1 and weakly dependent on R. At $\bar{R} \sim a$, the shape stiffness, $\partial^2 E_1/\partial R^2|_{R=\bar{R}}$ (where $\bar{R}$ minimizes 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 crystallization.

The plot of the spin polarization of the Skyrmion crystals at $T = 0, g = 0.1g_0$ is shown in Fig. 2. An interesting feature is that the Δ_1 to square structural transition is accompanied by a discontinuity of about 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.

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-ν plane (Fig. 3) 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. Moving Skyrmions experience a Magnus force equal to the Lorentz force produced by the external magnetic field [16]. This implies that if the orientation and the shape deformation of the Skyrmions are ignored, then the system is analogous to interacting charged particles in a strong magnetic field. Wigner crystallization of charged particles in a strong magnetic field B occurs when the magnetic length $l_c \sim 0.5a$ which happens at $\rho/B \sim 1/5$, where ρ is the charge density. We therefore expect that the Skyrmion crystal melts at $\rho_{\rm sky}/B \sim 1/5$, which corresponds to $\nu \sim 0.8$. This value could however be affected by the orientation and shape deformation of the Skyrmions. The quantum melting (QM) 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 ν 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 crystal is characterized by power-law correlations in the sublattice orientation.

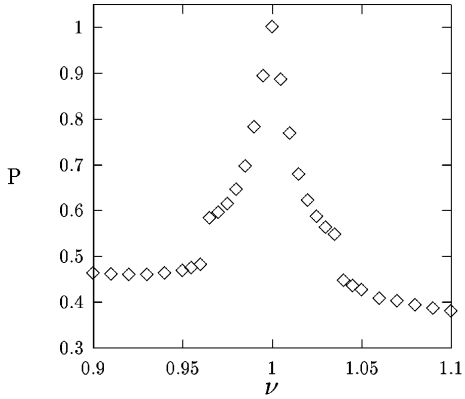

FIG. 2. Spin polarization P as a function of ν at $B = 10$ T and $g = 0.1g_0$. The structural transition predicted by our theory is accompanied by a discontinuity in the spin polarization at $|\nu - 1| \approx 0.04$.

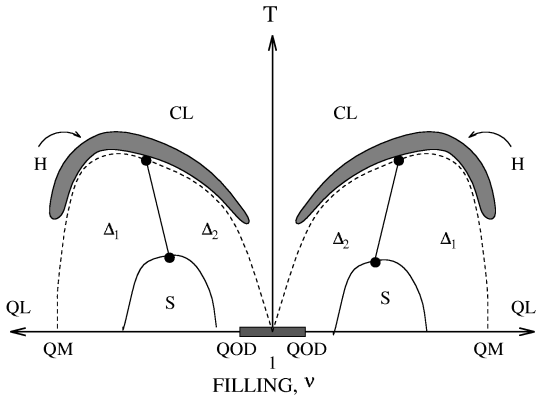

FIG. 3. Conjectured phase diagram as a function of filling ν and temperature. The solid and the dashed lines represent first-order and continuous boundaries, respectively. The various phases shown are defined in the text.

Quantum fluctuations would destroy this order when the fluctuations in the orientation become of the order of 2π, i.e., when $\hbar^2/2I \sim J(a)$, where I is the moment of inertia of the Skyrmion [13] 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 [17] 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 Δ_2 phase at $T = 0$ now diminishes, since the renormalized γ 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 Δ_1 and Δ_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. In this case a hexatic phase (H) intervenes between the solid and the classical liquid (CL) phase. Indeed there has been a recent suggestion [18] that the presence of an isostructural critical point might reveal a hexatic phase in the vicinity. As in the case of the Wigner crystal at $\nu \sim 0.2$ [19], 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 the Skyrmion lattice spacing and size are both around 10^3 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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