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Bond-orientational order, dislocation loops, and melting of solids and smectic-A liquid crystals

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A three-dimensional solid with an equilibrium concentration of unbound dislocation loops displays a resistance to torsion not present in isotropic liquids. There is residual bond-angle order analogous to that found in the two-dimensional hexatic phase. A bulk phase with bond orientational order may be observable in supercooled liquids. Such a phase would display an angular modulation in monodomain x-ray-diffraction patterns, and would give rise to an intrinsic asymmetry in the limits of supercooling and superheating. Bond-angle order may also be present in glasses. A dislocation-loop mechanism for the smectic-A—to—nematic transition implies anisotropic scaling and fixes the ratio of the transverse and longitudinal correlation length exponents.

I. INTRODUCTION

There is now considerable interest in the effect of defects like dislocations and disclinations on melting of two-dimensional solids.[1-5] Kosterlitz and Thouless[2] originally proposed that an unbinding of charge-neutral dislocation pairs would drive a continuous melting transition into a liquid. More recently, however, it has been argued that a second, disclination-unbinding transition is necessary to complete the transition from solid to liquid.[4] Interposed between the more familiar solid and liquid phases, one finds a phase with persistent order in the orientations of bond angles,[6] called a hexatic liquid crystal. The residual sixfold anisotropy characterizing the hexatic phase has nothing to do with the *shapes* of the atoms, but is instead a vestige of the singled-out crystallographic axes present in a triangular solid. Both the hexatic-to-solid and hexatic-to-liquid transitions can be continuous, in contrast to the first-order melting of bulk materials. It is as if the usual latent heat of melting had been spread out over an entire phase.

Although there is some support for dislocation-mediated melting in recent computer simulations,[7,8] other investigators find no evidence of the hexatic phase.[9-11] Tobochnik and Chester[12] find some evidence for a first-order melting transition at high densities and dislocation-mediated melting at low densities, in a simulation of a Lennard-Jones 6-12 potential. Experimental studies of melting of physiadsorbed rare-gas monolayers,[13] electrons trapped on the surface of helium,[14] "soap-bubble" liquid-crystal films,[15] monodispersed polystyrene spheres floating on water,[16] and lipid monolayer films[17] should ultimately provide detailed tests of the theory.

Although the situation in two-dimensions is unresolved at present, the discovery of a *bulk* analog of the hexatic phase has been reported by Moncton and Pindak.[18] Shortly after the dislocation theory was developed, Birgeneau and Litster[19] argued that stacking layers of hexatic material would result in a novel kind of smectic liquid crystal. This "stacked hexatic" phase would have long-range bond-orientational order, but short-range translational order in the smectic planes. The in-plane x-ray structure factor of such a material has the form[20]

$$S(\vec{q},T)=\sum_{n=0}^{\infty}c_n(q,T)[\cos(6n\theta_{\hat{q}})\operatorname{Re}\langle\psi^n(\vec{r})\rangle+\sin(6n\theta_{\hat{q}})\operatorname{Im}\langle\psi^n(\vec{r})\rangle]\ , \tag{1.1}$$

where $\theta_{\hat{q}}$ is the angle the scattering vector $\vec{q}$ makes with the $\hat{x}$ axis, and the coefficients $c_n(q,T)$ are weak functions of temperature. The dominant temperature dependence near a phase transition is given by thermal averages of powers of the bond-orientational order parameter.

$$\psi(\vec{r})\propto e^{6i\theta(\vec{r})}\ . \tag{1.2}$$

Here, $\theta(\vec{r})$ is the angle a line joining a pair of neighboring atoms makes with the $\hat{x}$ axis. The resulting diffraction pattern is shown schematically in Fig. 1. Moncton and Pindak observed a sixfold angular modulation in the x-ray diffraction off the smectic compound 650 BC consistent with Eq. (1.1). This modulation is accompanied by a large, but finite translational correlation length.[18]

Dislocations have long been proposed as a mechanism for melting of three-dimensional crystalline solids into isotropic liquids. Shockley,[21] for example, has argued that bulk melting may be viewed as a sudden

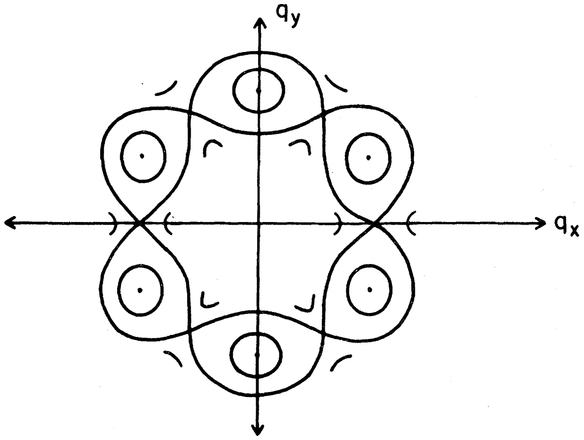

FIG. 1. Schematic contours of constant scattering density of the in-plane structure function of the "stacked hexatic" phase of smectic liquid crystals. The pattern of six maxima and six saddle points is indicative of short-range translational order, but long-range bond-orientational order in the smectic planes.

proliferation of a tangled array of dislocation loops in the solid. He showed that a finite density of mobile dislocation lines would result in a liquidlike viscosity. Shockley's ideas have been elaborated by a variety of subsequent workers whose efforts are reviewed by Cotterhill.[22] The most recent investigation is by Edwards and Warner,[23] who use methods developed in polymer physics to argue in favor of a dislocation-driven first-order melting transition. One problem with dislocation-mediated bulk melting is that current theories are not sophisticated enough to distinguish between interacting dislocation loops and interacting vortex lines in superfluid helium.[24] Superfluid helium usually displays a continuous λ transition, in contrast to the first-order bulk melting transition. The possible role of defects in three-dimensional phase transitions has been reviewed by Halperin.[25]

In this paper, we study the long-wavelength properties of a solid with an equilibrium concentration of "free" or "unbound" dislocation loops. Although all solidlike elastic constants vanish, we find a persistent resistance to torsion not present in an isotropic liquid. In this sense, a solid with unbound dislocations is not a liquid, as argued by Shockley, but is instead analogous to the hexatic phase discussed in Ref. 4. Assuming isotropic elastic properties, the stiffness constants characterizing the resistance to twist inhomogeneities are given explicitly in terms of edge and screw dislocation core energies. Although translational order is absent, the system remembers the singled-out crystallographic axes present in the solid.

To make this idea precise, consider the distribution of "bonds" joining a particle located at $\vec{r}$ to its near neighbors shown in Fig. 2. Expanding the density

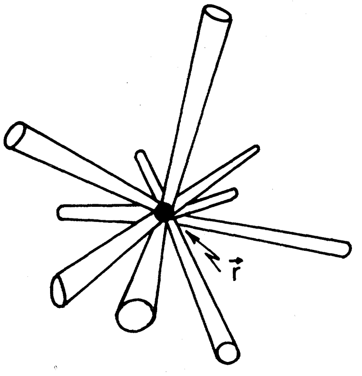

FIG. 2. Cluster of bonds surrounding a particle located at position $\vec{r}$. The bonds could be obtained by the Voronoi construction, or simply by searching for, say, the first 13 nearest neighbors of a given atom.

$\rho(\vec{r},\Omega)$ of points pierced by these bonds on a small sphere inscribed about $\vec{r}$, we have

$$\rho(\vec{r},\Omega)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Q_{lm}(\vec{r})\,Y_{lm}(\Omega)\ , \tag{1.3}$$

where the $Y_{lm}(\Omega)$ are spherical harmonics. The distribution of bonds as a function of solid angle Ω could be determined by, say, the Voronoi construction.[6] In a liquid, we expect that $\rho(\vec{r},\Omega)$ becomes isotropic upon averaging over particle positions $\vec{r}$,

$$\langle\rho(\vec{r},\Omega)\rangle=\rho_0\equiv\langle Q_{00}\rangle/\sqrt{4\pi}\ . \tag{1.4}$$

We find that a heavily dislocated solid has persistent bond-orientational order in the sense that Fourier coefficients with $l\neq 0$ in Eq. (1.3) fail to vanish upon averaging. For materials with a cubic rotational symmetry, the first coefficients which are nonvanishing correspond to $l=4$,

$$\begin{aligned}\langle\delta\rho(\vec{r},\Omega)\rangle&\equiv\langle\rho(\vec{r},\Omega)\rangle-\rho_0\\&\approx\sum_{m=-4}^{4}\langle Q_{4m}(\vec{r})\rangle\,Y_{4m}(\Omega)\ .\end{aligned} \tag{1.5}$$

In contrast to bcc, fcc and simple cubic crystals, where the $\langle Q_{4m}(\vec{r})\rangle$ are also nonvanishing, there is no translational order. Because this phase has some mathematical similarity to a nematic liquid crystal,[26] we shall refer to it as the "cubic-liquid-crystal phase."[27] It should be stressed that its cubic rotational anisotropy need not be associated with anisotropy in the constituent particles.

We have very little to say about dislocation loop unbinding as a *mechanism* for bulk melting. We are primarily interested in the concept of "a solid with a finite density of unbound dislocations" as a slightly awkward description of a phase which is not a crystal. Our analysis is intended to motivate a discussion of cubic liquid crystals in the more convenient language of fluctuations-corrected Landau theory. The fact that unbound dislocations alone are insufficient to destroy the rotational broken symmetry one associates with a crystal does represent an important constraint on dislocation mediated melting theories, however.

The resistance to torsion of a heavily dislocated solid makes the existence of a cubic-liquid-crystal phase at least plausible. It then becomes interesting to ask how it transforms into a liquid and, say, a bcc solid. A simple criterion due to Landau[28] suggests that both transitions are first order (see Sec. III). We shall argue, however, that fluctuations drive the liquid—to—cubic-liquid-crystal transition *second* order in $2+\epsilon$ dimensions. This transition is probably either continuous or weakly first order in $d=3$. A similar situation arises in nematic liquid crystals, where the nematic-to-isotropic first-order transition is anomalously small.[26] Fluctuations have less influence on the cubic-liquid-crystal—to—solid transition, which can be strongly first order.

Equilibrium cubic-liquid-crystal phases should be more rare than their two-dimensional hexatic counterparts. Upon warming up a solid, one can in principle both enter and leave the hexatic phase via continuous phase transitions.[4] The strong first-order melting of virtually all *bulk* crystals, however, usually leads directly to a liquid; the cubic-liquid-crystal phase may be bypassed entirely.[29] If the liquid—to—cubic-liquid-crystal phase transition is nearly continuous, one might nevertheless expect a liquid to drop into this new phase upon supercooling. As discussed in Sec. IV, this transition may be accompanied by a weak specific-heat singularity, and leads to an angular modulation in the monodomain x-ray-diffraction pattern, analogous to that shown for the stacked hexatic phase in Fig. 1. Near the phase transition, x rays provide a direct measure of the nine components of the cubic-liquid-crystal order parameter defined by Eq. (1.5). In an appropriate coordinate system, the only nonvanishing elements are $\langle Q_{40}\rangle$ and $\langle Q_{44}\rangle = \langle Q_{4-4}\rangle$. A characteristic feature of the cubic symmetry is that

$$|\langle Q_{4\pm4}\rangle/\langle Q_{40}\rangle| = \sqrt{5/14} \ . \tag{1.6}$$

We shall also argue that the existence of a metastable cubic-liquid-crystal phase leads to an intrinsic asymmetry in the limits of supercooling and superheating.

The bond angle order parameter may be useful in other contexts. The bond-angle density deviation from anisotropy can also be expressed in terms of a traceless, symmetric fourth-rank tensor Q_{ijkl},

$$\langle \delta\rho(\vec{r},\Omega)\rangle = \langle Q_{ijkl}(\vec{r})\rangle e_i e_j e_k e_l \ . \tag{1.7}$$

We have used the summation convention, and denoted by $\vec{e}$ the unit vector associated with the solid angle Ω. In terms of a singled out orthonormal triad $(\vec{l},\vec{m},\vec{n})$, we have[27]

$$\langle Q_{ijkl}(\vec{r})\rangle = Q_0[\,l_i l_j l_k l_l + m_i m_j m_k m_l + n_i n_j n_k n_l - \tfrac{1}{5}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\,] \ , \tag{1.8}$$

which defines the amplitude Q_0 of this tensor order parameter. This form for $\langle Q_{ijkl}\rangle$ allows us to associate an orthonormal triad with bond clusters like the one shown in Fig. 2. The traceless, symmetric, fourth-rank tensor one extracts from the $l=4$ part of the expansion (1.3) will not in general have the form (1.8). We can, however, define an optimal orthonormal triad associated with a given $Q_{ijkl}(\vec{r})$ by minimizing, say

$$\Delta(\vec{l},\vec{m},\vec{n}) = \sum_{ijkl}[\,(Q_{ijkl}/Q_0) - l_i l_j l_k l_l - m_i m_j m_k m_l - n_i n_j n_k n_l + \tfrac{1}{5}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\,]^2 \ , \tag{1.9a}$$

where

$$Q_0 \equiv (\tfrac{5}{6} Q_{ijkl} Q_{ijkl})^{1/2} \tag{1.9b}$$

over all potential order parameter triplets $(\vec{l},\vec{m},\vec{n})$. Note that all three coordinate axes are equivalent in the definition (1.8).

Having associated an orthonormal triad with the bond cluster surrounding a given atom one can assign a disclination field to every particle configuration. This has been done by McTague, Allen, and Frenkel in two dimensions, via the construction of Voronoi polygons.[7] In three dimensions, we imagine the triads associated with the particles rotating continuously into their configurations at neighboring sites by the shortest possible route.[30] To see if a closed ring of near-neighbor atoms contains a disclination, we make use of the standard definition[31] involving parallel transport of orthonormal triads around a closed circuit. Just as in two dimensions,[7] one can presumably build up more complicated defects like dislocations, vacancies, and interstitials from disclination complexions, and test via computer simulations the predictions of defect-mediated melting theories.

It would also be interesting to examine the bond angle order parameter in glassy materials. If a supercooled liquid transforms into a cubic liquid crystal, we expect a corresponding increase in the translational correlation length.[32] Enhanced translational order slows down the dynamics, and promotes glass formation. According to this argument, at least some glasses should be distinguished from liquids by a nonzero value of the bond-orientational order parameter. Alben *et al.*[33] have reported an intriguing angular anisotropy in various structural models of amorphous materials. It would be interesting to try to account for these results in terms of an appropriate bond-angle order parameter. The order parameter appropriate for structures with a *tetrahedral* seed, for example, is constructed from $l=3$ spherical harmonics. The density correlations expected in *equilibrium* cubic liquid crystals are discussed in Sec. IV B.

As temperature is lowered in a supercooled liquid, the dynamics slows down dramatically, and one apparently approaches, but never reaches, an asymptotic glass transition temperature T_0. Assuming that the supercooled liquid is in the cubic-liquid-crystal phase, it is intriguing to speculate that the cubic-liquid-crystal—to—solid transition has something to do with the temperature T_0. The transition to a bcc lattice structure is probably first order in equilibrium. It remains to be seen, however, if equilibrium concepts are appropriate in such a situation.

An analog of quenched bond-orientational order may exist in spin-glasses, with clusters of neighboring spins replacing the bond cluster in Fig. 2. Halperin and Saslow[34] have constructed a hydrodynamic theory of spin waves in such systems by following the dynamics of spin clusters. They associate an arbitrary orthonormal triad with each cluster at time $t=0$. The algorithm summarized by Eq. (1.9) allows a calculation of $\langle Q_{ijkl}(\vec{r})\rangle$, and could lead to a *unique* orthonormal triad associated with the spin-glass ground state. A nonzero average of $Q_{ijkl}(\vec{r})$ is certainly a sufficient condition for the nonvanishing spin-wave stiffness assumed by Halperin and Saslow. It would be interesting to map out the disclination field of a spin-glass by the technique proposed above for particle configurations.

The melting of smectic-*A* liquid crystals,[26] which are solidlike in one direction, but liquidlike in two, is an intriguing problem. These systems are known to be precisely at their lower critical dimension, where fluctuations prevent true long-range translational order.[35] Helfrich *et al.*[36] have argued that an unbinding of dislocation loops drives the melting of smectics-*A* into nematic liquid crystals. Experimentally, this transition seems to be second order.[37] Because a nematic has a singled out direction, one expects blobs of smectic-*A* fluctuations just above the transition to be anisotropic (see Fig. 3). Both theoretically[38] and on experimental grounds,[37] it has been suggested the correlation lengths parallel and perpendicular to the ordering actually diverge with different exponents:

$$\xi_\parallel \sim \frac{1}{|T-T_c|^{\nu_\parallel}}, \quad \xi_\perp \sim \frac{1}{|T-T_c|^{\nu_\perp}}, \qquad (1.10)$$

with $\nu_\parallel \neq \nu_\perp$. Singularities in a variety of physical properties can be expressed in terms of $\xi_\parallel$ and $\xi_\perp$.[38,39]

Smectics *A* can also transform directly into isotropic liquids, via a first-order phase transition. Indeed, the smectic-*A*, nematic, and isotropic phases are analogous, respectively, to the solid, cubic liquid crystal, and liquid phase discussed earlier for isotropic melting. It would be interesting to study experimentally a metastable nematic phase in a material with a direct smectic-*A*—to—isotropic transition. Such a metastable phase would be most easily obtained by superheating the smectic *A*, since the nematic-to-isotropic transition is first order. One might expect a larger intrinsic limit of superheating than supercooling, contrary to the situation in bulk melting (see Sec. IV A).

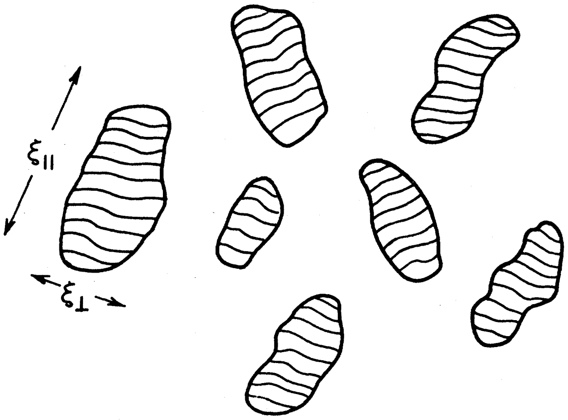

FIG. 3. Schematic illustration of smectic-*A* fluctuations in the nematic phase. The blobs of smectic ordering range in size up to a length $\xi_\parallel$ along the nematic ordering direction and up to a length $\xi_\perp$ perpendicular to this direction. An argument given in the text suggests that $\xi_\parallel \propto \xi_\perp^2$.

Here, we show explicitly that a smectic *A* permeated by an equilibrium density of unbound dislocation loops behaves like a nematic, rather than an isotropic liquid. The nematic Frank constants are given in terms of renormalized edge and screw dislocation core energies. We then argue that dislocation mediated melting of smectics *A* into nematics implies anisotropic scaling, with

$$\nu_\parallel = 2\nu_\perp . \qquad (1.11)$$

The suggestion that dislocation loops might lead to anisotropic scaling is due to Helfrich.[36] More generally, an adaptation of Josephson's scaling argument[40] for superfluid ^{4}He suggests that

$$\nu_\parallel = (5-d)\nu_\perp , \qquad (1.12)$$

for d between three and four dimensions. Lubensky and Chen[38] found a fixed point with this property within the $\epsilon = 4-d$ expansion. This fixed point is physically inaccessible to lowest order in ϵ, however. If correct, the relation (1.11) implies that both the smectic elastic constant $B(T)$ and the nematic Frank constant $K_2(T)$ remain finite at T_c. Independent of the result (1.11), we find that the exponent $\eta(T)$, describing the algebraic decay of translational order in bulk smectics,[35] is finite at T_c^-.

The properties of a solid with unbound dislocation loops are developed in Sec. II. Transitions out of the cubic liquid phase, including fluctuation effects, are discussed in Sec. III. In Sec. IV, we discuss the observability of the cubic-liquid-crystal phase in supercooled liquids, as well as its x-ray structure function and hydrodynamics. Results for melting of smectic-*A* liquid crystals are presented in Sec. V. In Appendix A, we show that unbound vortex rings in superfluid ^{4}He give rise to a normal liquid. This problem is simpler, but mathematically similar to the behavior of dislocations in solids. The generalization of the results of Sec. II to anisotropic solids is described in Appendix B. In Appendix C, we derive the "Josephson relations" for smectic liquid crystals.

II. BEHAVIOR OF A SOLID WITH UNBOUND DISLOCATION LOOPS

In this section, we summarize the behavior of a solid with an equilibrium density of "free" or "unbound" dislocation loops. The meaning of "free" and "unbound" will be made clear later. As we shall see, the behavior is not liquidlike at long wavelengths but instead reflects a residual resistance to torsion.

Following Shockley,[21] it is easy to see that a finite density of mobile dislocations gives rise to a liquidlike response to shear stresses. One arrives at an estimate for the shear viscosity,[41]

$$\eta \sim 1/\mu_D L_D \ , \tag{2.1}$$

where μ_D is a dislocation mobility, and L_D is the density of mobile dislocation line per unit volume. The basic assumption is that unbound dislocation lines move to relax uniform shear strains, at a rate proportional to the applied stress. Alternatively, we can say that all the shear elastic constants characteristic of the solid vanish.

More precise calculations exploit a continuum description of dislocation loops embedded in an isotropic solid.[42] The long-wavelength elastic properties are described by a free energy[43]

$$F_s = \frac{1}{2}\int d^3r\,(2\mu u_{ij}^2 + \lambda u_{kk}^2) \ , \tag{2.2a}$$

where the strain tensor $u_{ij}(\vec{r})$ is given in terms of the phonon displacement field $u_i(\vec{r})$,

$$u_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i}\right] \ , \tag{2.2b}$$

and μ and λ are "bare" elastic constants, unrenormalized by dislocations. Of course, real bulk crystalline solids are characterized by an anisotropic elasticity tensor. The extension to anisotropic media will be discussed later. Dislocation lines are characterized by a nonvanishing contour integral of the displacement field around such a line,

$$\oint du_i = -b_i \ , \tag{2.3}$$

which defines the Burger's vector $\vec{b}$. The direction of integration around the contour is that of a right-handed screw advancing parallel to a unit tangent vector $\vec{t}$ on the line. It is easily shown that the Burger's vector is constant along a line, and that Eq. (2.3) is equivalent to[42]

$$\epsilon_{ilm}\frac{\partial w_{mk}(\vec{r})}{\partial r_l} = -t_i b_k \delta^{(2)}(\vec{\xi}) \ , \tag{2.4}$$

where $\delta^{(2)}(\vec{\xi})$ is a two-dimensional δ function of the radius vector $\vec{\xi}$ taken from the axis of the dislocation line in a plane perpendicular to the tangent vector $\vec{t}$, and

$$w_{mk}(\vec{r}) = \frac{\partial u_k(\vec{r})}{\partial r_m} \ . \tag{2.5}$$

To study behavior at wavelengths long compared to the spacing between dislocation lines, we average over a small volume Ω_0 containing many dislocations (Fig. 4). Equation (2.4) becomes

$$\epsilon_{ilm}\frac{\partial w_{mk}(\vec{r})}{\partial r_l} = -\alpha_{ik}(\vec{r}) \ , \tag{2.6}$$

where $\alpha_{ik}(\vec{r})$ measure the density of Burger's vector "charge" carried by dislocation lines piercing Ω_0. This charge density tensor is defined such that its integral over a surface S spanning a contour C gives the sum of all Burger's vectors $\vec{b}^{(\alpha)}$ enclosed by that contour,

$$\oiint_S \alpha_{ij} n_i dA = -\sum_\alpha b_j^{(\alpha)} \ . \tag{2.7}$$

The unit vector $\vec{n}$ is normal to the surface, and the

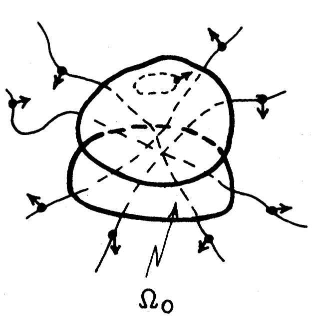

FIG. 4. Large but still microscopic averaging volume Ω_0 for a crystal pierced by many dislocation lines. Note that the Burgers vectors (arrows) carried by each line have a fixed direction. The closed loop in the volume makes no contribution to the dislocation line density tensor $\alpha_{ij}(\vec{r})$.

summation over α runs over those Burger's vectors encompassed by C. The strains $u_{ij}^{\text{sing}}(\vec{r})$ associated with a given complexion of dislocation lines are given by minimizing the free energy subject to the condition (2.6). We then decompose the strain field into $u_{ij}^{\text{sing}}(\vec{r})$ and a deviation $\phi_{ij}(\vec{r})$

$$u_{ij}(\vec{r}) = u_{ij}^{\text{sing}}(\vec{r}) + \phi_{ij}(\vec{r}) \ , \tag{2.8a}$$

where ϕ_{ij} is related to derivatives of a smoothly varying displacement field $\vec{\phi}(\vec{r})$,

$$\phi_{ij}(\vec{r}) = \frac{1}{2}\left[\frac{\partial \phi_i}{\partial r_j} + \frac{\partial \phi_j}{\partial r_i}\right] \ . \tag{2.8b}$$

The free energy associated with such a configuration is just

$$F_s = \frac{1}{2}\int d^3r\,(2\mu\phi_{ij}^2 + \lambda\phi_{kk}^2) + F_D \ , \tag{2.9}$$

where the dislocation part is[42]

$$F_D = -\frac{\mu}{8\pi}\int d^3r_1 \int d^3r_2\, \eta_{ij}(\vec{r}_1)|\vec{r}_1 - \vec{r}_2|\eta_{ij}(\vec{r}_2) - \frac{\mu\nu}{8\pi(1-\nu)}\int d^3r_1 \int d^3r_2\, \eta_{ii}(\vec{r}_1)|\vec{r}_1 - \vec{r}_2|\eta_{kk}(\vec{r}_2) \ . \tag{2.10}$$

Here, the tensor $\eta_{ij}(\vec{r})$ is related to the dislocation charge tensor,

$$\eta_{ij} = \frac{1}{2}\left[\epsilon_{ipl}\frac{\partial \alpha_{jl}}{\partial r_p} + \epsilon_{jpl}\frac{\partial \alpha_{il}}{\partial r_p}\right] \ , \tag{2.11}$$

and ν is Poisson's ratio,

$$\nu = \lambda/2(\mu + \lambda) \ . \tag{2.12}$$

The dislocation free energy may also be written in terms of the Fourier transformed charge-density tensor $\alpha_{ij}(\vec{q})$:

$$F_D = \frac{1}{2}\int \frac{d^3q}{(2\pi)^3}\left[\frac{\mu}{q^2}\left[Q_{ik}Q_{jl} + C_{il}C_{kj} + \frac{2\nu}{1-\nu}C_{ij}C_{kl}\right] + 2E_e\delta_{ik}\delta_{jl} + 2(E_s - E_e)\delta_{ij}\delta_{kl}\right]\alpha_{ij}(q)\alpha_{kl}(-q) \ . \tag{2.13}$$

The tensors Q_{ij} and C_{ij} are

$$Q_{ij} = \delta_{ij} - \frac{q_i q_j}{q^2} \ , \tag{2.14a}$$

$$C_{ij} = \epsilon_{ijl}q_l/q \ , \tag{2.14b}$$

and we have inserted edge and screw dislocation core energies per unit length E_e and E_s with contributions proportional to $|\vec{b}|^2$.

We would like to calculate statistical mechanical averages, weighted with e^{-F/k_BT}. One must integrate over the smoothly varying field $\phi_{ij}(\vec{r})$, and sum over distinct configurations of dislocation loops carrying a variety of allowed Burger's vectors. This second step is quite formidable in general, since $\alpha_{ij}(\vec{r})$ is made up of closed loops carrying discrete amounts of vector "charge." The calculation simplifies, however, if many different dislocation lines pierce the volume Ω_0. It then makes sense to integrate, rather than sum, over the allowed values of the charge-density tensor $\alpha_{ij}(\vec{r})$. The constraint that dislocation lines must either close or terminate at boundaries amounts to the condition,

$$\frac{\partial \alpha_{ij}(\vec{r})}{\partial r_i} = 0 \ . \tag{2.15}$$

The calculations become analogous to the statistical mechanics of magnetic fields subject to the constraint of no magnetic monopoles—magnetic field lines cannot start or stop inside the medium.

We are interested in the density of dislocation lines in the limit of large averaging volumes Ω_0, or, equivalently, at long wavelengths. Dislocation loops contained entirely within Ω_0 make no contribution to α_{ij}. If the number of loops drops off rapidly with increasing loop size, few lines will actually pierce large averaging volumes. The discrete nature of the Burger's vectors becomes important, and the approximation proposed above breaks down. Such a system presumably remains crystalline. Suppose, on the other hand, there is a finite density of "free" or "unbound" lines L_D which actually meander across the entire system. We can always ensure that a large number of these lines pierce Ω_0 by going to large averaging volumes. In this limit, we regard $\alpha_{ij}(\vec{r})$ as a continuous tensor field subject only to the constraint (2.15). A similar approximation was used in the theory of two-dimensional melting, to demonstrate the existence of the hexatic phase.[4] The approximation was called "Debye-Hückel theory," and the constraint analogous to Eq. (2.15) was overall Burger's vector charge neutrality. We identify the line density L_D of unbound loops with the quantity appearing in the viscosity estimate (2.1).

An analogous approximation may be applied to superfluid ^{4}He in the presence of unbound vortex rings. In Appendix A, we show explicitly that the rings cause the superfluid density (a quantity analogous to the elastic constants of a solid) to vanish. Thus, superfluid ^{4}He in the presence of unbound vortex rings is indeed a normal liquid, as originally suggested by Feynman.[24]

Here, we are interested in fluctuations in the bond-angle field

$$\theta_j(\vec{r}) = \tfrac{1}{2}\epsilon_{jkl} w_{kl}(\vec{r}) \ , \tag{2.16}$$

which gives the local twist in the material about different coordinate axes. Consider the singular part of the unsymmetrized strain tensor $w_{ij}^{\text{sing}}(\vec{r})$, defined as the solution of Eq. (2.6), subject to the condition

$$\partial_i \sigma_{ij} = 0 \ , \tag{2.17}$$

where $\sigma_{ij}(\vec{r})$ is the stress tensor. Inserting the decomposition

$$w_{jk}^{\text{sing}} = u_{jk}^{\text{sing}} + \epsilon_{jkl}\theta_l^{\text{sing}} \tag{2.18}$$

into Eq. (2.6), and solving for the Fourier transform $\theta_j^{\text{sing}}(\vec{q})$, we find

$$\theta_j^{\text{sing}}(\vec{q}) = \frac{-iq_k}{q^2}\alpha_{jk}(\vec{q}) + \tfrac{1}{2} i \frac{q_j}{q^2}\alpha_{kk}(\vec{q}) - \frac{iq_k q_m}{q^2}\epsilon_{jkl} u_{lm}^{\text{sing}}(\vec{q}) \ . \tag{2.19}$$

The last term in Eq. (2.19) vanishes, as can be seen by writing $u_{lm}^{\text{sing}}(\vec{r})$ in terms of the stress,[42]

$$u_{lm}^{\text{sing}} = \frac{1}{2\mu}\left(\sigma_{lm}^{\text{sing}} - \frac{\nu}{1+\nu}\sigma_{kk}^{\text{sing}}\delta_{lm}\right) \ , \tag{2.20}$$

and making use of Eq. (2.17). Combining the dislocation contribution to $\theta_j(\vec{r})$ with a part due to the smoothly varying background field $\vec{\phi}(\vec{r})$, we have finally

$$\theta_j(\vec{q}) = \tfrac{1}{2} i \epsilon_{jkl} q_k \phi_l(\vec{q}) - \frac{iq_k}{q^2}\alpha_{jk}(\vec{q}) + \tfrac{1}{2} i \frac{q_j}{q^2}\alpha_{kk}(\vec{q}) \ . \tag{2.21}$$

Making use of Eqs. (2.21) and (2.9), it is easy to see that

$$\langle \theta_i(q)\theta_j(-q)\rangle = \frac{k_B T}{4\mu}\left(\delta_{ij} - \frac{q_i q_j}{q^2}\right) + \frac{q_k q_l}{q^4}\langle \alpha_{ik}(q)\alpha_{jl}(-q)\rangle - \frac{1}{2}\frac{q_j q_k}{q^4}\langle \alpha_{ik}(q)\alpha_{ll}(-q)\rangle - \frac{1}{2}\frac{q_i q_l}{q^4}\langle \alpha_{kk}(q)\alpha_{jl}(-q)\rangle + \frac{1}{4}\frac{q_i q_j}{q^4}\langle \alpha_{kk}(q)\alpha_{ll}(-q)\rangle \ . \tag{2.22}$$

The first term comes from the smoothly varying phonon field $\vec{\phi}(\vec{r})$, while the remaining averages are to be evaluated in an ensemble specified by the dislocation free energy (2.13). It is tedious, but straightforward, to evaluate the charge correlation functions entering Eq. (2.22), provided $\alpha_{ij}(\vec{q})$ can be treated as the Fourier transform of a continuous tensor field. The constraint (2.15) is conveniently handled by adding a term

$$\tfrac{1}{2} M \int \frac{d^3 q}{(2\pi)^3}\left(\frac{q_i q_k}{q^2}\right)\alpha_{ij}(q)\alpha_{kj}(-q) \tag{2.23}$$

to Eq. (2.13), and taking the limit $M \to \infty$ at the end of the calculation. The correlation function which results is

$$\langle \alpha_{ij}(q)\alpha_{kl}(-q)\rangle = \left(\frac{k_B T}{4E_e}\right)(Q_{ik}Q_{jl} + C_{il}C_{jk} + 2Q_{ik}P_{jl}) + \frac{k_B T(E_e - E_s)}{2E_e(2E_s - E_e)}Q_{ij}Q_{kl} + \left(\frac{k_B T q^2}{4\mu}\right)\left(Q_{ik}Q_{jl} - C_{il}C_{jk} - \frac{2\lambda}{2\mu + 3\lambda}C_{ij}C_{kl}\right) \ , \tag{2.24}$$

where Q_{ij} and C_{ij} were defined previously, and

$$P_{ij}(\vec{q}) = q_i q_j / q^2 \ . \tag{2.25}$$

Upon inserting this expression into Eq. (2.22), we obtain the bond-angle correlation function, namely,

$$\langle \theta_i(\vec{q})\theta_j(-\vec{q})\rangle = \frac{k_B T}{(8E_s - 4E_e)q^2}P_{ij}(\vec{q}) + \left(\frac{k_B T}{4\mu} + \frac{k_B T}{2E_e q^2}\right)Q_{ij}(\vec{q}) \ . \tag{2.26}$$

Note that, as q tends to zero, all dependence on the bare elastic constants drop out.

At small wave vectors, $\langle \theta_i(q)\theta_j(-q)\rangle$ diverges like $1/q^2$. Evidently, the broken orientational symmetry of the crystal *remains* broken, even in the presence of a finite density of unbound dislocation loops. The loops are effective only in destroying the translational order, and driving the elastic constants to zero. We can summarize these conclusions by saying that there is a term in the long-wavelength free energy which resists deformations in $\vec{\theta}$, namely,

$$\delta F = \tfrac{1}{2}\int d^3 r \, [K_a(\vec{\nabla} \times \vec{\theta})^2 + K_b(\vec{\nabla} \cdot \vec{\theta})^2] \ . \tag{2.27}$$

The stiffness parameters K_a and K_b are analogous to the Frank constants in a nematic liquid crystal.[26] The free energy (2.27) is consistent with Eq. (2.26) at long wavelengths, provided

$$K_a = 2E_e, \quad K_b = 8E_s - 4E_e \ . \tag{2.28}$$

There is a residual resistance to torsion not present in an isotropic liquid. If the edge and screw dislocation core energies are approximately equal, both K_a and K_b are positive. Negative K_b means that higher order gradients must be taken into account in Eq. (2.28). We have not studied the spatial modulation of the bond-orientational order parameter which presumably occurs in this case. The generalization of these results to anisotropic solids is described in Appendix B.

The core energies per unit length entering Eq. (2.28) are long-wavelength quantities, and should be renormalized by the effect of short-wavelength fluctuations. We expect that, above the melting temperature, these quantities scale like a typical cross-sectional area divided by a typical length along the dislocation line. Just as in two dimensions,[4] one can argue that the characteristic length scale appropriate to unbound dislocations is the translational correlation length $\xi_+(T)$. This argument suggests that we can account for short-wavelength fluctuations by making the replacements,

$$E_e \to E_e(\xi_+/a) \ , \tag{2.29a}$$

$$E_s \to E_s(\xi_+/a) \ , \tag{2.29b}$$

in Eq. (2.29), where a is of order of the interparticle spacing.

III. TRANSITIONS OUT OF THE CUBIC LIQUID CRYSTAL PHASE

Evidently, a solid with a finite density of unbound dislocation loops is neither a solid nor a liquid. Here we discuss how such a material transforms into the solid and liquid states. Because there is a cubic broken rotational symmetry in bond orientations, we shall call this intermediate phase a "cubic liquid crystal." Although cubic liquid crystals may occur only rarely as equilibrium phases in nature, our discussion suggests they may be observable as metastable phases in supercooled liquids.

We shall consider transitions out of the cubic-liquid-crystal phase in the context of Landau's theory of phase transitions.[28] The transition directly from a liquid to a solid was originally considered by Landau himself.[24] The order parameter is composed of Fourier components of the density $\rho_{\vec{G}}(\vec{r})$ evaluated at a set of reciprocal-lattice vectors $\{\vec{G}\}$. In terms of the complex functions $\rho_{\vec{G}}(\vec{r})$, the density $\rho(\vec{r})$ of particles may be written[44]

$$\rho(\vec{r}) = \rho_0 + \mathrm{Re}\left[\sum_{\vec{G}} \rho_{\vec{G}}(\vec{r}) e^{i\vec{G}\cdot\vec{r}}\right] \ , \tag{3.1}$$

where ρ_0 is the density in a uniform liquid. The Fourier coefficients $\{\rho_{\vec{G}}(\vec{r})\}$, which vary slowly on a scale set by G^{-1}, have both an amplitude and a phase

$$\rho_{\vec{G}}(\vec{r}) = |\rho_{\vec{G}}(\vec{r})| e^{i\vec{G}\cdot\vec{u}(\vec{r})} \ . \tag{3.2}$$

Here, $\vec{u}(\vec{r})$ is the phonon displacement field in the solid. Landau observed that the expansion of the free energy in powers of the $\{\rho_G(\vec{r})\}$ admits third-order invariants, which in turn implies that three-dimensional melting is a first-order phase transition.[28,44]

A. Cubic-liquid-crystal–to–solid transition

It is easy to adapt Landau's analysis to the cubic-liquid-crystal–to–solid transition. We assume that the rotational symmetry of the liquid has already been broken, and that the system is characterized by a local set of rotation angles $\vec{\theta}(\vec{r})$, measured from a preferred orthonormal triad. The order parameter for this triad will be discussed in the next subsection. Density fluctuations leading to a crystal may be characterized by a discrete set of minimal reciprocal-lattice vectors $\{\vec{G}_\alpha\}$ with a fixed orientation relative to the preferred triad. (In a liquid, one must also consider a continuum of rotations of the $\{G_\alpha\}$.) If gradient terms are included in the free energy, care must be taken to ensure that the system is invariant under rotations. Upon rotating by a small amount $\vec{\theta}_0$, we have using Eq. (3.2) and the transformation properties of the phonon field,

$$\theta(\vec{r}) \to \theta(\vec{r}) + \theta_0 \ , \tag{3.3a}$$

$$\rho_{\vec{G}_\alpha}(\vec{r}) \to \rho_{\vec{G}_\alpha}(\vec{r}) \exp[i\vec{G}\cdot(\vec{\theta}_0 \times \vec{r})] \ . \tag{3.3b}$$

The rotationally invariant free energy density describing the tendency to form a solid is[45]

$$\begin{aligned}\mathfrak{F}_s = {} & \tfrac{1}{2}A \sum_\alpha |\vec{G}_\alpha \times (\vec{\nabla} - i\vec{G}_\alpha \times \vec{\theta})\rho_{\vec{G}_\alpha}|^2 + \tfrac{1}{2}B \sum_\alpha |\vec{G}_\alpha \cdot (\vec{\nabla} - i\vec{G}_\alpha \times \vec{\theta})\rho_{\vec{G}_\alpha}|^2 \\ & + \tfrac{1}{2}s \sum_\alpha |\rho_{\vec{G}_\alpha}|^2 + t \sum_{\substack{\alpha,\beta,\gamma \\ \vec{G}_\alpha+\vec{G}_\beta+\vec{G}_\gamma=0}} \rho_{\vec{G}_\alpha}\rho_{\vec{G}_\beta}\rho_{\vec{G}_\gamma} + O(\rho^4_{\vec{G}_\alpha}) + \tfrac{1}{2}K_a|\vec{\nabla}\times\vec{\theta}|^2 + \tfrac{1}{2}K_b(\vec{\nabla}\cdot\vec{\theta})^2 \ ,\end{aligned} \tag{3.4}$$

where s is assumed to decrease linearly with decreasing temperature, and t is a constant. The parameters A and B are related to the elastic constants of the solid which forms when, for sufficiently small s, we have

$$\langle \rho_{\vec{G}_\alpha} \rangle \neq 0 \ . \tag{3.5}$$

The Frank constants K_a and K_b are stiffnesses intrinsic to the cubic-liquid-crystal phase, and are the same as those entering Eq. (2.28). Since the expansion (3.4) admits a third-order invariant in $\rho_{\vec{G}_\alpha}$, where the $\{\vec{G}_\alpha\}$ are the minimal reciprocal lattice vectors appropriate to a bcc solid, the transition from liquid crystal to bcc solid is predicted to be first order.

Fluctuations sometimes lead to violations of the predictions of Landau theory. As discussed in Sec. III C, however, the cubic-liquid-crystal–to–bcc-solid transition probably remains first order, even in the presence of fluctuations. Well below the transition temperature, the gradient terms are minimized when $\theta(\vec{r})$ is locked to the curl of the phonon field,

$$\vec{\theta}(\vec{r}) = \tfrac{1}{2}[\vec{\nabla} \times \vec{u}(\vec{r})] \ . \tag{3.6}$$

Thus, translational and orientational order are not independent in a crystal.

Different crystal symmetries are represented by expansions of the form (3.4), but with different values of the couplings. Within mean-field theory, the precise crystal structure is determined by which t coupling first goes negative with decreasing temperature. Third-order terms are not possible for fcc and simple cubic lattices. Thus, transitions into these structures from the cubic-liquid-crystal phase could, in principle, be continuous.

A free energy expansion similar to Eq. (3.4) was constructed by de Gennes for the nematic–to–smectic-liquid-crystal transition.[46] Both theories resemble gauge-invariant free energies like that entering the phenomenological Landau-Ginzberg theory of superconductivity.[47] Here, the bond-orientation field plays the role of a vector potential, and the effect of a rotation is like a gauge transformation. It should be stressed, however, that neither theory is strictly gauge invariant. The only real symmetries are global translational and rotational invariance.

B. Liquid–to–cubic-liquid-crystal transition

The order parameter for the liquid–to–cubic-liquid-crystal phase transition was discussed in the Introduction. It consists of nine Fourier coefficients Q_{4m} measuring the deviation of the bond-angle field from isotropy [see Eq. (1.5)]. Close to equilibrium, we assume that the $Q_{4m}(\vec{r})$ vary smoothly on scales large compared to an interatomic spacing. The contribution of cubic-liquid-crystal fluctuations to the liquid free energy must be constructed from rotationally invariant combinations of the $Q_{4m}(\vec{r})$. There is only one quadratic invariant, namely,

$$I_2 = \sum_{m=-4}^{+4} |Q_{4m}|^2 \ . \tag{3.7}$$

Since a (unique) third-order invariant can be obtained from the Wigner $3j$ symbols,[48]

$$I_3 = \sum_{m_1+m_2+m_3=0} \begin{pmatrix} 4 & 4 & 4 \\ m_1 & m_2 & m_3 \end{pmatrix} Q_{4m_1} Q_{4m_2} Q_{4m_3} \ , \tag{3.8}$$

Landau theory predicts a first-order phase transition. As we shall see, this prediction may be altered by fluctuation effects.

Not all the Q_{4m} need be nonzero in a phase with a broken cubic rotational symmetry. In the right coordinate system, all the Q_{4m}'s will vanish except Q_{40} and $Q_{44} = Q_{4-4}$. In this special reference frame, corresponding to a singled out orthonormal triad, we have

$$I_2 = Q_{40}^2 + 2|Q_{44}|^2 \ . \tag{3.9}$$

Upon evaluating the $3j$ symbols, I_3 may be written

$$I_3 = I_2 \left[\operatorname{sgn}(Q_{40}) \frac{9+42z^2}{(1+2z^2)^{3/2}} \right] \ , \tag{3.10}$$

where

$$z = Q_{44}/Q_{40} \ . \tag{3.11}$$

If the transition is weakly first order, the ratio Q_{44}/Q_{40} is determined for fixed I_2 by minimizing the bracketed portion of Eq. (3.10). The minimum occurs when Q_{40} has a sign opposite that of the coefficient of the cubic term, and provided

$$|z| = \sqrt{5/14} \ . \tag{3.12}$$

Positive Q_{40} means that most bonds point along the cube axes, while negative Q_{40} signifies that they are predominantly along the cube diagonals.

To see how fluctuations affect the transition, it is convenient to introduce the traceless, symmetric fourth-rank tensor defined by Eqs. (1.7) and (1.8). The explicit connection between the two representations in the preferred coordinate system discussed above is

$$Q_{ijkl} e_i e_j e_k e_l = \sum_{m=-4}^{4} Q_{4m} Y_{4m}(\theta,\phi) = \sqrt{4\pi/9}\, Q_0 \{ \tfrac{2}{5} Y_{40}(\theta,\phi) + \sqrt{2/35} [Y_{44}(\theta,\phi) + Y_{4-4}(\theta,\phi)] \} \ . \tag{3.13}$$

Note that the ratio of the coefficients of $Y_{4\pm4}$ and Y_{40} is indeed $\sqrt{5/14}$. This ratio is an intrinsic feature of the cubic symmetry. The Landau free energy density is very similar to that describing the nematic to isotropic transition in liquid crystals.[26,27]

$$\mathfrak{F}_c = \tfrac{1}{2} K' (\vec{\nabla} Q_{ijkl})^2 + a Q_{ijkl}^2 + b Q_{ijkl} Q_{klmn} Q_{mnij} + O(Q^4) \ . \tag{3.14}$$

The coefficient a is assumed to change sign as temperature varies, while b is approximately temperature independent. The coefficient K' of the gradient term represents a one Frank constant approximation which sets $K_a = K_b$. The corresponding expression for nematic liquid crystals involves a traceless, symmetric second-rank tensor,

$$Q_{ij} = Q_0(n_i n_j - \tfrac{1}{3}\delta_{ij}) \ , \tag{3.15}$$

where Q_0 is the amplitude of the order parameter and $\vec{n}$ is a unit vector aligned with the nematogen axis. The third-order invariant present in the free energies of both systems suggests that these transitions are first order.[26,27]

C. Fluctuation Effects

The predictions of Landau theory for the cubic-liquid-crystal—to—liquid phase transition can be called into question, at least in the vicinity of two dimensions. Similar studies in $2+\epsilon$ dimensions[49–51] have illuminated the properties of spin systems. It is easy to see that fluctuations drive the critical temperature of the liquid—to—cubic-liquid-crystal phase transition to zero in precisely two dimensions. Fluctuations in the three Goldstone modes associated with the Euler angles of the order parameter triad prevent a genuine broken symmetry. Just above $d=2$, T_c is presumably very small, and well below the "mean-field" transition temperature associated with Eq. (3.14). In this limit, one can neglect fluctuations in the amplitude Q_0 of the order parameter defined by Eq. (3.18). Discarding a constant contribution, the free energy associated with (3.14) becomes

$$F_c = \tfrac{1}{2}K \int d^d r \, \{[\vec{\nabla}\vec{l}(\vec{r})]^2 + [\vec{\nabla}\vec{m}(\vec{r})]^2 + [\vec{\nabla}\vec{n}(\vec{r})]^2\} \ , \tag{3.16}$$

where

$$K = 4Q_0^2 K' \ . \tag{3.17}$$

The value of Q_0 is fixed by the polynomial part of Eq. (3.14). The partition function Z_c associated with Eq. (3.16) is obtained by integrating over all possible orthonormal triads $\vec{l}(\vec{r})$, $\vec{m}(\vec{r})$, and $\vec{n}(\vec{r})$. Discretizing space into a lattice of points $\{\vec{r}\}$, we have

$$\mathfrak{Z}_c = \prod_{\vec{r}} \left\{ 2\int_0^{\pi} [1-\cos\theta(\vec{r})]\, d\theta(\vec{r}) \int_0^{\pi} \sin[\vartheta(\vec{r})]\, d\vartheta(\vec{r}) \int_0^{2\pi} d\phi(\vec{r}) \right\} e^{-F_c/k_B T} \ . \tag{3.18}$$

At every point $\vec{r}$, we integrate over a set of rotations[52] from a reference triad $(\vec{l}_0, \vec{m}_0, \vec{n}_0)$. Each rotation is parametrized by an axis $\vec{N}(\vec{r})$ with polar angles $\vartheta(\vec{r})$ and $\phi(\vec{r})$, as well as by the amount rotated $\theta(\vec{r})$.

In principle, one could calculate the partition function (3.18) directly, using the methods described in Refs. 49–51. It is easier, however, to exploit the well-known homomorphism between the rotation group and SU(2).[53] Each orthonormal triad $(\vec{l}, \vec{m}, \vec{n})$ is replaced by a triplet of 2×2 complex matrices,

$$\vec{l} \rightarrow \vec{l}\cdot\vec{\sigma} = U^\dagger \sigma_x U \ , \tag{3.19a}$$

$$\vec{m} \rightarrow \vec{m}\cdot\vec{\sigma} = U^\dagger \sigma_y U \ , \tag{3.19b}$$

$$\vec{n} \rightarrow \vec{n}\cdot\vec{\sigma} = U^\dagger \sigma_z U \ . \tag{3.19c}$$

Here, $\vec{\sigma}$ is the vector of Pauli matrices, and we have brought the matrices into a canonical form by multiplying by a traceless Hermitian SU(2) matrix $U(\vec{r})$. In terms of the SU(2) matrices, the cubic-liquid-crystal free energy becomes, after some straightforward manipulations,

$$F_c = \tfrac{1}{2}(4K) \int d^d r \, \mathrm{Tr}(\vec{\nabla} U^\dagger \vec{\nabla} U) \ . \tag{3.20}$$

Each SU(2) matrix can be decomposed into a linear combination of the Pauli matrices and the identity[53]

$$U(\vec{r}) = x_0(\vec{r}) + i\vec{\sigma}\cdot\vec{x}(\vec{r}) \ , \tag{3.21a}$$

with

$$x_0^2 + |\vec{x}|^2 = 1 \ . \tag{3.21b}$$

In terms of the four-vector $x_\mu = (x_0, \vec{x})$, we have finally

$$F_c = \tfrac{1}{2}(8K) \int d^d r \, (\vec{\nabla} x_\mu)^2 \ . \tag{3.22}$$

Hence, the statistical mechanics of interacting orthonormal triads (neglecting amplitude fluctuations and in the one Frank constant approximation) is closely related to a theory of interacting four-component "spins," each with unit magnitude. The integration variables in Eq. (3.18) can be interpreted as the polar angles of these "spins."

We can now transcribe results tabulated for $n=4$ component spins in $2+\epsilon$ dimensions.[49–51] One finds that the cubic-liquid-crystal—to—liquid phase transitions is *continuous*, and occurs at a critical temperature

$$k_B T_c = 8\pi K(d-2) + O((d-2)^2) \ . \tag{3.23}$$

Note that the critical temperature vanishes as the dimension tends toward two from above. Just above this transition correlations in $Q_{ijkl}(\vec{r})$, should decay exponentially,

$$\langle Q_{ijkl}(\vec{r}) Q_{ijkl}(\vec{0}) \rangle \sim e^{-r/\xi_Q} \ , \tag{3.24}$$

with a diverging bond-orientational correlation length,

$$\xi_Q \sim |T - T_c|^{-\nu} \ . \tag{3.25}$$

The critical exponent ν has the expansion[50]

$$\nu^{-1} = d - 2 + \tfrac{1}{2}(d-2)^2 + \cdots \ ; \tag{3.26}$$

there are similar results for singularities in other quantities.

The critical behavior of cubic liquid crystals resembles that of four-component spins only in the limit that amplitude fluctuations are negligible. It is possible to treat cubic-liquid-crystal amplitude fluctuations perturbatively in $2+\epsilon$ dimensions,[54] and show formally that they are "irrelevant variables" in the sense used by Wilson and Kogut.[55] If T_c is not close to zero, however, the third-order invariant entering Eq. (3.14) may become important. There is, of course, no such third-order term in the Landau expansion for four-component spins. We cannot be certain that the cubic liquid crystal transition remains continuous all the way up to three dimensions. It is also worth emphasizing that the mapping of the rotation group onto SU(2) is not an isomorphism; the global properties of the two groups are different. Such differences manifest themselves in the $2+\epsilon$ expansion only in terms of order $\exp[-\text{const}/(d-2)]$. Even if the cubic-liquid-crystal phase transition remains continuous up to $d=3$, this transition could be in a universality class different from that of four-component spins.

It is instructive to consider the nematic-to-isotropic transition in $2+\epsilon$ dimensions as well. Neglecting amplitude fluctuations, the free energy associated with the order parameter (3.15) may be written

$$F_N = \tfrac{1}{2}K' \int d^2r\, |\vec{\nabla} Q_{ij}|^2 = \tfrac{1}{2}K \int d^2r\, (\vec{\nabla}\vec{n})^2 \ , \tag{3.27}$$

where $K = 2K'Q_0^2$. In this limit, the problem resembles a theory of interacting *three*-component spins. One would again predict a fluctuation-induced second-order phase transition near two dimensions, notwithstanding the third-order invariant appearing in the Landau theory of nematics. Experimentally, the nematic-to-isotropic transition is known to be first order in three dimensions.[26] The size of this transition is, however, anomalously small.[26,56] It is tempting to attribute this anomaly to fluctuations which drive the transition continuous near $d=2$. Presumably the transition becomes first order above a critical dimension d_c somewhat below $d=3$. Cubic liquid crystals have three low-energy Goldstone excitations (associated with Euler angles of the orthonormal triad), in contrast to two Goldstone modes associated with nematics. Thus, fluctuations should be even *more* effective in suppressing the first-order transition from liquids into bulk cubic liquid crystals. We believe that this transition is continuous or at most very weakly first order in three dimensions.

A similar situation arises in q-state Potts models as a function of continuous dimensionality.[57] For $q \geqslant 3$, such systems have a third-order invariant, and Landau theory predicts a first-order phase transition. Fluctuations drive the critical temperature of Potts models to zero in one dimension. Renormalization group studies have shown that all Potts models display second-order phase transitions sufficiently close to $d=1$.[58] These fluctuation-induced continuous transitions may again be attributed to the suppression of amplitude fluctuations. When amplitude fluctuations are introduced in the form of "vacancies," approximate renormalization schemes suggest that q-state Potts transitions become first order above a critical dimension $d_c(q) > 1$.[57] The three-state Potts transition actually remains continuous up to two dimensions. It is possible to treat cubic and nematic liquid-crystal phase transitions via an approximate recursion scheme due to Migdal and Kadanoff.[59] We are presently incorporating vacancies into this procedure, in order to determine the nature of these transitions over a range of dimensionalities between two and three. The results will appear in a future publication.[60]

One might also ask if fluctuations alter the cubic-liquid-crystal—to—bcc-solid transition. In our view, this is unlikely, although we have not investigated the problem in detail. In two dimensions, one does expect a continuous transition from hexatic to solid,[4] even though the corresponding Landau theory contains a third-order invariant.[45] Fluctuations are not strong enough to drive the melting temperature to zero, however. Fluctuations are generally more effective in systems with non-Abelian symmetries such as n-component Heisenberg spins with $n \geqslant 3$.[49–51] The translational symmetry of a solid is Abelian, and we expect that the corresponding Landau theory is reasonably trustworthy in three dimensions.

IV. PROPERTIES OF THE CUBIC-LIQUID-CRYSTAL PHASE

A. Observability in supercooled liquids

We have argued that cubic liquid crystals can condense from a liquid via a transition that is continuous or at most very weakly first order. This is an important conclusion, since it means that cubic liquid crystals may be observable in supercooled liquids, even if they occur only rarely in equilibrium. In Fig. 5, we show the free energy of a supercooled liquid schematically, as a function of a translational order parameter $|\rho_{\vec{G}}|$ and the bond-orientational order parameter Q_0. The system will remain near the metastable liquid minimum, provided there has been insufficient time to nucleate a fluctuation over the sad-

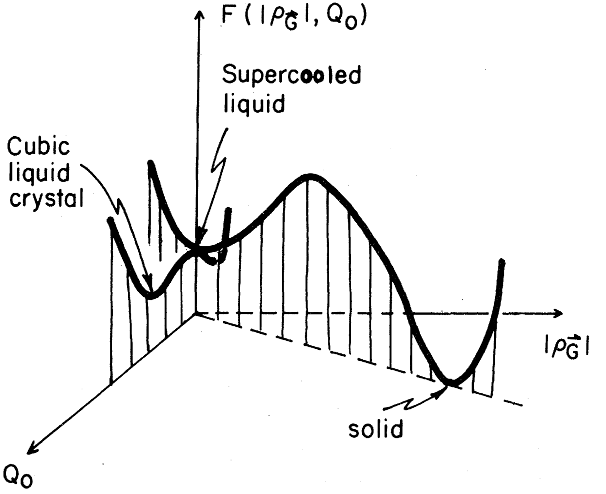

FIG. 5. Free energy F of a supercooled liquid, as a function of the translational order parameter $|\rho_{\vec G}|$ and the bond orientational order parameter Q_0. The solid phase is stable at this temperature. If a material remains liquid upon supercooling, it may eventually drop into the cubic liquid phase, as suggested by the figure.

dle point separating the liquid from the solid. We assume that the solid has a bcc lattice structure for simplicity. Note that both $|\rho_{\vec G}|$ and Q_0 are nonzero at the solid minimum. As shown in the figure, the system can drop upon sufficient supercooling into a metastable cubic-liquid-crystal phase, with no translational order, but with $Q_0 \neq 0$. We have assumed that the cubic liquid crystal is not present at the true melting temperature, i.e., when the liquid and solid minima have equal depths. In order to reach a cubic-liquid-crystal phase by supercooling, it is essential that it not be separated from the liquid by a large first-order transition.

It may be difficult to detect such a transition experimentally. If the phase change is continuous, there will be a weak singularity in the specific heat. Although the analogy with $n=4$ component spins may not carry over into three dimensions, it is interesting to note that the $n=4$ specific-heat exponent is[61]

$$\alpha(n=4) \approx -\tfrac{1}{3} \; . \tag{4.1}$$

The corresponding specific heat would be cusped. The specific-heat singularity associated with a weak first-order transition might also be difficult to observe experimentally. Other signatures of the cubic-liquid-crystal phase will be discussed below.

Figure 5 implies an intrinsic asymmetry in the limits of superheating and supercooling associated with three-dimensional melting. Once a supercooled liquid has dropped into the cubic-liquid-crystal phase, its free energy is lowered, and there will be an enhanced stability against fluctuations over the saddle point leading to a solid. According to this scenario, the cubic-liquid-crystal phase no longer exists by the time a heated solid becomes metastable. Thus, we expect a conventional limit of superheating, and an unconventional (large) limit of supercooling in the presence of a metastable cubic-liquid-crystal phase. Such an asymmetry has often been observed experimentally, but is usually attributed to surface effects.[62] Here, we predict an *intrinsic* asymmetry, present even when surface effects are unimportant.

B. X-ray structure function

Perhaps the most dramatic signature of the stacked hexatic smectic phase discussed in the Introduction is its in-plane x-ray-structure function (see Fig. 1). In-plane bond-orientational order is reflected in a sixfold angular modulation in reciprocal space. Here, we demonstrate an analogous angular modulation in the x-ray scattering from a monodomain cubic liquid crystal.

The x-ray-structure function measures fluctuations in the Fourier-transformed density $\hat\rho_{\vec q}$,

$$S(\vec q) = \langle |\rho_{\vec q}|^2 \rangle \; . \tag{4.2}$$

The coupling between density fluctuations and the bond-orientational order parameter Q_{ijkl} can be understood via a simple phenomenological model. The model makes sense provided density fluctuations at the wave vectors of interest decay rapidly on a scale set by variations in $Q_{ijkl}(\vec r)$. A modification of Eq. (3.14) which includes density fluctuations is the free energy density

$$\mathfrak{F}_d = \mathfrak{F}_c + \frac{1}{2} \int_{\Lambda_0 < q < \Lambda_1} \frac{d^3q}{(2\pi)^3} [A(q) |\hat\rho_{\vec q}|^2 + B(q) \hat q_i \hat q_j \hat q_k \hat q_l Q_{ijkl} |\hat\rho_{\vec q}|^2] \; . \tag{4.3}$$

The functions $A(q)$ and $B(q)$ depend only on the *magnitude* of $\vec q$, and $\hat q$ is a unit vector along $\vec q$. Only density fluctuations in an annulus of Fourier space $\Lambda_0 < |\vec q| < \Lambda_1$ have been considered. We take this annulus to encompass the interesting region surrounding the first maximum in the structure function of the liquid. Fluctuations in $\hat\rho_{\vec q}(\vec r)$ at each point $\vec r$ are assumed to be independent. The quantity $\hat\rho_{\vec q}(\vec r)$ is the average of $e^{i\vec q\cdot\vec R}\rho(\vec R)$ as $\vec R$ varies over a coarse graining volume Ω_0 centered at the point $\vec r$. Here, $\rho(\vec R)$ is the particle density.

If density fluctuations are integrated out of the partition function associated with Eq. (4.3), it can be shown that the resulting free energy functional, defined by

$$e^{-F_c'/k_BT}=\left[\prod_{\vec{r}}\prod_{\Lambda_0<q<\Lambda_1}\int d\hat{\rho}_{\vec{q}}(\vec{r})\right]\exp\left[-\int d^3r\,\frac{\mathfrak{F}_d}{k_BT}\right] \tag{4.4}$$

has the form of Eq. (3.14), with modified couplings $a,b,$ etc. It is also straightforward to evaluate

$$\begin{aligned}S(\vec{q})&=\langle|\hat{\rho}(\vec{q})|^2\rangle\\&=\left\langle\frac{1}{A(q)+B(q)\hat{q}_i\hat{q}_j\hat{q}_k\hat{q}_lQ_{ijkl}}\right\rangle_c\ .\end{aligned} \tag{4.5}$$

The subscript on the average means it is taken over by an ensemble with a cubic-liquid-crystal free energy of the form (3.14). Well below the cubic-liquid-crystal transition temperature, we can approximate Eq. (4.5) by

$$S(\vec{q})\approx\frac{1}{A(q)+B(q)\hat{q}_i\hat{q}_j\hat{q}_k\hat{q}_lQ^0_{ijkl}}\ , \tag{4.6}$$

where

$$Q^0_{ijkl}=\langle Q_{ijkl}(\vec{r})\rangle\ . \tag{4.7}$$

The function $A(q)$ presumably has a minimum in the range $\Lambda_0<q<\Lambda_1$ corresponding to the isotropic maximum in $S(q)$ which occurs when the material is a liquid. Provided $B(q)$ is well behaved in this region, Eq. (4.6) predicts an angular modulation in $S(\vec{q})$ near the liquid maximum associated with a nonzero bond-orientational order parameter. Whether the maxima occur predominantly along the cube axes or cube diagonals is determined by the sign of the third-order term in Eq. (3.14). We can also expand Eq. (4.5) in the spherical harmonics associated with the polar angles $\theta_{\vec{q}}$ and $\phi_{\vec{q}}$ of the vector $\vec{q}$,

$$\begin{aligned}S(\vec{q})=C_0(q)+\sum_{l=4}^{\infty}\sum_{m=-l}^{l}C_l(q)\langle Q_{lm}(\vec{r})\rangle_c\\\times Y^*_{lm}(\theta_{\hat{q}},\phi_{\hat{q}})\ .\end{aligned} \tag{4.8}$$

The coefficients of the Y_{lm}'s are functions $C_l(q)$ of the magnitude of $\vec{q}$ only, multiplied by expectations of the bond-angle order parameter, and its harmonics with $l>4$. Near the cubic-liquid-crystal—to—liquid transition, harmonics with $l>4$ should vanish rapidly compared to the $\langle Q_{4m}\rangle_c$. If this transition is truly continuous, the angular modulation in $S(\vec{q})$ then provides a direct experimental measure of the primary bond-orientational order parameter. As was discussed in Sec. III, one can always find a coordinate system such that only $Q_{4\pm4}$ and Q_{40} are nonzero. It would be interesting to test experimentally via x-ray scattering the prediction that, in this special frame of reference,

$$\left|\frac{Q_{4\pm4}}{Q_{40}}\right|=\sqrt{5/14}\ . \tag{4.9}$$

C. Hydrodynamics

The dynamics of cubic liquid crystals resembles that of nematic liquid crystals,[26] and provides in principle a way of distinguishing this phase from solids and liquids experimentally. Residual bond-angle order couples to the momentum density, and alters the transverse hydrodynamic excitations. Each transverse shear mode in the liquid is replaced by a pair of excitations whose frequencies vanish like q^2 at long wavelengths. Depending on the values of hydrodynamic parameters, these frequencies can be purely diffusive, or else acquire a real part proportional to q^2. The transverse part of the hydrodynamics is very similar to that worked out for the hexatic phase in two dimensions.[63]

We start with a generalization of Eq. (2.28) which includes transverse momentum fluctuations, namely,

$$\begin{aligned}\bar{F}=\tfrac{1}{2}\int d^3r\,[K_a|\vec{\nabla}\times\vec{\theta}|^2+K_b(\vec{\nabla}\cdot\vec{\theta})^2]\\+\frac{1}{2\rho_0}\int d^3r\,|\vec{g}_T|^2\ ,\end{aligned} \tag{4.10}$$

where $\vec{g}_T(\vec{r})$, the transverse part of the momentum density, satisfies

$$\vec{\nabla}\cdot\vec{g}_T=0\ . \tag{4.11}$$

Within linearized hydrodynamics, the bond-angle field decouples from the longitudinal degrees of freedom. The quantity ρ_0 is the equilibrium mass density. Hydrodynamics for systems with broken symmetries begins by considering nonzero "Poisson brackets" between quantities at long wavelengths. Nonzero Poisson brackets imply reversible dynamic couplings,[64] just as nonvanishing commutation relations do in quantum mechanics. Since $\vec{\theta}$ is the generator of rotations in $\vec{g}$, we have the Poisson bracket

$$[g_i,\theta_j]_{\text{PB}}=\tfrac{1}{2}\epsilon_{ijk}\frac{\partial}{\partial r_k}\ . \tag{4.12}$$

The dynamics must then be supplemented with all irreversible couplings consistent with the underlying symmetries and conservation laws.

The cubic-liquid-crystal hydrodynamics which results from the above procedure can be summarized by the equations,

$$\begin{aligned}\frac{\partial\vec{g}_T(\vec{r},t)}{\partial t}=-\tfrac{1}{2}\vec{\nabla}\times\frac{\partial\bar{F}}{\partial\vec{\theta}(\vec{r},t)}\\-\eta\nabla^2\frac{\delta\bar{F}}{\delta\vec{g}(\vec{r},t)}+\vec{\zeta}(\vec{r},t)\ ,\end{aligned} \tag{4.13a}$$

$$\begin{aligned}\frac{\partial\vec{\theta}(\vec{r},t)}{\partial t}=\tfrac{1}{2}\vec{\nabla}\times\frac{\delta\bar{F}}{\delta\vec{g}(\vec{r},t)}\\-\Gamma\frac{\delta\bar{F}}{\delta\vec{\theta}(\vec{r},t)}+\vec{\Upsilon}(\vec{r},t)\ .\end{aligned} \tag{4.13b}$$

The functions $\vec{\zeta}(\vec{r},t)$ and $\vec{Y}(\vec{r},t)$ are Gaussian Langevin noise sources designed to bring the system into thermal equilibrium. Upon Fourier transforming in space, their autocorrelations may be written

$$\langle \zeta_i(\vec{q},t)\zeta_j(\vec{q}\,',t')\rangle = 2\eta k_B T q^2\left(\delta_{ij} - \frac{q_i q_j}{q^2}\right) \times \delta(\vec{q}+\vec{q}\,')\delta(t-t') \ , \tag{4.14a}$$

$$\langle Y_i(\vec{q},t)Y_j(\vec{q}\,',t')\rangle = 2\Gamma k_B T\delta_{ij} \times \delta(\vec{q}+\vec{q}\,')\delta(t-t') \ . \tag{4.14b}$$

The first term in Eq. (4.13a) shows that the fluid moves to relax inhomogeneities in the bond-angle field, while the corresponding term in Eq. (4.13b) causes the bond-angle field to process at a rate determined by the local vorticity. The quantity η is the dynamic shear viscosity, while Γ is a relaxational kinetic coefficient. It is straightforward to demonstrate that Fokker-Planck equation associated with Eqs. (4.13) relaxes to a probability distribution proportional to e^{-F/k_BT}.

The equations (4.13) are most easily solved by Fourier transforming in space, and decomposing $\vec{\theta}(\vec{q},t)$ in transverse and longitudinal parts,

$$\vec{\theta}_T(\vec{q},t) = \vec{q} \times \vec{\theta}(\vec{q},t)/q \ , \tag{4.15a}$$

$$\theta_L(\vec{q},t) = \vec{q}\cdot\vec{\theta}(\vec{q},t)/q \ . \tag{4.15b}$$

Neglecting the Langevin noise sources, we have

$$\frac{\partial \vec{g}_T(\vec{q},t)}{\partial t} = -\tfrac{1}{2} i K_a q^3 \vec{\theta}_T(\vec{q},t) - \nu q^2 \vec{g}_T(\vec{q},t) \ , \tag{4.16a}$$

$$\frac{\partial \vec{\theta}_T(\vec{q},t)}{\partial t} = -\frac{1}{2\rho_0} i q \vec{g}_T(\vec{q},t) - \kappa_a q^2 \vec{\theta}_T(\vec{q},t) \ , \tag{4.16b}$$

$$\frac{\partial \theta_L(\vec{q},t)}{\partial t} = -\kappa_b q^2 \theta_L(\vec{q},t) \ , \tag{4.16c}$$

where

$$\nu = \eta/\rho_0 \tag{4.17}$$

is the kinematic viscosity, and we have defined two other quantities with the dimensions of diffusion constants,

$$\kappa_a = \Gamma K_a, \quad \kappa_b = \Gamma K_b \ . \tag{4.18}$$

There is one longitudinal eigenfrequency

$$\omega_L(q) = -\kappa_b q^2 i \ , \tag{4.19}$$

and two pairs of transverse eigenmodes $\omega_\pm(q)$ whose properties depend on the sign of

$$\Delta = \frac{K_a}{\rho_0} - (\nu - \kappa_a)^2 \ . \tag{4.20}$$

For positive Δ, these eigenfrequencies acquire a real part,

$$\omega_\pm(q) = \pm\tfrac{1}{2}\sqrt{\Delta}q^2 - \tfrac{1}{2}(\nu + \kappa_a)q^2 i \ , \tag{4.21}$$

while, for Δ negative, they are purely diffusive,

$$\omega_\pm(q) = -\tfrac{1}{2}(\nu + \kappa_a \pm \sqrt{|\Delta|})q^2 i \ . \tag{4.22}$$

It is difficult to decide between these two possibilities without knowing the relaxational kinetic coefficient Γ. At present, all we can say is that frequencies with a nonzero real part are favored when K_b is large.

Physically, one would expect the effective shear viscosity in a cubic liquid crystal to be larger than in a liquid, since there are twice as many transverse modes available to dissipate energy. An effective viscosity can be defined in terms of the transverse momentum correlation function,

$$\nu_{\text{eff}} = \lim_{q\to 0}\lim_{\omega\to 0}\left(\frac{q^2\langle|\vec{g}_T(\vec{q},\omega)|^2\rangle}{4k_B T\rho_0}\right)^{-1} \ . \tag{4.23}$$

Alternatively, one can consider a conventional macroscopic viscosity experiment with the bond orientations pinned at the walls, as was done in Appendix A of Ref. 63. In either case, one finds an effective long-wavelength shear viscosity,

$$\nu_{\text{eff}} = \nu[1 + (1/4\rho_0\Gamma\nu)] \ , \tag{4.24}$$

which is increased over the value it would have in a liquid.

At the level of linearized hydrodynamics, a cubic liquid crystal has propagating longitudinal sound and thermal diffusion modes similar to those in a liquid. Mode coupling nonlinearities, however, allow compressional sound to decay into coupled bond-angle–vorticity excitations. Near the phase transition to a liquid, where the transverse modes probably exhibit critical slowing down, one might expect an anomaly of the sound absorption due to these nonlinear effects.

V. MELTING OF SMECTIC-*A* LIQUID CRYSTALS

As discussed in the Introduction, it has been suggested that the smectic-*A*–to–nematic transition is actually driven by an unbinding of dislocation loops.[36] Differences between layered systems and crystalline solids are reflected in the continuum elastic free energy appropriate to smectics *A*, namely,[26]

$$F_s = \tfrac{1}{2}\int d^3r \left[B\left(\frac{\partial u}{\partial z}\right)^2 + K_1\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)^2\right] \ , \tag{5.1}$$

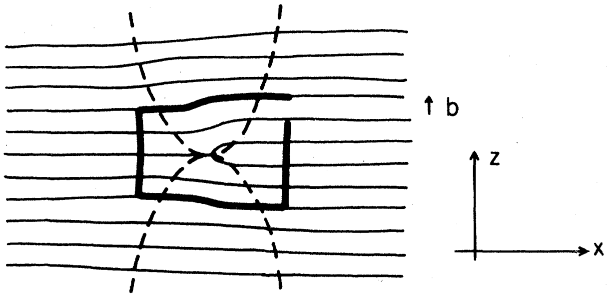

FIG. 6. Cross section of an edge dislocation in a smectic-*A* liquid crystal. The heavy line shows the construction which defines a Burger's vector of magnitude *b*, and always points along the *z* axis. The dashed parabolas bound a region of maximum strain. In a coordinate system centered at the dislocation, these lines are given by $z = \pm x^2/\lambda$.

which should be contrasted with Eq. (2.2). Here, $u(\vec{r})$ is a displacement from a density wave in the $\hat{z}$ direction. The quantities B and K_1 are elastic constants parametrizing the parabolic continuum elastic theory embodied in Eq. (5.1). It can be shown that there is no true long-range translational order in three dimensions; instead, translational correlations decay algebraically to zero. In contrast to crystalline solids, the energy per unit length of dislocation line in a smectic *A* is *finite;* a cross section of an edge dislocation line is shown in Fig. 6. As pointed out by Helfrich,[36] the energy and entropy of an isolated dislocation loop both grow linearly with the loop perimeter. He predicts a continuous phase transition when the free energy of such an excitation changes sign. This argument is similar to a heuristic one constructed for two-dimensional melting by Kosterlitz and Thouless.[2]

Here we show explicitly that a smectic *A* with a finite concentration of unbound dislocations behaves like a nematic, with Frank constants K_2 and K_3 that depend on the edge and screw dislocation core energies. When expressed in terms of correlation lengths parallel and perpendicular to the layering, K_2 and K_3 behave as predicted by the anisotropic scaling theory of Lubensky and Chen.[38] We also argue that, in precisely three dimensions, this picture of the transition implies that

$$\xi_\parallel \propto \xi_\perp^2 \ . \tag{5.2}$$

This relation sharpens the predictions of anisotropic scaling,[38,39] and allows more detailed confrontations with experiment.

A. Smectic-*A* liquid crystals with unbound dislocation loops

Dislocation lines[65] in a smectic *A* carry Burgers's vectors which point perpendicular to the layering (see Fig. 6). As a line twists and turns, it acquires both an edge and screw character. The magnitude of the Burger's vector is determined by a contour integral around the line of the displacement in the $\hat{z}$-direction

$$\oint du = -b \ . \tag{5.3}$$

It is convenient to introduce a strain field $\vec{w}(\vec{r})$ which, in the absence of dislocations, is just the gradient of the displacement,

$$\vec{w}(\vec{r}) = \vec{\nabla} u(\vec{r}) \ . \tag{5.4}$$

As can be seen from Eq. (5.3), $\vec{w}(\vec{r})$ acquires a nonzero curl in the presence of dislocations. Introducing a vector dislocation charge density $\vec{B}(\vec{r})$, we have the relation,

$$\vec{\nabla} \times \vec{w}(\vec{r}) = -\vec{\mathcal{B}}(\vec{r}) \ , \tag{5.5}$$

where the integral of $\vec{B}(\vec{r})$ over a surface S gives the total Burger's "charge" $\sum_\alpha b^{(\alpha)}$ piercing that surface,

$$\iint_S \vec{\mathcal{B}} \cdot \vec{n}\, dA = -\sum_\alpha b^{(\alpha)} \ . \tag{5.6}$$

The requirement that dislocation lines not stop or start in the interior of the medium amounts to the constraint,

$$\vec{\nabla} \cdot \vec{\mathcal{B}}(\vec{r}) = 0 \ . \tag{5.7}$$

Passing to Fourier-transformed variables, the solution of Eq. (5.5) may be written

$$\vec{w}(\vec{q}) = \frac{-i\vec{q} \times \vec{\mathcal{B}}(\vec{q})}{q^2} + i\vec{q}\,\psi(\vec{q}) \ , \tag{5.8}$$

where $\psi(\vec{q})$ is an as yet undetermined function. For a given configuration of dislocation lines, $\vec{w}(\vec{r})$ must minimize Eq. (5.1), which amounts to the condition,

$$\frac{\partial w_z}{\partial z} = \lambda^2 \nabla_\perp^2 (\vec{\nabla}_\perp \cdot \vec{w}_\perp) \ , \tag{5.9a}$$

where

$$\lambda^2 = K_1/B \ . \tag{5.9b}$$

The operator $\vec{\nabla}_\perp$ is a gradient acting perpendicular to the $\hat{z}$ direction, and $\vec{w}_\perp$ consists of the corresponding perpendicular components of $\vec{w}$. Equation (5.9) suffices to determine $\psi(\vec{q})$,

$$\psi(\vec{q}) = \frac{q_z}{q^2(q_z^2 + \lambda^2 q_\perp^4)} \times (1 - \lambda^2 q_\perp^2)\hat{z} \cdot [\vec{q} \times \vec{\mathcal{B}}(\vec{q})] \ . \tag{5.10}$$

Equations (5.8) and (5.10) now completely specify the singular part of the strain in the presence of dislocation lines.

Just as in our discussion of solids, we break up a configuration of displacements in thermal equilibrium into a part due to dislocations and a smoothly varying background field $\phi(\vec{r})$. The elastic free energy becomes

$$F_s=\frac{1}{2}B\int d^3r\left[B\left(\frac{\partial\phi}{\partial z}\right)^2+K_1\left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}\right)^2\right]+F_D\ ,\tag{5.11}$$

where

$$F_D=\frac{1}{2}B\int d^3r\,[w_z^2+\lambda^2(\vec{\nabla}_\perp\cdot\vec{w}_\perp)^2]\ .\tag{5.12}$$

Here, $\vec{w}(\vec{r})$ represents the singular part of the strain only. The dislocation part of the free energy is most conveniently evaluated in Fourier space. Making use of Eq. (5.9a), we find

$$\begin{aligned}F_D&=\frac{1}{2}B\int\frac{d^3q}{(2\pi)^3}[\,|w_z(q)|^2+\lambda^2|\vec{q}_\perp\cdot\vec{w}_\perp(q)|^2]\\&=\frac{1}{2}B\int\frac{d^3q}{(2\pi)^3}\left(\frac{q_z^2+\lambda^2q_\perp^4}{\lambda^2q_\perp^4}\right)|w_z(q)|^2\ .\end{aligned}\tag{5.13}$$

According to Eqs. (5.8) and (5.10), the function $w_z(\vec{q})$ is

$$w_z(\vec{q})=\frac{-i\lambda^2q_\perp^2\hat{z}\cdot[\vec{q}\times\vec{\mathcal{B}}(\vec{q})]}{q_z^2+\lambda^2q_\perp^4}\ ,\tag{5.14}$$

so we have finally

$$F_D=\frac{1}{2}\int\frac{d^3q}{(2\pi)^2}\left(\frac{K_1|\hat{z}\cdot[\vec{q}\times\vec{\mathcal{B}}(\vec{q})]|^2}{q_z^2+\lambda^2q_\perp^4}+2E_s|\mathcal{B}_z(q)|^2+2E_s|\vec{\mathcal{B}}_\perp(\vec{q})|^2\right)\ .\tag{5.15}$$

We have supplemented the elastic contribution to the dislocation free energy with phenomenological screw and edge core energies E_s and E_e. The screw dislocation core contribution is assumed proportional to the square of the projection of the lines into the $\hat{z}$ direction, while edge dislocations contribute proportionally to the square of the part of $\vec{\mathcal{B}}(\vec{q})$ which lies perpendicular to this direction.

The statistical mechanics associated with Eq. (5.11) follows from integrating e^{-F_s/k_BT} over the smooth phonon field $\phi(\vec{r})$ and over different configurations of dislocation loops. Adapting the discussion for solids with dislocations presented in Sec. II, we imagine that a finite density of "unbound" dislocation loops actually stretch across the entire system. At long enough wavelengths, it then becomes permissible to treat $\vec{\mathcal{B}}(\vec{q})$ as the Fourier transform of a continuous vector field subject only to the constraint $\vec{q}\cdot\vec{\mathcal{B}}(\vec{q})=0$. We are interested in fluctuations in the angles $\theta_x(\vec{r})$ and $\theta_y(\vec{r})$ describing deviations of the smectic layer normal from the $\hat{z}$ direction. It is easily seen that, for small deviations,

$$\begin{aligned}\theta_x(\vec{q})&=-w_x(\vec{q})-iq_x\phi(\vec{q})\ ,\\\theta_y(\vec{q})&=-w_y(\vec{q})-iq_y\phi(\vec{q})\ .\end{aligned}\tag{5.16}$$

It is tedious, but straightforward to evaluate correlations between $\theta_x(\vec{q})$ and $\theta_y(\vec{q})$ in the presence of unbound dislocation loops, making use of Eqs. (5.8), (5.10), (5.15), and (5.16). One finds that the fluctuations are described by a nematic-like free energy,

$$\begin{aligned}F_N=\frac{1}{2}\int\frac{d^3q}{(2\pi)^3}[\,&(K_1q_x^2+2E_sq_y^2+2E_eq_z^2)|\theta_x(\vec{q})|^2+(K_1q_y^2+2E_sq_x^2+2E_eq_z^2)|\theta_y(\vec{q})|^2\\&-2(2E_s-K_1)q_xq_y\theta_x(\vec{q})\theta_y(-\vec{q})]\ .\end{aligned}\tag{5.17}$$

The expected form for a nematic free energy characterized by a director field $\vec{n}(\vec{r})$ is[26]

$$F_N=\frac{1}{2}\int d^3r\,\{K_1(\vec{\nabla}\cdot\vec{n})^2+K_2[\vec{n}\cdot(\vec{\nabla}\times\vec{n})]^2+K_3|\vec{n}\times(\vec{\nabla}\times\vec{n})|^2\}\ .\tag{5.18}$$

Assuming alignment in the $\hat{z}$ direction and making the identifications

$$\theta_x(\vec{r})=\delta n_x(\vec{r}),\quad\theta_y(\vec{r})=\delta n_y(\vec{r})\ ,\tag{5.19}$$

we find that Eqs. (5.17) and (5.18) are consistent for small

$$\delta n\equiv\vec{n}-\hat{z}\ ,\tag{5.20}$$

provided the Frank constants K_2 and K_3 are

$$K_2=2E_s,\quad K_3=2E_e\ .\tag{5.21}$$

A smectic with a finite density of unbound dislocation loops does indeed behave like a nematic. The calculation is completely analogous to the one carried out for solids in Sec. II.

We expect nematiclike behavior at wavelengths long compared to the distance between unbound dislocations. The long-wavelength elastic constants and core energies should be renormalized by fluctuations at shorter length scales. Suppose the medium behaves like a smectic out to a translational correlation length $\xi_\parallel$ in the $\hat{z}$ direction, and a length $\xi_\perp$ perpendicular to this direction. The core energy per unit length of a screw dislocation should scale proportionally with $\xi_\perp^2$ and inversely with $\xi_\parallel$. This suggests the replacement

$$E_s \to (\xi_\perp^2/\xi_\parallel a)E_s \ , \qquad (5.22)$$

where E_s now signifies a microscopic core energy, and a is a microscopic length. A similar argument for edge dislocations gives

$$E_e \to (\xi_\perp \xi_\parallel/\xi_\perp a)E_e = (\xi_\parallel/a)E_e \ , \qquad (5.23)$$

where E_e is again microscopic quantity. Our final result for the Frank constants K_2 and K_3 is thus

$$K_2 = 2E_s\xi_\perp^2/\xi_\parallel a, \quad K_3 = 2E_e\xi_\parallel/a \ . \qquad (5.24)$$

The correlation length dependence agrees with the anisotropic scaling theory of Lubensky and Chen.[38] No singularity is expected in the elastic constant K_1, which remains finite below T_c.

B. Anisotropic scaling

There is, at present, no first-principles theory of the smectic A to nematic transition. Lubensky and Chen[38] have constructed a general scaling theory which allows for different power law divergences in translation correlation lengths parallel and perpendicular to the ordering. Analogous predictions for the dynamics have been given by Swift and Mulvaney.[39] If a finite density of unbound dislocation line is the dominant mechanism for breaking up translational order above T_c, the two anisotropic scaling correlations lengths have a definite relation.

The amount of unbound dislocation line can be parametrized by the areal densities n_s and n_e of screw and edge dislocations contained in planes oriented perpendicular and parallel to the z axis. Implicit in the scaling analysis leading to Eqs. (5.23) and (5.24) are the relations

$$n_s \approx 1/\xi_\perp^2 \ , \qquad (5.25)$$

$$n_e = 1/\xi_\parallel \xi_\perp \ . \qquad (5.26)$$

Thus, unbound screw dislocation lines are on average a distance $\xi_\perp$ apart, while unbound edge dislocation lines are separated by $\xi_\parallel$ in the z direction and by $\xi_\perp$ in the smectic planes.

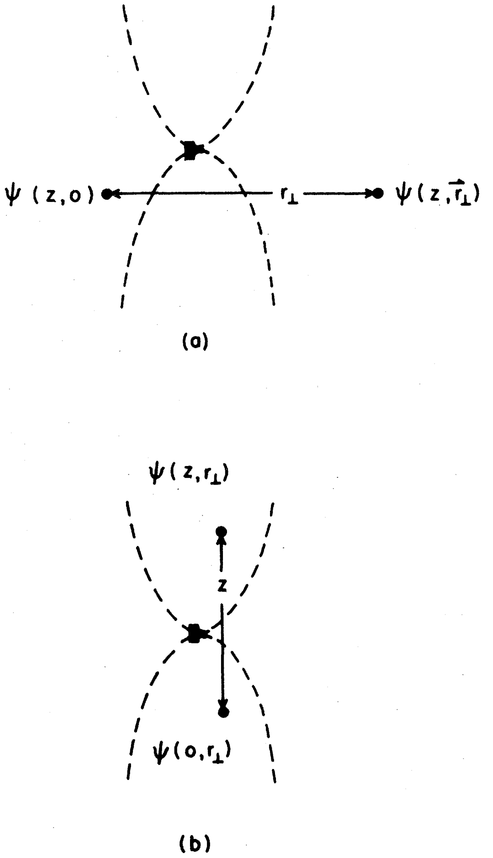

FIG. 7. Effect of an edge dislocation in decorrelating translational order. In (a), the points being considered must be on opposite sides of the parabolic regions of maximum strain to be significantly dephased by the dislocation. For fixed $\vec{r}_\perp$, an edge dislocation will have this effect if it pierces the plane of the figure anywhere in a region of area $r_\perp^3/\lambda$. In (b), the two points must both be within the parabolas, but on opposite sides of the dislocation, to be affected. Dephasing will occur if the edge dislocation pierces a region of area $z(z\lambda)^{1/2}$.

To derive a relation between $\xi_\parallel$ and $\xi_\perp$, consider first the decay of correlations in the translational order parameter

$$\psi(\vec{r}) \propto e^{iq_0 u(\vec{r})} \ , \qquad (5.27)$$

where q_0 is a wave vector which specifies the layering in the $\hat{z}$ direction. We first examine the correlation

$$G(\vec{r}_\perp, z) = \langle \psi^*(\vec{r}_\perp, z)\psi(\vec{0}, 0)\rangle \ , \qquad (5.28)$$

where $\vec{r} \equiv (\vec{r}_\perp, z)$, for the special case of separations perpendicular to the $\hat{z}$ direction. As shown in Fig. 7(a), an edge dislocation will decorrelate $G(\vec{r}_\perp, 0)$ if it falls in an elongated region between the two points in question. If $\psi^*(\vec{r}_\perp, 0)$ and $\psi(\vec{0}, 0)$ are on opposite sides of the parabolic region of maximum stress associated with a straight edge dislocation, they will be 180° out of phase. For the dislocation in Fig. 6, the region of maximum stress is bounded by the lines $z = \pm x^2/\lambda$. Thus, an edge dislocation line must pierce a region of cross-sectional area $r_\perp^3/\lambda$ in order to significantly reduce $G(\vec{r}_\perp, 0)$. A straight screw dislocation [which would run vertically in Fig. 7(a)] whose projection onto the plane of Fig. 7 cuts $\vec{r}_\perp$, can also decorrelate $G(\vec{r}_\perp, 0)$. Any screw dislocation within $r_\perp$ of the plane of the figure will have this effect. Thus, the probability that either an edge or screw dislocation will dephase correlations at a separation $r_\perp$ is

$$n_e r_\perp^3/\lambda + n_s r_\perp^2 \ . \tag{5.29a}$$

We expect that this probability is of order unity when $r_\perp = \xi_\perp$, which gives

$$n_e \xi_\perp^3/\lambda + n_s \xi_\perp^2 = 1 \ . \tag{5.29b}$$

A second relation follows from considering the correlations in the z direction as shown in Fig. 7(b). Only edge dislocations are significant in decorrelating $G(0,z)$. The two points being correlated must now fall on opposite sides of the dislocation core itself, but *within* the parabolic region of maximum stress. The probability that $G(0,z)$ is decorrelated is now

$$n_e z(z\lambda)^{1/2} \ . \tag{5.30a}$$

Since $G(0,z)$ will be dephased with unit probability when $z = \xi_\parallel$, we require

$$n_e \xi_\parallel^{3/2} \lambda^{1/2} \approx 1 \ . \tag{5.30b}$$

Combining Eqs. (5.30b) and (5.26), we find the desired relation between $\xi_\parallel$ and $\xi_\perp$, namely,

$$\xi_\parallel \sim \xi_\perp^2/\lambda \ . \tag{5.31}$$

Inserting this result, together with Eqs. (5.25) and (5.26), into the relation (5.29b), we find that *both* edge and screw dislocations contribute to dephasing $G(r_\perp, 0)$. An identical relation between parallel and perpendicular translational correlation lengths was found for the nematic to smectic-A "transition" which occurs at $T=0$ in two dimensions.[66]

Some predictions of anisotropic scaling in three dimensions are tabulated below,[38]

$$K_2 \sim \xi_\perp^2/\xi_\parallel, \quad K_3 \sim \xi_\parallel \ , \tag{5.32a}$$

$$B \sim \xi_\parallel/\xi_\perp^2, \quad D \sim \xi_\parallel^{-1} \ . \tag{5.32b}$$

The quantities K_2 and K_3 are the Frank constants discussed in the previous subsection, and B is the smectic elastic constant appearing in Eq. (5.1). The parameter D is related to the penetration depth for bend and twist deformations in the smectic. According to Eq. (5.31), both K_2 and B should be finite at T_c. "Corrections to scaling" terms would superimpose cusps on these quantities. Although there is some experimental evidence for anisotropic scaling,[37] the existing data on K_2, K_3, B, and D are not completely consistent with either Eq. (5.32) or the specific relation (5.31).

It is possible to measure $\xi_\parallel$ and $\xi_\perp$ directly, via x-ray scattering.[37] Upon parametrizing these diverging correlation lengths as in Eq. (1.10), anisotropic scaling suggests a specific relation between $\nu_\parallel$, $\nu_\perp$, and the specific-heat exponent α, namely,[67]

$$2\nu_\perp + \nu_\parallel = 2 - \alpha \ . \tag{5.33}$$

Taking the representative value $\alpha \approx 0.24$ from the experiments of Garland *et al.*,[67] we find using Eq. (5.31) that

$$\nu_\parallel \approx 0.88, \quad \nu_\perp \approx 0.44 \ . \tag{5.34}$$

The experimentally observed exponents[37] do not exhibit quite so pronounced an anisotropy. The value $\alpha \approx 0.0$ obtained by Johnson *et al.*[68] leads to an even larger difference between $\nu_\parallel$ and $\nu_\perp$. Hopefully, more precise experiments in the future will unambiguously confirm or deny the anisotropic scaling results (5.32), and the specific prediction (5.31) of the dislocation loop mechanism.

There is another reason to believe that $\xi_\parallel \propto \xi_\perp^2$ in precisely three dimensions. In Appendix C we show using Josephson-like scaling arguments[40] that, for $d > 3$,

$$B \sim \xi_\parallel/\xi_\perp^{d-1}, \quad K_1 \sim \xi_\perp^{5-d}/\xi_\parallel \ . \tag{5.35}$$

The result for B agrees with anisotropic scaling.[38] The behavior of K_1 is surprising, since K_1 is not expected to diverge on physical grounds.[37,38] In order for K_1 to remain finite at T_c, we must have

$$\xi_\parallel \propto \xi_\perp^{5-d} \ , \tag{5.36}$$

which agrees with Eq. (5.31) in the limit $d \to 3+$.

Lubensky and Chen have analyzed a variety of possible fixed points relevant to the smectic-A—to—nematic transition, to lowest order in the $\epsilon = 4-d$ expansion.[38] Near four dimensions, they find the first-order transition predicted by earlier studies.[69] A small first-order transition, of course, cannot be ruled out experimentally. Another possibility is a "superconducting fixed point," with $K_1 = 0$. Lubensky and Chen emphasized crossover effects related to an unstable fixed point with $K_1 = \infty$. They uncovered yet another fixed point, which although physically inaccessible to lowest order in ϵ, has precisely the property Eq. (5.36). If one accepts that $d=3$ is the lower critical dimension for smectics, three dimensions is in some sense very far from $d=4$. The dislocation loop mechanism could be reconciled with Lubensky and Chen's renormalization group analysis, provided this last fixed point became both physically accessible and stable as the spatial dimension tends toward 3. It would be worth checking for such a trend by extending the Lubensky-Chen calculations to $O(\epsilon^2)$.

The Fourier transform of the correlation function (5.28) is directly related to the smectic-A structure factor $S(\vec{q}_\perp, q_z)$. At all temperatures below T_c in three dimensions, there is an algebraic singularity at $\vec{q}_\perp = 0$, $q_z = q_0$. Hydrodynamics predicts that, near this singularity[35,37]

$$S(0,q_z) \sim \frac{1}{|q_0 - q_z|^{2-\eta(T)}} \ , \tag{5.37a}$$

$$S(q_\perp, q_0) \sim \frac{1}{q_\perp^{4-2\eta(T)}} \ , \tag{5.37b}$$

where the temperature-dependent critical exponent $\eta(T)$ is

$$\eta(T) = k_B T (q_0^2/8\pi)/\sqrt{BK_1} \ . \tag{5.38}$$

Inserting the Josephson scaling results (5.35) for the elastic constants, we find that

$$\eta \sim \xi_\perp^{d-3} \ . \tag{5.39}$$

There is strong experimental evidence[37] that the perpendicular correlation length exponent $\nu_\perp$ is finite above T_c. If the same exponent describes $\xi_\perp$ below T_c, we have

$$\eta(T) \sim \frac{1}{|T-T_c|^{(d-3)\nu_\perp(d)}} \ . \tag{5.40}$$

Provided $\nu_\perp(d)$ does not diverge before reaching its finite value $\nu_\perp(3)$ in the limit $d \to 3+$, $\eta(T)$ must remain *finite* as T approaches T_c from below. This prediction is *independent* of the precise relation between $\nu_\perp$ and $\nu_\parallel$.

It should be emphasized that $\eta(T_c^-)$ need not be the same as the corresponding critical exponent measured precisely at T_c. The qualitative renormalization group flows we expect for the smectic-A –to–nematic transition are shown in Fig. 8. Temperature is measured in terms of the function $\eta(T)$ defined by Eq. (5.38), and we have introduced a dislocation fugacity per unit length y. The dashed locus of initial conditions is given by

$$y = e^{-E_c\lambda/k_BT} \ , \tag{5.41}$$

where E_c is a typical edge or screw dislocation core energy per unit length. Below T_c, dislocation loop excitations are irrelevant at long wavelengths, and y is renormalized to zero. All trajectories then terminate in a line of fixed points parametrized by $\eta(T)$. There is a critical fixed point at *finite* y which controls the actual phase transition. The exponent $\eta(T_c^-)$ is given by the terminus of the heavy trajectory leaving this fixed point and ending in the line $y = 0$. There is a separate critical exponent η^* determined by an eigenvalue of the finite y fixed point. That such a fixed point exists can be inferred from Helfrich's entropy argument,[36] which suggests that E_c, and hence, y, are finite at T_c. The situation we envision is quite different than in, say, two dimensional melting, where the fixed point controlling the transition is part of a fixed line.[3–5] Of course, the renormalization flows of Fig. 8 are a physically motivated *conjecture*, and are not the result of an actual calculation.

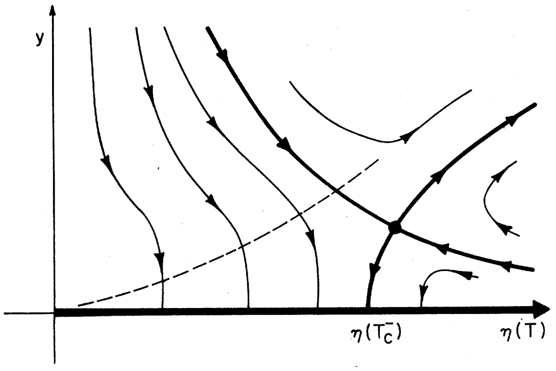

FIG. 8. Conjectured renormalization group flows for the smectic-A –to–nematic transition. there is both a fixed line describing the behavior for $T < T_c$, and a fixed point at finite dislocation line fugacity y describing the phase transition.

Stripped of renormalization group jargon, we can summarize our conclusions in terms of a scaling ansatz. Upon defining

$$\delta q_\parallel = q_z - q_0 \ , \tag{5.42}$$

and a reduced temperature,

$$t \propto (T-T_c)/T_c \ , \tag{5.43}$$

the scaling hypothesis for $S(\delta q_\parallel, q_\perp, t)$ takes the form

$$S(\delta q_\parallel, q_\perp, t) = b^{4-2\eta^*} S(b^2 \delta q_\parallel, b q_\perp, b^{1/\nu_\perp} t) \ , \tag{5.44}$$

where b is an arbitrary scale factor. When $t = 0$, Eq. (5.44) predicts that $S(q_\parallel, q_\perp)$ behaves as in Eq. (5.37), with the replacement $\eta(T) \to \eta^*$. For t very small and negative, we choose b such that $b^{1/\nu_\perp} t$ is near the point $\eta(T_c^-)$ in Fig. 8, and find that S takes the form

$$S(\delta q_\parallel, q_\perp, t) = \xi_\perp^{4-2\eta^*} \Phi(\xi_\perp^2 \delta q_\parallel, \xi_\perp q_\perp) \ . \tag{5.45}$$

The behavior of $\Phi(x,y)$ for small x and y is fixed by the hydrodynamic predictions of Eq. (5.37). When $q_\perp = 0$ one finds that

$$S(\delta q_\parallel, 0, t) \sim \xi_\perp^{\eta^- - \eta^*}/|\delta q_\parallel|^{2-\eta^-} \ , \tag{5.46a}$$

while, for $\delta q_\parallel = 0$, the result is

$$S(0, q_\perp, t) \sim \xi_\perp^{2\eta^- - 2\eta^*}/q_\perp^{4-2\eta^-} \ . \tag{5.46b}$$

The amplitudes have a singular temperature dependence, provided

$$\eta^- \equiv \eta(T_c^-) \neq \eta^* \ . \tag{5.47}$$

This picture of the smectic-A –to–nematic transition is summarized in Fig. 9. Because the hydrodynamic elastic constant $B(T)$ remains finite at T_c^-, there should be smecticlike behavior not only at long wavelengths below T_c, but also in the center regions of the figure.

The nature of the smectic-A –to–nematic transition is one of the few remaining unresolved problems in equilibrium critical phenomena. Although this question is far from settled at present, we hope the

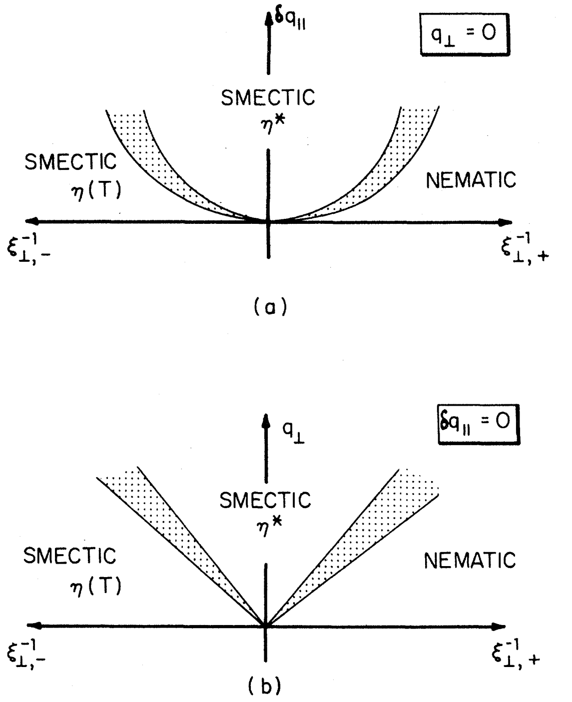

FIG. 9. Different regions of temperature and wave vector for the x-ray structure function $S(\delta q_{\parallel}, q_{\perp}, t)$. Temperature above and below T_c is measured by the reciprocal transverse correlation lengths $\xi^{-1}_{\perp,\pm}$. (a) is for $q_{\perp}=0$, while (b) corresponds to $\delta q_{\parallel}=0$.

points raised here will encourage further investigations of interacting dislocation loops, as well as more precise experiments.

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APPENDIX A: BEHAVIOR OF A SUPERFLUID WITH UNBOUND VORTEX RINGS

Feynman has speculated that the λ transition in superfluid ^{4}He could be understood in terms of a sudden proliferation of unbound vortex rings.[24] The behavior near the λ point is now quite well understood in terms of the $\epsilon = 4 - d$ expansion,[55] which focuses very little on defects like vortex rings. Both the diameter of a vortex core and the width of the interface between the core and the surrounding superfluid are believed to scale like the superfluid coherence length $\xi_-(T)$. Since $\xi_-(T)$ diverges as $T \to T_\lambda^-$, a "vortex ring" becomes indistinguishable at long wavelengths from an amorphous blob of normal material. There is no great advantage in describing this phase transition in terms of a set of line singularities like vortex rings. The situation is quite different in two dimensions, where point vortices have finite cores right up to the transition.[70] The assumption that vortices remain sharp singularities even at long wavelengths is basic to the Kosterlitz-Thouless theory[2] of superfluid helium films.

There is, of course, nothing fundamentally wrong with a point of view that models excitations in superfluid helium by a set of interacting vortex rings. We shall show explicitly that a finite density of unbound vortex rings gives rise to a superfluid density which vanishes at long wavelengths; such a material behaves like a normal liquid in this limit. Although this result is certainly not surprising, it provides a test of the calculational method which produced the novel cubic liquid phase in Sec. II.

The basic relation defining the strength of the vorticity carried by a vortex line is

$$\oint \vec{v}_s \cdot d\vec{l} = \frac{2\pi\hbar}{m} n \ . \tag{A1}$$

where n is an integer. The field $\vec{v}_s$ is the superfluid velocity field (whose circulation is quantized in units of $2\pi\hbar/m$), and m is the mass of a ^{4}He atom. In the continuum limit, Eq. (A1) may be restated in the form

$$\vec{\nabla} \times \vec{v}_s(\vec{r}) = \frac{2\pi\hbar}{m} \vec{M}(\vec{r}) \ , \tag{A2}$$

where the integral of $\vec{M}(r)$ over a surface S gives the total vorticity contained within the contour C which bounds S. To ensure that the dislocation loops close, we impose the condition

$$\vec{\nabla} \cdot \vec{M} = 0 \ . \tag{A3}$$

Equations (A2) and (A3) completely determine the part of $\vec{v}_s(\vec{r})$ due to vortex rings. In Fourier space, we find

$$\vec{v}_s(\vec{q}) = -i \frac{2\pi\hbar}{m} \frac{\vec{q} \times \vec{M}(\vec{q})}{q^2} \ . \tag{A4}$$

To model the free energy associated with a superfluid velocity field $\vec{v}_s(\vec{r})$, we imagine that the ^{4}He is embedded in a porous medium, which clamps the normal velocity $\vec{v}_n$ to zero. The free energy is then

$$F_s = \frac{1}{2} \rho_s \int d^3r \, |\vec{v}_s(\vec{r})|^2 \ . \tag{A5}$$

In general, $\vec{v}_s(\vec{r})$ will have an irrotational part, proportional to the gradient of a smoothly varying phase function, as well as a contribution from a distribution of vortex rings. If $\phi(\vec{r})$ is the smooth phase field, we have

$$\vec{v}_s(\vec{q}) = -i\frac{\hbar}{m}\vec{q}\phi(\vec{q}) - i\frac{2\pi\hbar}{m}\frac{\vec{q}\times\vec{M}(\vec{q})}{q^2} \quad . \tag{A6}$$

Inserting this decomposition into Eq. (A5) we find

$$\frac{F_s}{k_B T} = \frac{1}{2}K\int d^3r\,|\vec{\nabla}\phi|^2 + \frac{F_v}{k_B T} \quad , \tag{A7}$$

where the vortex contribution is

$$\frac{F_v}{k_B T} = \frac{1}{2}\int\frac{d^3q}{(2\pi)^3}\left(\frac{4\pi^2 K}{q^2} + \frac{2E_c}{k_B T}\right)|\vec{M}(q)|^2 \quad , \tag{A8}$$

and

$$K = \hbar^2\rho_s/m^2 k_B T \quad . \tag{A9}$$

The quantity E_c gives the core energy per unit length of vortex line.

The renormalized superfluid density can be defined in terms of the transverse and longitudinal parts of the momentum correlation function. The momentum is

$$\vec{g}^s(\vec{r}) = \rho_s\vec{v}_s(\vec{r}) \quad , \tag{A10}$$

and, upon defining

$$\begin{aligned} C_{ij}(\vec{q}) &= \langle g_i^s(\vec{q})g_j^s(-q)\rangle \\ &\equiv C_L(q)\frac{q_i q_j}{q^2} + C_T(q)\left(\delta_{ij} - \frac{q_i q_j}{q^2}\right) \end{aligned} \tag{A11}$$

we have[71]

$$K_R(q) = C_L(q) - C_T(q) \quad , \tag{A12}$$

where $K_R(q)$ is related to a wave-vector-dependent renormalized superfluid density $\rho_s^R(q)$,

$$K_R(q) = \hbar^2\rho_s^R(q)/m^2 k_B T. \tag{A13}$$

In a normal fluid, $C_L(q)$ and $C_T(q)$ become equal as q tends to zero. In an "unbound vortex ring approximation" of the kind used for dislocations in solids and smectics in Secs. II and V, we readily find from Eqs. (A6), (A7), and (A8) that

$$C_L(q) = K, C_T(q) = \frac{4\pi^2 K^2}{4\pi^2 K + 2E_c q^2} \quad . \tag{A14}$$

It follows from Eq. (A12) that $K_R(q)$ vanishes like q^2 at long wavelengths

$$K_R(q) \approx \frac{E_c}{2\pi^2}q^2 \quad . \tag{A15}$$

To incorporate fluctuations on scales less than a superfluid coherence length $\xi_+(T)$, we make the replacement

$$E_c \rightarrow \xi_+ E_c/a \quad , \tag{A16}$$

where a is a microscopic vortex core diameter. The result agrees with the Josephson scaling form for $K_R(q,\xi_+)$,[40]

$$K_R(q,\xi_+) = qf(q\xi_+) \quad , \tag{A17}$$

provided the scaling function $f(x)$ vanishes linearly with x for small x. Since $\rho_s^R(q)$ vanishes for small q, the behavior is that of a normal liquid.

There is nothing analogous to a bond-angle field in superfluid helium. It may be possible to construct a demonstration (along the lines taken here for the superfluid density) that the elastic constants of a solid do indeed vanish in the presence of unbound dislocations. The original physical argument of Shockley[21] seems quite compelling, however.

APPENDIX B: BOND-ANGLE FREE ENERGY FOR ANISOTROPIC SOLIDS

In this Appendix, we demonstrate that bond-angle order persists despite the presence of unbound dislocation loops in anisotropic crystalline solids. We begin with the incompatibility condition (2.6), which may be written

$$\alpha_{kl} = i(\epsilon_{kmn}q_m u_{nl} + Q_{klm}\theta_m) \quad , \tag{B1a}$$

where

$$Q_{ijm} = \delta_{ij}q_m - \delta_{im}q_j \quad . \tag{B1b}$$

In this Appendix, u_{lm} and θ_l denote the singular parts of the strain and bond-angle fields, due to a distribution of dislocations. The relation (B1a) holds for any crystal. The only changes from the isotropic case occur in the dislocation free energy, which no longer has its relatively simple isotropic form. It is, however, presumably still possible to separate the free energy density into a contribution from the dislocation cores

$$\mathcal{F}_{\text{core}} = E_{ijkl}\alpha_{ij}(q)\alpha_{kl}(-q) \tag{B2}$$

and a long-range interaction due to the elastic energy

$$\mathcal{F}_{\text{el}} = \frac{1}{2}C_{ijkl}u_{ij}(q)u_{kl}(-q) \quad . \tag{B3}$$

In general, the tensors C_{ijkl} and E_{ijkl} reflect the symmetries of the crystal in question. It should be noted, however, that while the elastic tensor C_{ijkl} can always be chosen to be symmetric under the interchanges of $i \rightleftarrows j$ and $k \rightleftarrows l$, the core energy tensor E_{ijkl} cannot, since α_{ij} need not be symmetric.

Combining these energies and writing α_{ij} in terms of dislocation bond angle and strain fields as in Eq. (B1), we can obtain an effective free energy density for those fields, which is, to lowest order in q

$$\mathfrak{F}_D = \tfrac{1}{2}\{2E_{ijkl}Q_{ijm}(q)Q_{kln}(q)\theta_m(q)\theta_n(-q) + 4A_{ijk}[u_{ij}(q)\theta_k(-q)] + C_{ijkl}u_{ij}(q)u_{kl}(-q)\}\ , \tag{B4}$$

where

$$A_{ijk} = E_{ljmn}\epsilon_{ilp}q_pQ_{mnk}(q)$$

and the superscript d has been suppressed. An effective free energy for the bond-angle field $\vec{\theta}$ can now be obtained by integrating out u_{ij} from the probability distribution

$$\mathcal{P}(\{\theta\},\{u_{ij}\}) \propto \exp\left[-\int \frac{d^3q}{(2\pi)^3}\frac{F_D}{k_BT}\right]\ . \tag{B5}$$

This functional integral over u_{ij} is constrained, since, by our definition of the "field of a dislocation," u_{ij} must give rise to no body forces. In Fourier space, this means that

$$q_i\sigma_{ij} = 0\ , \tag{B6}$$

where the stress σ_{ij} is related to the strain u_{ij} in the usual manner of continuum elasticity theory

$$\sigma_{ij} = C_{ijkl}u_{kl}\ . \tag{B7}$$

The constraint (B6) is easily incorporated into the functional integral over Eq. (B5) by adding a sort of "longitudinal mass" as was done (in a different context) in Sec. II. That is, we add to the free energy (B4) an additional term

$$\frac{M}{q^2}q_i\sigma_{ij}q_j\sigma_{jk} \tag{B8}$$

and then perform all functional integrals over u_{ij} without constraint, enforcing the constraint at the end of the calculation by letting M tend to infinity. Carrying out this procedure, we find for an effective free energy density for θ above,

$$\mathfrak{F}_{\text{eff}}(\theta) = \tfrac{1}{2}[2E_{ijkl}Q_{ijm}(q)Q_{kln}(q) + D_{ijkl}(\hat{q})A_{ijm}(q)A_{kln}(q)] \times \theta_m(q)\theta_n(-q)\quad (\hat{q} = \vec{q}/|\vec{q}|)\ , \tag{B9}$$

where

$$D_{ijkl} = \lim_{M\to\infty}\left(C_{ijkl} + \frac{M}{q^2}C_{ijmn}q_nC_{klmp}q_p\right)^{-1}\ . \tag{B10}$$

We shall not need to evaluate D_{ijkl}, since it is bounded above as $M \to \infty$ and gives rise to a contribution which is higher order in q than the first term of Eq. (B9). The first term of Eq. (B9) is of order q^2 at long wavelengths. To lowest order in q, then, the effective bond-angle free energy density becomes

$$F_{\text{eff}} = \tfrac{1}{2}\int \frac{d^3q}{(2\pi)^3}\,2E_{ijkl}Q_{ijm}Q_{kln}\,\theta_m(q)\theta_n(-q)\ . \tag{B11}$$

Note that the elastic constants have completely dropped out of this calculation; the symmetry of the crystal enters *only* through the core energy tensor E_{ijkl}. Using the definition of Q_{ijk} and Fourier transforming back into real space, we determine that the integrated free energy is

$$F_{\text{eff}} = \tfrac{1}{2}\int d^3r\,K_{ijkl}\partial_i\theta_j(r)\partial_k\theta_l(\vec{r})\ , \tag{B12a}$$

with

$$K_{ijkl} = 2(E_{ijkl} - 2E_{mmlk}\delta_{ij} + E_{mmnn}\delta_{ij}\delta_{kl})\ . \tag{B12b}$$

K_{ijkl} is a sort of "orientational elastic tensor." It clearly has the same symmetries as the core energy tensor, which in turn has all the symmetries of the crystal lattice. It must be remembered, however, that it does *not* have the symmetries of the elasticity tensor of the solid, since it is not symmetric under interchange of its first two or last two indices. Thus, more independent constants are required to describe a "bond-oriented liquid crystal" than are necessary to describe the corresponding solid.

For cubic symmetries, we have

$$\begin{aligned} F_{\text{eff}} = \tfrac{1}{2}\int d^3r\,\{&K_1[(\partial_x\theta_x)^2 + (\partial_y\theta_y)^2 + (\partial_z\theta_z)^2] + K_2[\partial_x\theta_x\partial_y\theta_y + \partial_x\theta_x\partial_z\theta_z + \partial_y\theta_y\partial_z\theta_z] \\ &+ K_3[(\partial_x\theta_y)^2 + (\partial_x\theta_z)^2 + (\partial_y\theta_x)^2 + (\partial_y\theta_z)^2 + (\partial_z\theta_x)^2 + (\partial_z\theta_y)^2] \\ &+ 2K_4[(\partial_x\theta_y)(\partial_y\theta_x) + (\partial_x\theta_z)(\partial_z\theta_x) + (\partial_y\theta_z)(\partial_z\theta_y)]\}\ . \end{aligned} \tag{B13}$$

Note that although the last term in square brackets in this expression can be converted into the 1st by suitable integration by parts, such a trick will *not* work in the presence of *disinclination* lines, which force the introduction of cuts to keep the strain field single valued. These cuts will give contributions to the energy from the surface term by which the last term in square brackets and the 1st differ. For systems with a hexagonal symmetry,

$$F_{\text{eff}}=\frac{1}{2}\int d^3r\,\{K_1(\partial_x\theta_x+\partial_y\theta_y)^2+K_2[(\partial_x\theta_x)^2+(\partial_y\theta_y)^2+(\partial_x\theta_y)^2+(\partial_y\theta_x)^2]$$
$$+K_3(\partial_x\theta_y)(\partial_y\theta_x)+K_4(\partial_z\theta_z)^2+K_5\partial_z\theta_z(\partial_x\theta_x+\partial_y\theta_y)+K_6[(\partial_x\theta_z)^2+(\partial_y\theta_z)^2]$$
$$+K_7(\partial_x\theta_z\partial_z\theta_x+\partial_y\theta_z\partial_z\theta_y)+K_8[(\partial_z\theta_x)^2+(\partial_z\theta_y)^2]\}\ .$$

Spherical harmonics other than those for $l=4$ used here would be required to study bond-angle order in hexagonal systems.

One can also imagine a more general situation than that considered throughout this paper in which dislocations with some types of Burgers vectors remain bound (in the sense of Sec. II) while others become free.[72] In such a "partly dislocated solid," some translational order will persist, together with a type of orientational order similar to that which we have considered already. An example of such a phase is the stacked hexatic phase discussed in the Introduction. By permeating a crystal with hexagonal symmetry with a finite density of free dislocations whose Burgers vectors lie in the hexagonal plane, we thereby destroy translational order within that plane. However, if we allow no dislocations with Burgers vectors perpendicular to this plane, translational order in that direction will persist. Furthermore, we would expect sixfold orientational order within the hexagonal planes, since, as we have seen, free dislocation loops are not sufficient to destroy such order. Thus we have a phase with long-range translational order in one direction, and in-plane orientational order. This is exactly the type of order exhibited by the proposed "stacked hexatic" phase.[19] It is equally easy to see that the so-called "discotic" or "pokerchip" phase, with translational order in two out of three directions, can be created by permeating a crystal of the same hexagonal symmetry with dislocation loops whose Burger's vectors point in the direction *normal* to the hexagonal planes, while leaving all other loops bound. This point of view is similar in spirit to that taken by Martin *et al.*,[73] who consider successively less correlated phases of matter by discarding various elastic constants.

APPENDIX C: JOSEPHSON RELATIONS FOR SMECTIC-*A* LIQUID CRYSTALS

In 1966, Josephson[40] published a scaling argument which relates the behavior of the superfluid density in ^{4}He near T_λ to conventional critical exponents. Hohenberg *et al.*[74] have presented a particularly transparent derivation of Josephson's result. In d dimensions, the hydrodynamic "stiffness" $\rho_s(T)$ is related to a suitably defined transverse correlation length $\xi_T(T)$,

$$\rho_s \propto \xi_T^{2-d}\ . \tag{C1}$$

Here we adapt the Hohenberg *et al.* argument to determine how the hydrodynamic parameters B and K_1 entering a d-dimensional generalization of Eq. (5.1) depend on suitably defined parallel and perpendicular correlation lengths.

The generalization of Eq. (5.1) to d dimensions is

$$F=\frac{1}{2}\int d^dr\,[B(\partial_z u)^2+K_1(\nabla_\perp^2 u)^2]\ , \tag{C2}$$

where $\nabla_\perp^2$ is a $(d-1)$-dimensional Laplacian corresponding to the $d-1$ directions within layers normal to the $\hat{z}$-direction. We work in $d>3$ dimensions, and assume genuine long range order in

$$\psi(r)\equiv\psi_0 e^{iq_0u(\vec{r})}\ . \tag{C3}$$

Fluctuations in the magnitude of $\psi(\vec{r})$ will be neglected (this is always permissible in the hydrodynamic limit), and we chose the phase of the order parameter such that $\langle\psi(r)\rangle$ is real and positive.

The large-distance behavior of correlations in the transverse part of the order parameter,

$$\psi_T(\vec{r})=\psi_0\sin[q_0u(\vec{r})]\ , \tag{C4}$$

is entirely determined by hydrodynamics. It is easy to show given the Gaussian free energy functional (C2) that

$$\begin{aligned}C_T(\vec{r})&\equiv\langle\psi_T(\vec{r})\psi_T(\vec{0})\rangle\\&=|\langle\psi(\vec{r})\rangle|^2\sinh[Q(r)]\ ,\end{aligned} \tag{C5}$$

where

$$|\langle\psi(\vec{r})\rangle|=\psi_0\exp[-\tfrac{1}{2}q_0^2\langle u^2(\vec{r})\rangle] \tag{C6a}$$

and

$$Q(\vec{r})=q_0^2\langle u(\vec{r})u(\vec{0})\rangle\ . \tag{C6b}$$

The averages are evaluated in an ensemble specified by the free energy (C2). Since $Q(\vec{r})$ tends to zero for large r, the large r behavior of $C_T(\vec{r})$ is just that of $Q(r)$, which may be written

$$Q(\vec{r})=q_0^2\int\frac{d^dq}{(2\pi)^d}\frac{e^{i\vec{q}\cdot\vec{r}}}{Bq_z^2+K_1q_\perp^4}\ . \tag{C7}$$

Considering now $Q(\vec{r})\equiv Q(\vec{r}_\perp,z)$ as a function of separations perpendicular and parallel to the smectic layer normal, it is straightforward to show from Eq.

(C7) that

$$Q(r_\perp,0) \underset{r_\perp\to\infty}{\sim} \frac{1}{\sqrt{BK_1}} r_\perp^{3-d} \quad , \tag{C8a}$$

$$Q(0,z) \underset{z\to\infty}{\sim} \left(\frac{B}{K_1}\right)^{(d-1)/4} \frac{1}{B} z^{(3-d)/2} \quad . \tag{C8b}$$

Because of the broken translational symmetry in the smectic phase, correlations decay as power laws rather than exponentially. The particularly simple power law decay of $C_T(\vec{r}) \equiv C_T(\vec{r}_\perp, z)$, however, can be used to extract correlation lengths via the definitions

$$C_T(r_\perp,0) \underset{r_\perp\to\infty}{\sim} |\langle\psi(\vec{r})\rangle|^2(\xi_\perp/r_\perp)^{(3-d)} \quad , \tag{C9a}$$

$$C_T(0,z) \underset{z\to\infty}{\sim} |\langle\psi(r)\rangle|^2(\xi_\parallel/z)^{(3-d)/2} \quad . \tag{C9b}$$

Making use of Eqs. (C5) and (C8), we readily find

$$B_1 \sim \xi_\parallel/\xi_\perp^{d-1}, \quad K_1 \sim \xi_\perp^{5-d}/\xi_\parallel \quad , \tag{C10}$$

which are the results quoted in Sec. V. It is interesting to note that the behavior of K_1 below T_c matches that predicted by anisotropic scaling[38] for the Frank constant K_2 above T_c.

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