Disclination unbinding transition in quantum Hall liquid crystals

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We derive the long-wavelength elastic theory for the quantum Hall smectic state starting from the Hartree-Fock approximation. Dislocations in this state lead to an effective nematic model for $T > 0$, which undergoes a disclination unbinding transition from a phase with algebraic orientational order into an isotropic phase. We obtain transition temperatures that are in qualitative agreement with recent experiments that have observed large anisotropies of the longitudinal resistivities in half-filled Landau levels, lending credence to the liquid crystal interpretation of experiments.

Recent experiments[1–3] in high-mobility two-dimensional electron systems (2DES) have revealed remarkable phenomena in the transitional regions between the different plateau of the Hall conductance. In particular, striking anisotropies and nonlinearities in the magnetotransport were observed for Landau level (LL) filling factors near $\nu = n + 1/2$, for $n \geq 4$, corresponding to partially filled LL indices $L \geq 2$. This anisotropy tends to align with the crystalline axes of the sample, but can be reoriented by the application of in-plane magnetic fields,[4,5] and resistance ratios as high as R_{xx}/R_{yy} ~ 3500 have been observed.[6] This anisotropic behavior has been attributed to the formation of a striped phase. A unidirectional charge density wave (UCDW) had been predicted several years ago[7] for nearly-half-filled high LL's; exact diagonalizations for systems of up to 12 electrons[8] corroborate this picture for $L \geq 2$, and many experimental results can be qualitatively understood under the assumption of a UCDW. The presence of stripes has already been directly observed in a large class of low-dimensional, strongly correlated electronic systems,[9] and the present experimental evidence in quantum Hall devices is compelling, even if still somewhat circumstantial.[10]

Due to the similarities of the UCDW state with a classical smectic liquid crystal, these states have been dubbed *quantum Hall smectics* by Fradkin and Kivelson.[11,12] In two dimensions thermal fluctuations destroy the positional order,[13] but the system should still exhibit anisotropic transport as long as there is some remnant of orientational order (algebraic order in the *quantum Hall nematic*).[14] As the temperature is increased, the algebraic orientational order will disappear in a Kosterlitz-Thouless (KT) disclination-unbinding transition.[15]

To study this process we have mapped the interacting electron system (in the Hartree-Fock approximation) onto a classical smectic (the UCDW). We then consider the role of thermal fluctuations (phonons and dislocations) in reducing the order from smectic to nematic at larger distances. Without the use of any fitting parameters, and using only experimentally accessible values for the electron density and the width of the 2DES, we are able to estimate values for the disclination-unbinding transition temperature, which are in qualitative agreement with the transport measurements.

(I) Hartree-Fock approximation for the charge-density-wave state. In order to study the energetics of a charge density wave (CDW) in the 2DES we closely follow the strategy developed in Refs. 16–18, and use the Hartree-Fock (HF) approximation, which corresponds to the assumption that the electronic state can be described as a Slater determinant of single-electron states. In the Landau gauge, $\mathbf{A}(\mathbf{r}) = (0, Bx, 0)$, and the eigenstates of the noninteracting problem are

$$\psi_{i\sigma n x_0}(\mathbf{r}) = \frac{\zeta_i(z) e^{i x_0 y / l_b^2} H_n((x - x_0)/l_b) e^{-(x - x_0)^2 / 2 l_b^2}}{\pi^{1/4} (2^n n! l_b L_y)^{1/2}}, \quad (1)$$

where i, σ, n, and x_0 indicate the electric subband index (due to the confinement in the z direction), spin index, LL index, and guiding center, respectively; $l_b = (\hbar/eB)^{1/2}$ is the magnetic length, L_y is the length of the system in the y direction, and H_n are Hermite polynomials.

Since the electric subband splitting is very large (about 9.8 meV in the sample of Ref. 1), in what follows we consider only states with $i = 0$. The Coulomb interaction between the basis states above can be replaced by the effective interaction[16–18]

$$V_{x_1, x_2}^{n_1, n_2}(q_x, q_y) = \frac{4\pi e^2}{\kappa} \int dq_z \frac{|M_{x_1, x_2}^{n_1, n_2}(\mathbf{q})|^2}{q^2}, \quad (2)$$

where κ is the dielectric constant of the semiconductor (~ 13 in GaAs/Al$_x$Ga$_{1-x}$As), with the matrix element

$$M_{x_1, x_2}^{n_1, n_2}(\mathbf{q}) = \int d^3 x e^{i\mathbf{q} \cdot \mathbf{r}} \psi_{0\sigma n_1 x_1}^*(\mathbf{r}) \psi_{0\sigma n_2 x_2}(\mathbf{r}), \quad (3)$$

which may be expressed in terms of associated Laguerre polynomials.[16–18] Since the anisotropic states occur for moderately weak magnetic fields, the effect of a CDW on the valence LL is to polarize the fully occupied LL's below. This polarization may be accounted for with an effective dielectric constant $\epsilon(\mathbf{q})$, which can be calculated in the random phase approximation[17–19] (RPA). This effective interaction greatly simplifies the calculation, as we only need to consider states within the valence LL for the determination of CDW energies.
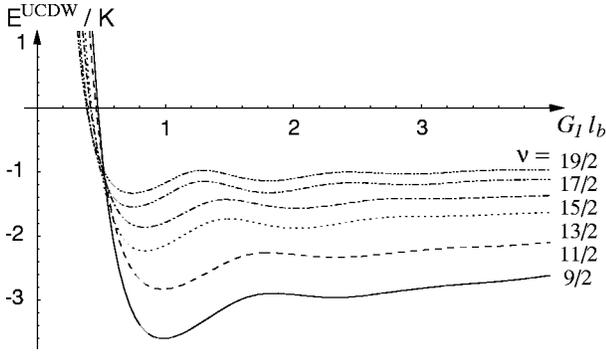
FIG. 1. Dependence of the average energy per electron state E^{UCDW} for various filling factors of Ref. 1 ($n_e = 2.67 \times 10^{11}$ cm^{-2}, $z_{rms} = 58.3$ Å).

In the absence of LL mixing, the state of the system is uniquely specified by the particle density function.[16,20] The energy per electron in a CDW state at a fractional filling ν^* is given by[21]

$$E = \frac{1}{2\nu^*} \sum_j U(\mathbf{G}_j) |\Delta(\mathbf{G}_j)|^2, \quad (4)$$

where $\Delta(\mathbf{G}_j)$ is the Fourier coefficient of the occupation number at the reciprocal lattice vector $\mathbf{G}_j$ and the kernel $U(\mathbf{q}) = H(\mathbf{q}) + X(\mathbf{q})$ with the direct and exchange contributions

$$H(\mathbf{q}) = \frac{1}{2\pi l_b^2 \epsilon(q)} V^{n,n}_{x_1, x_1 + l_b^2 q_y}(q), \quad (5)$$

$$X(\mathbf{q}) = -\int \frac{d^2 p}{(2\pi)^2 \epsilon(p)} e^{i(p_x q_y - p_y q_x) l_b^2} V^{n,n}_{x_1, x_1 + l_b^2 p_y}(p). \quad (6)$$

In the UCDW state, we have $\mathbf{G}_j = \mathbf{e}_x G_1 j$ with j an integer, and

$$\Delta(\mathbf{G}_j) = \frac{\sin(\nu^* \pi j)}{\pi j}, \quad (7)$$

where $G_1 = 2\pi/a$, with a the period of the UCDW. Inserting this into Eq. (4) we find $E^{UCDW}(G_1)$, the average energy per electron in the UCDW (see Fig. 1). The optimal UCDW corresponds to the minimum E^{UCDW}, and is observed at a
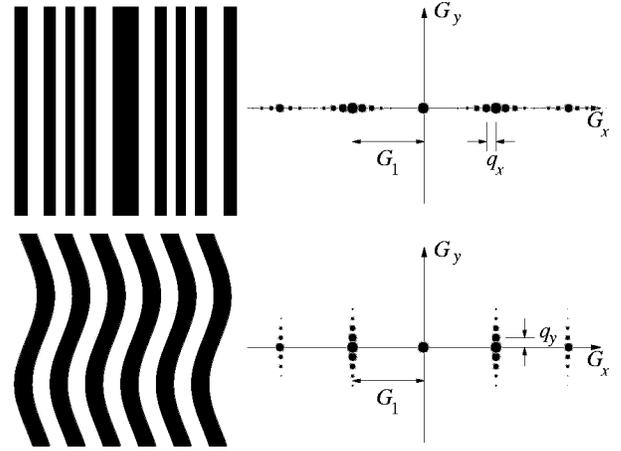

FIG. 2. Two characteristic examples of low-energy perturbations of the UCDW. Top: the *longitudinal modulation*. Bottom: the *transverse modulation*. On each panel, the right-hand side shows the Bragg peaks of $\Delta(\mathbf{G})$ in reciprocal space. G_1 is the wave vector of the UCDW, and q_x, q_y are the wave vectors of the modulation. See Eqs. (8)–(10).

$\simeq R_c \simeq 2.84 l_b \sqrt{2L+1}$ (in general agreement with Ref. 7, even though we are far from $L \to \infty$), where each electron gains one to a few degrees; see Table I. Since the anisotropic-isotropic transition is observed at temperatures much smaller than this, it is clear that the observed transition is not related to the formation of the stripes but, as we shall see, to the unbinding of topological defects in the stripes.

(II) Low-energy excitations of the UCDW. Here we consider low-energy states that correspond to long-wavelength fluctuations of the UCDW. We take care to construct modulations of the stripes that do not accumulate charge over large distances since this would significantly increase the Coulomb energy of the system. These modulations add extra "Bragg peaks" to the density function $\Delta(\mathbf{G})$ (see Fig. 2), and of the many modulations one can devise, very few avoid adding significant peaks far from where $U(\mathbf{G})$ is near its minimum.[22] These can be described by a distortion in the position of the UCDW stripe edges of the form

$$u(x,y) = \alpha \cos(q_x x) \cos(q_y y), \quad (8)$$

where α, q_x, q_y are the amplitude and wave-vector components of the modulation, respectively. Longitudinal ($q_y = 0$) and transverse ($q_x = 0$) modulations are illustrated in Fig. 2.

TABLE I. UCDW: optimal wave vector G_1, period a, energy gain per electron E^{UCDW} and elastic constants B and K. The calculations were performed for the realization of Ref. 1.

ν	B(T)	l_b(Å)	$G_1 l_b$	a(Å)	E^{UCDW} (K)	B (μK/Å^2)	K (mK)
9/2	2.46	164	0.983	1048	-3.603	25.5	189
11/2	2.02	181	0.978	1163	-2.830	15.7	144
13/2	1.70	197	0.842	1470	-2.234	13.0	192
15/2	1.48	211	0.839	1580	-1.864	9.07	158
17/2	1.30	225	0.746	1895	-1.549	7.58	196
19/2	1.16	239	0.744	2018	-1.332	5.66	167

To determine the energy of this excited state to $O(\alpha^2)$, we need to retain the following peaks:

$$\Delta[\mathbf{e}_x G_1 j] = \frac{\sin(\nu^* \pi j)}{\pi j}\left(1 - \frac{G_1^2 j^2 \alpha^2}{8}\right), \quad (9)$$

$$\Delta[\mathbf{e}_x (G_1 j \pm q_x) \pm \mathbf{e}_y q_y] = -\frac{\sin(\nu^* \pi j)}{\pi j}\frac{G_1 j \alpha}{4}, \quad (10)$$

where j is an integer. The energy per electron, relative to the optimal UCDW is then given by

$$\Delta E = \frac{G_1^2 \alpha^2}{16\pi^2 \nu^*}\sum_{j=-\infty}^{\infty}\sin^2(\nu^* \pi j)[U(\sqrt{(G_1 j + q_x)^2 + q_y^2})$$

$$+ U(\sqrt{(G_1 j - q_x)^2 + q_y^2}) - 2U(G_1 j)]. \quad (11)$$

Keeping terms up to $O(q_x^4, q_y^4, q_x^2 q_y^2)$, the energy *per unit area* is

$$\Delta\mathcal{E} = \frac{\alpha^2}{8}[Bq_x^2 + Kq_y^4 + K'q_x^2 q_y^2 + K''q_x^4], \quad (12)$$

with the elastic coefficients given by

$$B = \frac{\nu^*}{2\pi l_b^2}\frac{G_1^2 \partial^2 E^{\text{UCDW}}}{\partial G_1^2}, \quad (13)$$

$$K = \frac{1}{16\pi^3 l_b^2}\sum_{j=-\infty}^{\infty}\frac{\sin^2(\pi \nu^* j)}{j^2}\left[U''(G_1 j) - \frac{U'(G_1 j)}{G_1 j}\right], \quad (14)$$

$$K' = \frac{G_1}{4\pi^3 l_b^2}\sum_{j=-\infty}^{\infty}\frac{\sin^2(\pi \nu^* j)}{j}\left[\frac{U'''(G_1 j)}{2} - \frac{U''(G_1 j)}{G_1 j}\right.$$

$$\left. + \frac{U'(G_1 j)}{G_1^2 j^2}\right], \quad (15)$$

$$K'' = \frac{G_1^2}{48\pi^3 l_b^2}\sum_{j=-\infty}^{\infty}\sin^2(\pi \nu^* j)U''''(G_1 j). \quad (16)$$

It is easy to see from energetics above [Eq. (12)] that the low-energy perturbations of a UCDW correspond one-to-one to those of a smectic liquid crystal:[14]

$$E_{\text{sm}} = \frac{1}{2}\int d^2 r\{[B(\partial_x u)^2 + K(\partial_y^2 u)^2]$$

$$+ [K'(\partial_x \partial_y u)^2 + K''(\partial_x^2 u)^2]\}. \quad (17)$$

Results for the elastic moduli B and K are presented in Table I for parameters relevant to the sample used in Ref. 1. The terms between the second set of brackets in Eq. (17) are not expected to be relevant since they only become large for momenta near the edge of the Brillouin zone (where the validity of the elastic theory is doubtful). We now use the energy functional E_{sm} (without the terms involving K' and K'') for all further analysis of the quantum Hall liquid crystal.

TABLE II. Frank elastic constants K_1 and K_3, renormalized elastic constant K and KT disclination unbinding temperature calculated for the experimental realization of Ref. 1. Note the characteristic oscillations with the spin index.

ν	σ	K_1 (mK)	K_3 (mK)	K(mK)	T_{KT} (mK)
9/2	↑	189	1030	610	206
11/2	↓	144	783	463	156
13/2	↑	192	1041	616	208
15/2	↓	158	848	503	170
17/2	↑	196	1034	615	208
19/2	↓	167	875	521	176

(III) Effects of thermal fluctuations: from smectics to nematics. The energy functional for a smectic [Eq. (17)] has been extensively studied. We follow closely the formulation of Toner and Nelson.[14] Since the dimensionality of the system ($d=2$) is one below the lower critical dimension for layered materials, phonon fluctuations readily destroy positional order for $T>0$ (the Landau-Peierls argument), while preserving order in the layer orientation. However, this argument omits dislocations, which have finite energy; their energy can be estimated as[22]

$$E_D = \frac{Ba^2}{4\pi}[\sqrt{2q_c \lambda + 1} - 1], \quad (18)$$

where $\lambda^2 = K/B$ and $q_c \sim \pi/a$ is a large-momentum cutoff. Therefore, for $T>0$ we expect a density of dislocations given by $n_D \approx a^{-2}e^{-E_D/k_B T}$. At distances larger than $\xi_D = n_D^{-1/2}$, and as long as $E_D \gg dk_B T$, dislocations can be treated in a Debye-Hückel approximation. Then, to lowest order in q_x^2 and q_y^2, the correlation function for the layer normal angle $\theta = -\partial_y u$ can be written as[14]

$$\langle\tilde{\theta}(\mathbf{q})\tilde{\theta}(-\mathbf{q})\rangle = \frac{k_B T}{2E_D q_x^2 + Kq_y^2}, \quad (19)$$

which is precisely the correlation function of a two-dimensional nematic, with a free energy

$$F_{\text{nm}} = \frac{1}{2}\int d^2 r[K_1(\mathbf{\nabla}\cdot\mathbf{n})^2 + K_3[\mathbf{n}\times(\mathbf{\nabla}\times\mathbf{n})]^2], \quad (20)$$

where $\mathbf{n} = (\cos\theta, \sin\theta)$ is the director field, and the two Frank constants are given by

$$K_1 = K, \quad K_3 = 2E_D. \quad (21)$$

Orientational correlations in the director $\mathbf{n(r)}$ should decay algebraically at distances much larger than ξ_D. Table II summarizes the values of K_1 and K_3. The values of these elastic constants are determined at distances comparable to ξ_D ($\sim 10a$ at $T\sim 100$ mK).

(IV) The nematic to isotropic transition. At sufficiently long wavelengths Nelson and Pelcovits,[23] using a momentum-shell renormalization approach, have shown that

deviations from the one-Frank-constant approximations $K_1 = K_3$ are irrelevant, and the system is equivalent to a two-dimensional XY model:

$$F_{XY} = \frac{1}{2} K(T) \int d^2r (\nabla \theta)^2, \qquad (22)$$

with $K \to [K_1(\xi_D) + K_3(\xi_D)]/2$ at very large distances. For our values of K_1 and K_3, at the characteristic temperatures of the experiments, convergence is achieved at distances around $(20-100)\xi_D$. We then expect unbinding of disclination pairs at the KT temperature:[15]

$$k_B T_{KT} = \frac{\pi}{8} K(T_{KT}), \qquad (23)$$

where the $\pi/8$ comes instead of the more common $\pi/2$ for vortices since each disclination winds up the angle by π rather than 2π. In general, $K(T_{KT})$ corresponds to the large-distance elastic constant (reduced by disclination pairs) to the bare elastic constant at small distances $K(0)$ by means of the KT renormalization group (RG) formulas:[15]

$$\frac{dk^{-1}}{dl} = \pi^3 y^2(l), \quad \frac{dy}{dl} = [8 - \pi k(l)] \frac{y(l)}{4}, \qquad (24)$$

where $k = K/k_B T$ and we have introduced the fugacity $y \sim \exp[-\pi^2 K(0)/k_B T]$. In practice, these RG equations can be approximated by $k_B T_{KT} \simeq (\pi/8)K(0)/\{1 + 2\pi \exp[-\pi^2 K(0)/8 k_B T_{KT}]\} \simeq 0.86(\pi/8)K(0)$. This reduction is in general agreement (although somewhat less important) to results for Monte Carlo simulations.[12]

Table II presents the resulting estimates for the disclination-unbinding transition temperatures for half-filled LL's. Although these can only be considered estimates due to the approximations used, they are in qualitative agreement with the temperatures at which the anisotropies are seen to vanish. For comparison, Fradkin et al.[12] find $T_{KT} \simeq 65$ mK with significant rounding by 5% intrinsic anisotropy for $\nu = 9/2$ by fitting the results of a Monte Carlo simulation of an XY model to the resistivity data of Ref. 1. We also see the characteristic spin oscillation of the transition parameters.[1,24] The reason for this spin oscillation is simple: in the energetics of Eqs. (4)–(6), there is an energy scale e^2/R_c that decreases with increasing filling factor ν (both because of the change in LL index *and* the reduction of the magnetic field);

simultaneously the matrix elements of the Coulomb interaction [Eq. (3)] increase with increasing LL index L, resulting in the observed spin dependence.

There are a couple of caveats that apply to our results. First, we have left out the native anisotropy of the sample that tends to align the smectic structure (similar effects arise from an in-plane component of the magnetic field). Uniaxial anisotropy will produce a term of the form $B'(\partial_y u)^2$ in the smectic energy density; although the experiments indicate that $B' \ll B$, at sufficiently long length scales (of order $\sqrt{K/B'}$) the anisotropy will dominate over the bending energy. In this case the dislocation energy diverges as the logarithm of the system size, and the transition to the isotropic phase occurs through the unbinding of dislocations. Second, as is customary in studies of smectics, we have dropped terms in the smectic free energy, Eq. (17), of $O(q_x^2 q_y^2)$. To check the validity of this truncation we have calculated the elastic coefficients K' and K'', and find that while $K'' > 0$, it is possible for K' to be negative.[25] This does not seem to cause any problems in the long-wavelength limit, but it may change our estimates of the dislocation energy. This issue is currently under study.[22]

In conclusion, we have mapped a 2DES with half-filled LL's to a liquid crystal with smectic/nematic order at short/long distances and that undergoes a KT disclination-unbinding transition, after which the system becomes isotropic, as seen by transport measurements. Without the use of any fitting parameters we have obtained transition temperatures in qualitative agreement with experimental evidence. A particularly robust feature is the spin dependence of the nematic elastic moduli and transition temperature (Table II): they are larger for the lower-spin subband ($\nu = 9/2, 13/2, 17/2$). While precise experimental values for the transition temperatures have not been established and the transition is rounded by disorder, the same characteristic spin dependence is observed in the transport anisotropy[1,24] ρ_{xx}/ρ_{yy}.

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