Renormalization-group treatment of the dislocation loop model of the smectic-A–nematic transition

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A dislocation model for the smectic-A–nematic transition is mapped onto a peculiar sort of anistropic superconductor, which is then studied using a momentum-shell renormalization group. The elastic constants behave according to the helium analog, while the specific heat displays an *inverted* λ anomaly. The x-ray correlation-length exponents are $\nu_{\parallel}^{x} \simeq \frac{4}{5}$ and $\nu_{\perp}^{x} \simeq \frac{8}{15}$, in fairly good agreement with experiment.

There are many theories of the nematic to smectic-A transition currently extant,[1–5] none of which have succeeded in correctly predicting the experimentally observed critical exponents. DeGennes's[1] argument that the transition should be equivalent to the superfluid-normal transition was disputed by Halperin, Lubensky, and Ma,[2] who argued that it should rather be equivalent to the *superconductor*-normal transition, with director fluctuations driving the transition to first order. Unfortunately some experimentally observed[6] transitions appear continuous down to reduced temperatures $t \sim 10^{-6}$—orders of magnitude smaller than that at which the predicted first-order transition should occur. In contrast with both these theories, the experimentally observed critical behavior appears to be anisotropic, with different correlation-length exponents $\nu_{\perp}(\nu_{\parallel})$ for fluctuations within (normal to) the layers.

It has been conjectured[3,4] that a dislocation[7] unbinding theory of this transition might explain some of these anomalies. I will show in this paper that, at least for some finite range of values of the parameters, the dislocation loop model has the thermodynamic properties of an inverted X-Y transition, i.e., one with the high- and low-temperature sides of the transition reversed. This is in agreement with the recent work of Dasgupta and Halperin[8] on the three-dimensional superconductor. (There are theoretical reasons[2,9] for believing that this model has the same critical properties as a smectic, although this does not appear to be the case experimentally.) The x-ray correlation length exponents are given *exactly* by $\nu_{\parallel}^{x} = 6\nu_s/5$ and $\nu_{\perp}^{x} = 4\nu_s/5$, where ν_s is the superfluid correlation-length exponent.

The dislocation loop model that I will use here is a lattice version of that considered in Ref. 4, and assumes that dislocation loops are the sole excitation responsible for the smectic-A–nematic transition. These loops are the boundaries of extra layers inserted into the smectic; we can characterize them by a vector $\vec{m}_i$ that points along the boundary and whose magnitude is the number of such extra layers. (Since only an integral number of layers can be inserted, $\vec{m}_i$ is integer valued.) The partition function for this system was derived in Ref. 4; on a lattice it is[4,10]

$$Z = \sum_{\{\vec{m}_i\}} \delta(\vec{\Delta} \cdot \vec{m}_i) \exp(-\bar{H}) , \quad (1)$$

with

$$\bar{H} = \frac{1}{2} \sum_{\vec{q}} \left(\frac{\bar{K}_1 q_{\perp}^2}{q_z^2 + \lambda^2 q_{\perp}^4} P_{ij}^{\perp} + 2E_c \delta_{ij} \right) m_i(\vec{q}) m_j(-\vec{q}) . \quad (2)$$

Here $\vec{m}_i$ is an integer valued vector field that measures the charge (i.e., the number of extra layers inserted) of the dislocation at the site i, $\vec{m}(\vec{q})$ is its Fourier transform, $z(\perp)$ is the direction normal to (within) the layers, $P_{ij}^{\perp} = (\delta_{ij} - q_i^{\perp} q_j^{\perp}/q_{\perp}^2)(1 - \delta_{iz}\delta_{jz})$, $\bar{K}_1 \equiv K_1 d^2/k_B T$ is a reduced elastic constant, d is the smectic layer spacing, and E_c is the dislocation core energy. The constraint $\vec{\Delta} \cdot \vec{m}_i = 0$, where $\vec{\Delta}$ is a lattice gradient operator, simply requires that dislocation lines form closed loops. The length λ is related to the elastic constants B and K_1 that control compression and bending of the layers, respectively, by $\lambda^2 = K_1/B$.

Following Peskin,[11] I apply a Hubbard-Stratonavich transformation to this model, i.e., I introduce a continuous vector field $\vec{A}_i$ to mediate the interaction:

$$Z' = \int \prod_i d\vec{A}_i \sum_{\{\vec{m}_i\}} \delta(\vec{\Delta} \cdot \vec{m}_i) \exp\left[-H_A(\{\vec{A}_i\}) + \sum_i i\vec{m}_i \cdot \vec{A}_i - E_c |\vec{m}_i|^2 \right] \delta(A_z) \delta(\vec{\Delta} \cdot \vec{A}_i) \quad (3)$$

with

$$H_A(\{\vec{A}_i\}) = \frac{1}{2} \sum_{\vec{q}} [(q_z^2/\bar{K}_1 q_{\perp}^2) + (q_{\perp}^2/\bar{B})] |\vec{A}_q|^2 , \quad (4)$$

where $\vec{A}_q$ is the Fourier transform of $\vec{A}_i$ and $\bar{B} \equiv Bd^2/k_BT$.

It is easily verified by performing the Gaussian integrals over $\vec{A}$ that Z' is equal to Z as given by Eq. (1) up to a multiplicative constant.

Now I cope with the constraint $\vec{\Delta}\cdot\vec{m}_i=0$ by introducing another auxiliary field ϕ_i:

$$Z'=\int\prod_i d\vec{A}_i\int_{-\pi}^{\pi}\frac{d\phi_i}{2\pi}\sum_{\{\vec{m}_i\}}\exp\left[-H_A(\{\vec{A}_i\})+\sum_i(i\vec{m}_i\cdot\vec{A}_i-E_c|\vec{m}_i|^2+\phi_i\vec{\Delta}\cdot\vec{m}_i)\right]\delta(A_z)\delta(\vec{\Delta}\cdot\vec{A}_i)\ . \tag{5}$$

Integrating out ϕ_i will recover the constraint. I can now integrate by parts in the exponential; i.e., use $\sum_i\phi_i\vec{\Delta}\cdot\vec{m}_i=-\sum_i\vec{m}_i\cdot\vec{\Delta}\phi_i$ and rewrite the partition function as

$$Z'=\int\prod_i d\vec{A}_i\int_{-\pi}^{\pi}\frac{d\phi_i}{2\pi}\exp[-H_A(\{\vec{A}_i\})]\left[\sum_{\{\vec{m}_i\}}\exp\left(\sum_i-E_c|\vec{m}_i|^2+i\vec{m}_i\cdot(\vec{A}_i-\vec{\Delta}\phi_i)\right)\right]\delta(A_z)\delta(\vec{\Delta}\cdot\vec{A}_i)\ . \tag{6}$$

Recognizing the term in large square brackets as the Fourier transform of a periodic Gaussian allows me to express the partition function as a Villain model for peculiar superconductor

$$Z'=\int\prod_i d\vec{A}_i\int_{-\pi}^{\pi}\frac{d\phi_i}{2\pi}\sum_{\{\vec{S}_i\}}\exp\left[-H_A(\{\vec{A}_i\})-\frac{1}{4E_c}\sum_i|\vec{A}_i-\vec{\Delta}\phi_i+2\pi\vec{S}_i|^2\right]\delta(A_z)\delta(\vec{\Delta}\cdot\vec{A}_i) \tag{7}$$

in which the magnetic energy $|\vec{\nabla}\times\vec{A}|^2/8\pi\mu$ has been replaced by the Hamiltonian (4), and there is a new constraint $A_z=0$ in addition to the usual $\vec{\nabla}\cdot\vec{A}=0$ that holds for superconductors in the Coulomb gauge. I expect this Villain model to have the same critical properties as the Hamiltonian

$$H=H_A(\{\vec{A}_i\})+J\sum_i\sum_\mu\cos(\phi_{i+\hat{\mu}}-\phi_i-A_{i\mu})\ , \tag{8}$$

where the index μ denotes different lattice directions, and with $J\approx 1/4E_c$ as $E_c\to 0$. In turn, this system should have the same critical properties[12,13] as the following "soft-spin" model:

$$H=H_A(\{\vec{A}(\vec{r})\})+\tfrac{1}{2}\int d^dr[r|\psi|^2+u|\psi|^4+c_\perp|(\vec{\nabla}-i\vec{A})\psi|^2+c_z|\partial_z\psi|^2+O(\psi^6)]\ , \tag{9}$$

where ψ is a complex order parameter, and I have replaced the three-dimensional discrete lattice with a continuous space of dimension d. As always,[12] I will assume that r is proportional to the reduced temperature $t\equiv(T-T_c/T_c)$ and that u is roughly independent of t near the transition. The equivalence between this model and the original dislocation loop model [Eq. (1)] only holds in $d=3$; nonetheless, the continuation to arbitrary dimension is useful in that it enables me to do an ϵ expansion about $d=4$. The conclusion that this model has an inverted XY transition is, as we shall see, independent of the ϵ expansion.

I proceed by the usual momentum shell techniques, with the modification that (for computational convenience) I choose a hypercylindrical Brillouin zone of infinite extent in the z direction, rather than the usual hyperspherical one.

After integrating out all Fourier components of $\vec{A}$ and ψ in a hypercylindrical shell with $b^{-1}\le q\le 1$, I anisotropicly rescale wave vectors: $q_\perp\to b^{-1}q_\perp$, $q_z\to b^{-1-a}q_z$ and fields: $\psi(\vec{q}_\perp,q_z)=b^{(d+2-\eta_\psi)/2}\times\psi(b\vec{q}_\perp,b^{1+a}q_z)$, $\vec{A}(\vec{q}_\perp,q_z)=b^{d+a-1}\vec{A}(b\vec{q}_\perp,\ b^{1+a}q_z)$. I have rescaled q_z and $\vec{q}_\perp$ differently to allow for the possibility of anisotropic scaling.

In practice, both a and the equally arbitrary parameter η_ψ will be chosen to produce fixed points. The rescaling of $\vec{A}$ is chosen to keep the coefficient of the $\vec{A}|\psi|^2$ term in H (the "charge") from renormalizing. Taking $b=e^l$ with the l differential leads to the following recursion relations:

$$\frac{dr}{dl}=(2-a-\eta_\psi)r+\frac{8C_{d-1}u}{[(c_\perp+r)c_z]^{1/2}}+\left(\frac{d-2}{2}\right)C_{d-1}(\bar{B}\bar{K}_1)^{1/2}c_\perp+O(\bar{B}\bar{K}_1,u^2), \tag{10a}$$

$$\frac{du}{dl}=(\epsilon-3a-2\eta_\psi)u-\frac{10C_{d-1}u^2}{c_z^{1/2}(c_\perp+r)^{3/2}}-\frac{C_{d-1}(\bar{B}\bar{K}_1)^{1/2}\bar{B}c_\perp^2}{2}+O(u^3,\bar{B}^3\bar{K}_1), \tag{10b}$$

$$\frac{d\bar{K}_1}{dl}=(a+\epsilon-2)\bar{K}_1, \tag{10c}$$

$$\frac{d\bar{B}}{dl}=(\epsilon-a)\bar{B}-\frac{\bar{B}^2C_{d-1}c_\perp^2}{2(d-1)c_z^{1/2}}\times\left[\frac{3c_\perp}{2[(c_\perp+r)]^{5/2}}-\frac{5c_\perp^2}{(d+1)[(c_\perp+r)c_z]^{7/2}}\right], \tag{10d}$$

$$\frac{dc_z}{dl}=-(\eta_\psi+3a)c_z+O(\bar{B}^3,u^2,u\bar{B}^2), \tag{10e}$$

$$\frac{dc_\perp}{dl}=-(\eta_\psi+a)c_\perp-\frac{c_\perp^2}{c_z^{1/2}}\frac{C_{d-1}[\bar{K}_1\bar{B}(c_\perp+r)]^{1/2}}{\lambda[\lambda+(c_\perp+r)^{1/2}]}+O(\bar{K}_1\bar{B},u^2)\ , \tag{10f}$$

where C_d is the surface area of a d-dimensional sphere divided by $(2\pi)^d$. It is important to note that the recursion relation (10c) for K_1 is *exact* to all orders in perturbation theory; there are no graphs that renormalize K_1, since it is the coefficient of a nonanalytic (in $\vec{q}$) term in the Hamiltonian [Eq. (4)]. Hence all conclusions based on (10c) (i.e., most of the conclusions of this paper) are independent of the ϵ expansion.

In precisely three dimensions, these recursion relations have fixed plane with $r=\infty$, $c_\perp=c_z=u=0$, $\overline{B}=$const, and $\overline{K}_1=$const, if we choose $a=1$ and $\eta_\psi=0$. This plane is characterized by algebraic decay of correlations–i.e., $G(r_\perp,0)\propto(r_\perp)^{-\eta_\perp}$ and $G(\vec{0},z)\propto(z)^{-\eta_\parallel}$–of the smectic order parameter (which should not be confused with the artificial order parameter introduced here) with $\eta_\parallel=\pi/2\sqrt{\overline{B}\overline{K}}$ and $\eta_\perp=(1+a)\eta_\parallel=2\eta_\parallel$. The last relation is just a simple consequence of anisotropic scaling.

These are all just well-known properties of the *ordered* smectic-A phase.[14,15] Since $r\to\infty$ corresponds to the *disordered* phase of ψ, it follows that these transformations have had the dualitylike property of interchanging the high- and low-temperature sides of the transition.

The transition itself is controlled by an isolated fixed point with $a=0=\overline{K}_1$. The thermal eigenvalue of this fixed point (which would be the inverse of the correlation-length exponent ν in the absence of the complications discussed by LDI) is $\lambda=2-2\epsilon/5$, which is just that of the XY model, to lowest order in ϵ. Since in addition the scaling is isotropic $(a=0)$, this fixed point has precisely the properties of the XY fixed point. In renormalization-group jargon, the vector potential terms in (9) constitute an "irrelevant perturbation" to the XY behavior.

How are these results modified when ϵ grows to unity $(d=3)$? One thing that *cannot* change is the recursion relation (10c) for K_1, for the reasons given earlier. Thus for $a<1$, the conclusion that K_1 *renormalizes to zero, even in* $d=3$, is unaltered. But for small K_1, we must choose $a=O(\sqrt{\overline{B}\overline{K}_1})$ in order to keep $c_\perp$ and c_z from renormalizing $(a=C_{d-1}\sqrt{\overline{B}\overline{K}_1}$ for $\overline{K}_1<<\overline{B}$ and $\epsilon<<1)$; hence a is indeed $<<1$ when $K_1\to0$ (unless $\overline{B}\to\infty$) and a *zero* K_1, *the finite* $\overline{B}$ *fixed point will be stable even in* $d=3$. Such a fixed point will always have X-Y exponents, since all terms involving $\overline{B}$ and $\overline{K}_1$ drop out of the recursion relations for u and r [and, clearly those for the coefficients of higher-order terms in (9) as well].

Likewise, the existence of a fixed plane in $d=3$ is independent of the ϵ expansion. Note that the topology of the Hamiltonian flows (fixed plane controlling the smectic A phase, isolated fixed point controlling the NA transition) is just that conjectured in Ref. 4 on the basis of crude physical arguments. They failed to anticipate, however, that $\overline{K}_1=0$ (in their language, $\eta^*=\infty$) at the isolated fixed point.

As pointed out by Lubensky *et al.*,[5] the existence of an isotropic fixed point does not imply that the two correlation lengths ($\xi_\parallel^x$ and $\xi_\perp^x$) experimentally observed in x-ray scattering need diverge with the same exponents. This is a consequence of the fact that $\overline{K}_1$ is a "dangerous irrelevant variable" in the sense that the correlation lengths diverge when $\overline{K}_1$ goes to zero. We can calculate the behavior of these correlation lengths using the arguments of Ref. 4, which suggest that $\xi_\parallel^x=n_e^{-2/3}\lambda^{-1/3}$ and $\xi_\perp^x=n_e^{-1/3}\lambda^{1/3}$, where n_e is the areal density of free-edge dislocations piercing a given plane, provided that we allow λ to depend on the length scale we are considering ($\lambda\to\infty$ at long wavelengths in the nematic phase, since $B\to0$ there).

From the renormalization group constructed here one can show[16] that $n_e\propto\xi_s^{-2}$ and $\lambda\propto\xi_s^{2/5}$ at the relevant length scales near T_c, where ξ_s is a superfluid correlation length. This gives $\nu_\parallel^x=6\nu_s/5\approx0.8$ and $\nu_\perp^x=4\nu_s/5\approx0.533$, where in the numerical estimates I have used for the superfluid correlation length exponent $\nu_s\approx\frac{2}{3}$. This compares reasonably well with the experimental values $\nu_\parallel^x=0.763$ and $\nu_\perp^x=0.623$ reported by Kortan *et al.*[17]

Since the transition is controlled by an X-Y fixed point, the elastic constants B, K_2, and K_3 obey the helium analog; i.e., $B\propto|t|^{\nu_s}$, $K_{2,3}\propto|t|^{-\nu_s}$, near T_c.

The anharmonic effects considered in Ref. 14 [which are neglected in the model Eq. (1)] are controlled by a parameter $w=\overline{B}^{1/2}/\overline{K}_1^{3/2}$. The above results imply that this parameter vanishes like $|t|^{\nu_s/2}$ as the transition is approached; thus the harmonic theory used here should give an accurate description of the transition.

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