

## Smectic, cholesteric, and Rayleigh-Benard order in two dimensions

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(Received 29 February 1980)

Order in layered smectic and cholesteric liquid-crystal films is investigated. Although long-wavelength fluctuations in the layer displacements destroy translational order at any finite temperature, one must also account for effects of free dislocations. The combined action of layer fluctuations and dislocations is to produce a phase at finite temperatures with persistent orientational order in the local normal to the layers. At length scales greater than  $\xi_D \sim \exp(E_D/2k_B T)$  where  $E_D$  is the energy of an isolated dislocation, the properties are those of a two-dimensional nematic, with the local layer normal playing the role of a director field. An intermediate phase of this kind could conceivably exist in bulk cholesteric liquid crystals as well. In two dimensions, an unbinding of disclination pairs eventually produces an isotropic phase. The low-temperature nematic Frank constants  $K_1(T)$  and  $K_3(T)$  are worked out, and compared with the diamagnetic susceptibility expected in a two-dimensional superconductor. We determine the characteristic nematic frequencies at low temperatures, using a simple model of dislocations interacting with a layer displacement field. Our analysis may also be relevant to the behavior of Rayleigh-Benard convective rolls in the presence of thermal noise fluctuations.

### I. INTRODUCTION

#### A. Purpose

There has been considerable interest recently in systems where fluctuations are strong enough to destroy conventional long-range order. This seems to be the case for superfluids, solids, and magnets with a continuous symmetry in both one and two dimensions. For Heisenberg ferromagnets with three or more components, ordinary spin-wave fluctuations seem sufficient to produce paramagnetic behavior at any finite temperature, even in two dimensions.<sup>1</sup> Although spin waves cause exponential decay of correlations in two-component  $XY$  models of magnetism in one dimension,<sup>2</sup> this is not the case in  $d=2$ . Instead, one finds a low-temperature phase characterized by algebraically decaying correlations with temperature-dependent exponents. According to Kosterlitz and Thouless,<sup>3-5</sup> vortex pairs unbind above a finite critical temperature, producing the exponential decay one expects in a paramagnet. Very similar ideas apply to the superfluid transition in thin helium films, where the superfluid density drops discontinuously to zero.<sup>3-5</sup>

Bound pairs of dislocations are believed to play an analogous role in melting two-dimensional solids.<sup>3,5-9</sup> Although long-wavelength phonon excitations alone are sufficient to replace the usual  $\delta$ -function Bragg peaks in the structure factor by power-law singularities,<sup>10</sup> a finite density of dislocations is necessary to actually produce liquidlike behavior. It appears that order in the orientations of bond angles, which is not significantly affected by phonons,<sup>11</sup> persists even in

the presence of unbound dislocations.<sup>7</sup> One finds a "hexatic" liquid-crystalline phase with algebraic decay of bond-angle correlations, and exponential decay of translational order. A second, disclination unbinding transition is necessary to complete the transition to an isotropic liquid [see Fig. 1(a)].

The purpose of this paper is to examine the effects of phononlike fluctuations, dislocations, and disclinations on layered materials in two dimensions. In particular, our analysis should apply to smectic liquid-crystal films with layering in the plane. As discussed by DeGennes,<sup>12,13</sup> it is possible in principle to make a two-dimensional nematic liquid crystal, floating on water, from nematogens with two hydrophilic ends. Although monolayer films of this kind have not yet been made, one can certainly imagine smectic ordering in these systems [see Fig. 2(a)]. Freely suspended films of smectic-C liquid crystals, which have, in fact, been made,<sup>14-16</sup> mimic a two-dimensional nematic, with the projection of the tilted molecules onto the plane playing the role of "nematogens." Layered order may occur in these projections provided the film does not crystallize into an ordinary tilted solid phase first. In most physical systems, one would expect crystallization into this kind of anisotropic solid at a sufficiently low temperature  $T_m$ . The detailed temperature dependence determined here for Frank constants, kinetic coefficients, etc., would then hold only for temperatures  $T \gg T_m$ . The divergences we find in Frank constants, kinetic coefficients, etc., at low temperatures (see Sec. I C) would be replaced by diverging behavior as  $T \rightarrow T_m^+$ . Ostlund and Halperin<sup>17</sup> have recently analyzed the melting of anisotropic solids using the methods of Refs.

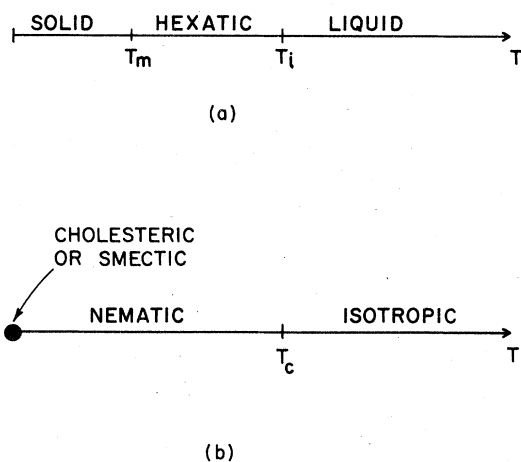


FIG. 1. Different phases involved in the melting of triangular solids and layered systems in two dimensions. (a) shows a triangular solid at low temperatures, which first melts at  $T_m$  via a dislocation unbinding transition into a hexatic liquid crystal. The sixfold bond orientational order in this phase is destroyed at a higher temperature  $T_i$  by an unbinding of disclination pairs. (b) shows a zero-temperature smectic or cholesteric, which becomes a kind of nematic, with persistent order in the orientations of layer normals, at finite temperatures. This phase, which arises from effects of phonon fluctuations and free dislocations on layered order, transforms into an isotropic phase via a disclination unbinding transition at  $T_c$ .

6–8. They find that such solids can melt via a dislocation unbinding transition into a phase with the kind of layered order discussed in this paper.

Anisotropic solids can also occur for molecules physisorbed onto periodic substrates. Recently, Coulomb *et al.*<sup>18</sup> have reported evidence for an anisotropic solid phase of ethane physisorbed onto exfoliated graphite. They find a first-order transition into an intermediate phase which may possess only “partial” translational order, followed by a continuous transition to a fluid. The intermediate phase could be an example of the layered structures considered here. The periodicity of the layers appears to be commensurate with the substrate.<sup>18</sup> Although we have not studied the effect of a periodic substrate potential, it appears likely that such a potential could stabilize a layered phase at finite temperatures. As will be discussed in Sec. IC, layered order is particularly susceptible to breakup by thermal fluctuations in the absence of a periodic substrate.

Cholesteric liquid crystals provide examples of layered structures where the wavelength associated with the periodicity is thousands of angstroms, instead of the 20–30 Å repeat distance one might expect in a smectic. In cholesterics, chiral nematogens rotate slowly in space along a preferred axis, as in Fig. 2(b). Although the properties are those of a nematic at dis-

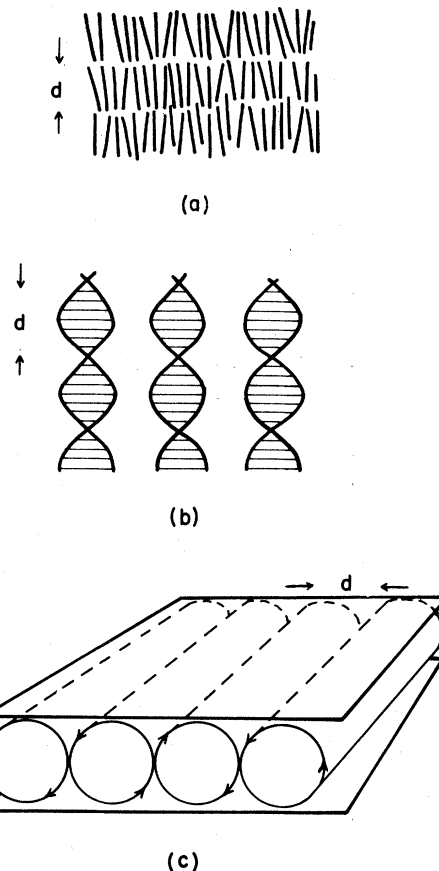


FIG. 2. (a) Arrangement of the constituent molecules (nematogens) in the smectic-*A* phase. Note the orientational ordering, the layering, and the lack of translational order within each layer. (b) Arrangement of nematogens in the cholesteric phase. As one moves along the vertical helical axis, the nematogens rotate slowly in a plane perpendicular to this axis. There is no translational order in the centers of mass of the nematogens, although this is not clear from the figure. (c) Rayleigh-Benard convective rolls. Above a threshold temperature gradient across the two plates, a roll pattern of circulation forms, with the fluid within each roll moving in an opposite sense to its two neighbors.

tances short compared to the pitch, the ordered state resembles a one-dimensional crystal when the pitch is short compared to a nematic correlation length.<sup>19</sup> Evidently, one can prepare cholesteric films with thicknesses less than or comparable to the pitch which form layers in the plane of the substrate.<sup>20</sup> If the thickness is much greater than the nematic healing length, most nematogens in the film will be free to rotate about the local helical axis, independent of the boundary conditions at the substrate. In principle, one might hope to study the effects of fluctuations on layering in such systems. The energy scale for the effects discussed in this paper is a dislocation

energy, which for cholesterics may be written

$$E_D \sim K_2 d, \quad (1.1)$$

where  $K_2$  is a twist nematic Frank constant and  $d$  is the film thickness. Unfortunately, the temperatures necessary to obtain a reasonable density of oppositely charged dislocations in equilibrium may be prohibitively high at film thicknesses comparable to the pitch.

The Rayleigh-Benard instability<sup>21</sup> provides an interesting example of layered two-dimensional order out of equilibrium. Above a threshold temperature difference applied across two confining plates, heat is often transferred through fluids by a layered pattern of convective rolls [see Fig. 2(c)]. The effect of fluctuations on the convective instability have been treated by a number of authors.<sup>22-24</sup> Swift and Hohenberg<sup>24</sup> have argued that thermal fluctuations cause a linear combination of the temperature deviation and fluid velocity to relax to a steady-state probability distribution of the kind commonly used to describe smectics and cholesterics in equilibrium. If so, our results will describe the effect of thermal fluctuations on the Rayleigh-Benard convective rolls.<sup>25</sup>

Although this is an intriguing problem, it may be of academic interest only, since estimates of thermal-fluctuation effects<sup>23</sup> suggest that they will be unobservable experimentally. Our results could be quite relevant, however, if the developing chaos in a Benard cell produced a high density of dislocations. The model of dislocation *dynamics* discussed here could be used to study nonequilibrium processes above the convection threshold.

### B. Layered order in three dimensions

Considerable experimental and theoretical attention has been focused on *three*-dimensional smectic and cholesteric liquid crystals. Before summarizing our results in two dimensions, we discuss layered order in these bulk systems. The experimental and theoretical situation is rather controversial, and we believe our conclusions for  $d = 2$  may have some bearing on this important problem.

At sufficiently low temperature, smectic-*A* and cholesteric liquid crystals should be describable at long wavelengths by a free-energy functional of the layer spacing  $u(\vec{\tau})$  alone. If the layers are oriented on average in the  $z$  direction, we have, to lowest order in gradients of  $u$ ,<sup>12</sup>

$$F = \frac{1}{2} B \int d^3r [(\partial_z u)^2 + \lambda^2 (\partial_i^2 u)^2], \quad (1.2)$$

where  $B$  is an elastic parameter,  $\partial_i$  is a gradient acting on directions perpendicular to  $\hat{z}$ , and  $\lambda$  is a length comparable to the layer spacing  $d$ . More generally, one can imagine a functional of a complex field,  $\psi(\vec{\tau})$ , which is the amplitude of the first harmonic of the one-dimensional density wave associated with the

ordering,

$$\rho(r) = \rho_0 \text{Re}[1 + \psi(\vec{\tau}) e^{i\vec{q}_0 \cdot r}] \quad (1.3)$$

Here,  $\rho_0$  is the average density and  $\vec{q}_0$  is the wave vector associated with the periodicity. At low enough temperatures, we can take

$$\psi(\vec{\tau}) = \psi_0 \exp[iq_0 u(\vec{\tau})], \quad (1.4)$$

where  $\psi_0$  is real, independent of  $\vec{\tau}$ , and less than unity, and  $u(\vec{\tau})$  is the layer displacement field.

If Eq. (1.1) is used to model smectic-*A* liquid crystals, it may be important to include explicitly a coupling to the director field of the nematogens. When this is done, and fluctuations in the magnitude of  $\psi_0$  are allowed, the resulting free-energy functional resembles the Landau-Ginzburg phenomenological model of superconductivity.<sup>26</sup> (See Sec. II.) This model of a smectic is only approximately gauge invariant, however, in contrast to a real superconductor. Renormalization-group studies<sup>27,28</sup> suggest that the coupling to the director field drives the smectic-to-nematic transition first order, at least near four dimensions. This conclusion rests on the equivalence at long wavelengths of superconductors and smectic-*A*'s near their transition temperatures. In particular, "asymptotic gauge invariance" of a smectic requires that the rescaled Frank constants satisfy  $\tilde{K}_2 = \tilde{K}_3 \gg \tilde{K}_1$  just above the transition temperature. Although this requirement can be checked near four dimensions,<sup>28</sup> its justification in  $d = 3$  is an open question. Lubensky and Chen<sup>29</sup> have argued that an anisotropic fixed point, with  $\tilde{K}_1 \gg \tilde{K}_2, \tilde{K}_3$ , may also be important in the critical region. Unfortunately, no first-order smectic-to-nematic transition has been observed experimentally,<sup>30</sup> and the entire situation seems very unclear.

Unlike smectics, cholesteric liquid crystals are believed to undergo a transition directly to an isotropic phase in three dimensions.<sup>12</sup> A conventional nematic phase does not usually occur in nonracemic materials, since a cholesteric is itself already a kind of twisted nematic. When the pitch is long compared to a nematic correlation length, the transition should be weakly first order, just as for a nematic-isotropic transition. When the pitch is short compared to a nematic correlation range, however, one can argue<sup>19</sup> that the ordered phase is better described as a kind of one-dimensional "solid." To model the melting of this "crystal," Brazovskii and Dmitriev<sup>19</sup> have proposed a Landau free-energy functional of the form

$$F = \int d^3r \left\{ \frac{1}{2} [(|\vec{\nabla}| - iq_0)w]^2 + rw^2 + uw^4 \right\}, \quad (1.5a)$$

where  $w(\vec{\tau})$  is a scalar density. The operator  $|\vec{\nabla}|$  is understood to give  $i|\vec{q}|$  when acting on the Fourier transform  $\hat{w}(\vec{q})$ . Well below the mean-field transition temperature (i.e., for  $r$  large and negative),

$w(\vec{r})$  becomes spatially modulated in some direction  $\vec{q}_0$  and we can write

$$w(\vec{r}) = 2 \operatorname{Re}[\psi(\vec{r})e^{i\vec{q}_0 \cdot \vec{r}}], \quad (1.5b)$$

where the complex quantity  $\psi(r)$  varies slowly on a scale set by  $q_0^{-1}$ . Assuming fluctuations in the amplitude  $\psi_0$  are negligible, the decomposition (1.4) leads to a free energy of the form (1.2). This simple model of a cholesteric was studied in detail by Brazovskii,<sup>31</sup> who concluded that there would again be a first-order transition, due in this case to fluctuations in the neighborhood of a preferred sphere in Fourier space. There are, at present, few experimental checks of Brazovskii's detailed predictions. The cholesteric "blue phases," which are in a sense intermediate between the usual cholesteric and isotropic phases, will be discussed briefly in Sec. IC.

It is important to remember that fluctuations in the layer displacements of smectics and cholesterics are logarithmically divergent in three dimensions.<sup>32</sup> Indeed one has immediately from Eq. (1.2) that

$$\langle u^2(\vec{r}) \rangle \sim \frac{k_B T}{B} \int \frac{d^3 q}{q_z^2 + \lambda^2 q_1^4} \sim \ln \left( \frac{R}{d} \right), \quad (1.6)$$

where  $R$  is of order the system size. As a result, there is no long-range order,

$$\langle \psi(\vec{r}) \rangle = 0, \quad (1.7)$$

and one finds power-law decay of correlations in  $\psi(\vec{r})$ ,<sup>32</sup> with different exponents in directions parallel and perpendicular to  $\hat{z}$ . In this sense, smectic and cholesteric liquid crystals may be at a "lower critical dimensionality" in  $d=3$ , just as crystals, superfluids, and  $XY$  magnets are in  $d=2$ . One might guess that defects would be important in understanding bulk smectic and cholesteric transitions, although such excitations were not considered explicitly in the theoretical treatments described above. Helfrich<sup>33</sup> has, in fact, suggested that the smectic- $A$ -nematic transition may be understood as a break up of order by dislocation loops. It is not yet clear whether this point of view can resolve the discrepancies between theory and experiment.

### C. Results and outline

Because  $d=2$  is one below an apparent lower critical dimensionality of layered materials, phonon fluctuations are quite effective in destroying translational order at any finite temperature. Both phonon and dislocation excitations are necessary to describe these materials properly at low temperatures, however. To characterize the effect of phonons on layered order, we consider correlations of the translational order parameter  $\psi(\vec{r}) = \psi_0 \exp[iq_0 u(\vec{r})]$ , discussed in Sec. IB. Using the free energy (1.2), one readily finds<sup>23</sup>

that

$$\langle \psi(\vec{r}) \psi^*(\vec{0}) \rangle \sim \exp \left[ -\frac{q_0^2 k_B T}{B} \left( \frac{|z|}{4\pi\lambda} \right)^{1/2} \right], \quad (1.8a)$$

$$x^2 \ll \lambda z,$$

$$\langle \psi(\vec{r}) \psi^*(\vec{0}) \rangle \sim \exp \left[ -\frac{q_0^2 k_B T}{4B\lambda} |x| \right], \quad (1.8b)$$

$$\lambda z \ll x^2$$

for  $d=2$ , in contrast to the power-law decay of this correlation function in three dimensions.<sup>32</sup> In deriving Eq. (1.8), we have set  $\vec{r} = (x, z)$ , and assumed layering in the  $z$  direction. The decay is more rapid in the  $x$  direction, since this is chiefly due to the fluctuations displayed in Fig. 3(a). These have a lower energy than the fluctuations displayed in Fig. 3(b), which decorrelate correlations in the  $z$  direction. Phonons are much less important in decorrelating layer orientations, which can be described by the angle the layer normal deviates from the  $z$  direction,

$$\theta(\vec{r}) = -\partial_x u(\vec{r}). \quad (1.9)$$

Upon defining a nematiclike orientational order parameter,

$$\vec{N}(\vec{r}) = \begin{pmatrix} \cos\theta(\vec{r}) \\ \sin\theta(\vec{r}) \end{pmatrix}, \quad (1.10)$$

we find from Eq. (1.2) that long-range order in  $\vec{N}(\vec{r})$  persists, even in the presence of phonons,

$$\lim_{\vec{r} \rightarrow \infty} \langle \vec{N}(\vec{r}) \cdot \vec{N}(\vec{0}) \rangle = \text{const} \neq 0. \quad (1.11)$$

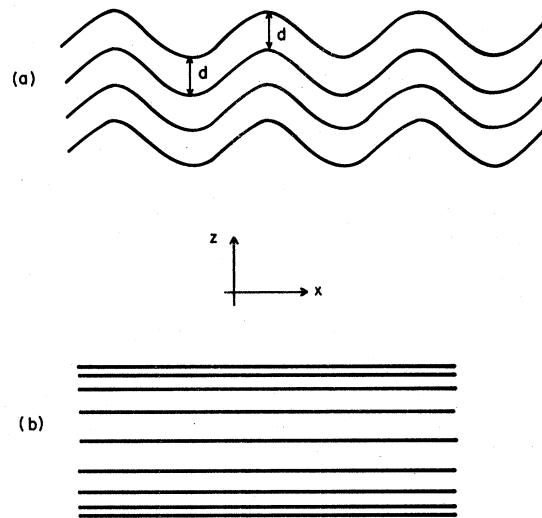


FIG. 3. Different kinds of phonon excitations in layered systems. (a) shows a phonon with  $q_x \neq 0$  and  $q_z = 0$ , which keeps the interlayer spacing  $d$  fixed. This has a lower energy than the phonon in (b), where  $q_x = 0$  and  $q_z \neq 0$ .

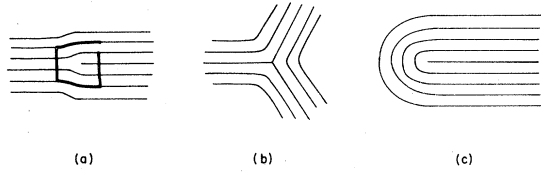


FIG. 4. Dislocation and disclinations in layered materials. (b) and (c) show two oppositely charged disclinations. Ordinarily, isolated disclinations would have much too high an energy to exist in thermal equilibrium. Note, however, that bringing the two disclinations together forms a dislocation of the kind shown in (a). Isolated dislocations have a finite energy, and may be characterized by their Burger's vector, which is the amount by which the path shown as a heavy line fails to close.

Since the behavior summarized by Eqs. (1.8) and (1.11) is rather peculiar, one might expect that a description of layered materials purely in terms of phonon fluctuations is incomplete. Other excitations possible at low temperatures include dislocations and disclinations (see Fig. 4). Isolated dislocations have a finite energy  $E_D$  in layered substances,<sup>26,34</sup> so one expects them to occur with density

$$n_D \approx a^{-2} \exp(-E_D/k_B T) \quad (1.12)$$

at finite temperatures, where  $a$  is a dislocation core diameter. Disclinations are much less important, since their energy diverges with the size of the system. Note, however, that a dislocation can itself be regarded as a tightly-bound pair of oppositely charged disclinations.

When effects due to a finite density of free dislocations are accounted for, the properties of layered systems at length scales greater than

$$\xi_D \approx n_D^{-1/2} \approx a \exp(E_D/2k_B T) \quad (1.13)$$

are those of a nematic liquid crystal. In a kind of Debye-Hückel approximation, we find that the behavior at long wavelengths is given by an effective free energy,

$$F_N = \frac{1}{2} \int d^2r \{ K_1(T) (\vec{\nabla} \cdot \vec{N})^2 + K_3(T) [\vec{N} \times (\vec{\nabla} \times \vec{N})]^2 \} \quad (1.14)$$

The "twist" elastic constant  $K_2$  is absent in two dimensions. Although nematic order is to be expected in materials which are smectics at  $T=0$ , it is certainly surprising to see this kind of persistent orientational order in the layer normal of cholesterics and Rayleigh-Benard convective rolls. Orientational correlations in the director field  $\vec{N}(\vec{r})$  should decay algebraically when  $|\vec{r}| \gg \xi_D$ . Figure 5 provides a rough illustration of the physical picture we have in mind. Although the blobs are anisotropic, the area per blob is just  $\xi_D^2$ . There is some evidence of aniso-

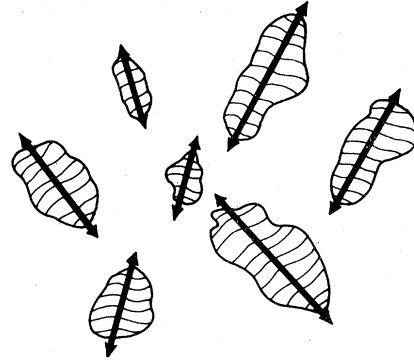


FIG. 5. Crude physical picture of the "nematic phase" of layered systems at low temperatures. Layered order is decorrelated only by phonon fluctuations in blobs, or "cybotactic groups" (see Ref. 12), of sizes controlled by the dislocation correlation length  $\xi_D$ . The width of the blobs varies like  $\xi_D^{2/3}$ , while the length varies as  $\xi_D^{4/3}$ . The nematic order parameter is the average layer normal within each blob. The directions of these average normals are indicated by double-headed arrows. The distortion energy associated with spatial variations in this direction has the same form as the Frank expression for a nematic. A phase of this kind is predicted for cholesterics as well as smectics.

tropic correlation lengths in the bulk smectic- $A$  to nematic transition.<sup>30</sup>

At sufficiently long wavelengths, it can be shown<sup>35</sup> that a nematic free energy of the form (1.14) can be replaced by a free energy characterized by a *single* Frank constant, namely,

$$F_N = \frac{1}{2} K(T) \int d^2r (\vec{\nabla} \theta)^2 \quad (1.15)$$

The decay of orientational order is then given by

$$\langle e^{2i\theta(\vec{r})} e^{-2i\theta(0)} \rangle \sim r^{-\eta_2(T)} \quad (1.16)$$

with

$$\eta_2(T) = 2k_B T / \pi K(T) \quad (1.17)$$

At high enough temperatures, one expects an unbinding of logarithmically bound disclination pairs at a temperature  $T_c$  into an isotropic phase. Just below this Kosterlitz-Thouless transition, one has the exact result,<sup>36</sup>

$$K(T_c^-) / k_B T_c^- = 8/\pi \quad (1.18)$$

The persistent orientational correlations found here for layered materials are very analogous to the persistent bond angle order of the hexatic phase in recent two-dimensional melting theories applied to triangular crystals.<sup>7</sup> The sequence of phases—smectic, nematic, isotropic—corresponds to the sequence—solid, hexatic, liquid—found in this theory [see Fig.

1(b)]. In layered systems, the dislocation unbinding transition has been pushed down to  $T=0$ , because of the peculiar nature of parabolic elasticity theory.

These results may be relevant to bulk cholesteric liquid crystals. Recent light scattering experiments<sup>37</sup> show two apparently distinct "blue phases," intermediate between ordinary cholesteric and isotropic phases. It is intriguing to speculate that one of these blue phases could be a "nematic," of the kind found here for two-dimensional cholesterics. Translational order in the pitch would persist over large chunks of material, with the average normal playing the role of a "nematogen." If this order parameter really behaved like a nematic at long wavelengths, one would expect a first-order transition to an isotropic phase in three dimensions.

Our conclusions differ from those reached by Swift and Hohenberg,<sup>24</sup> who argued that the transition to Rayleigh-Benard convective rolls should be first order with no nematic phase, in analogy to the conclusions of Brazovskii<sup>31</sup> for three-dimensional layered systems. They recognized, however, difficulties associated with the lack of long-range order, which are especially severe in two dimensions. Their analysis was restricted to situations such as  $Lq_0 \ll g^{-2/5}$ , where  $L$  is the lateral extent of the system and  $g$  is a dimensionless coupling constant. Strictly speaking, our results apply only to infinite aspect ratio convection problems. We hope to explore the precise connection, if any, of our results with the Rayleigh-Benard problem in a future publication.

Although properties of the disclination unbinding transition follow from a transcription of Kosterlitz's results<sup>4</sup> for  $XY$  models, it is also interesting to ask how layered order sets in at low temperatures in the nematic phase of smectics and cholesterics. The critical point at  $T=0$  is a two-dimensional analog of the bulk smectic- $A$ -nematic transition. The wave-vector-dependent renormalized Frank constants  $K_1^R(q, T)$  and  $K_3^R(q, T)$  behave differently in regions of the  $(\xi_D^{-1}, q)$  plane shown in Fig. 6. For sufficiently small  $q$ , the Frank constants become equal to their common value  $K(T)$  and appear to diverge like  $\xi_D^2$ ,

$$K_1^R \approx K_3^R = K \sim \xi_D^2. \quad (1.19)$$

As  $T$  tends to zero for any fixed, finite  $q$ , the Frank constants ultimately acquire a different temperature dependence,

$$\begin{aligned} K_1^R(q, T) &\sim \xi_D^{2/3} [\ln(1/qd)]^{2/3}, \\ K_3^R(q, T) &\sim \xi_D^2. \end{aligned} \quad (1.20)$$

This crossover between these two behaviors occurs at temperatures and wave vector such that

$$k_B T \approx E_D / |\ln[\ln(1/qd)]|. \quad (1.21)$$

This condition means that the behavior (1.20) will al-

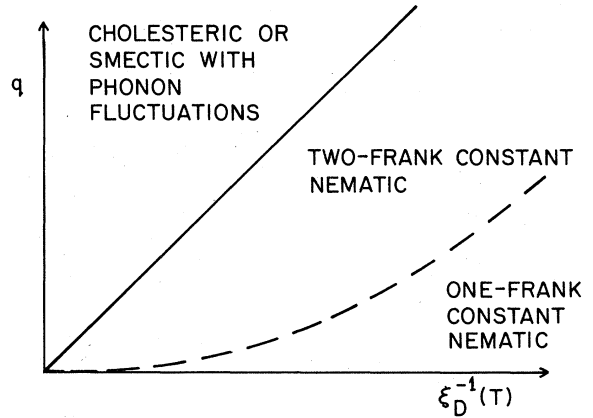


FIG. 6. Summary of the behavior of layered systems as a function of wave vector  $q$  and the inverse dislocation correlation length,  $\xi_D^{-1}(T) \approx (1/a) \exp(-E_D/k_B T)$ . As temperature decreases with small, fixed  $q$ , one in principle first encounters a one-Frank-constant nematic, followed, by two-Frank-constant nematic behavior. Finally, the behavior becomes like that of a smectic or cholesteric decorrelated by phonons at temperatures such that  $q \xi_D(T) \geq 1$ . As discussed in the text, the boundary between one- and two-Frank-constant nematic behavior occurs at astronomically small wave vectors.

most always be encountered in practice for temperatures less than  $E_D/k_B$ . The vanishing of the ratio  $K_1(q, T)/K_3(q, T)$  at low temperatures in this case signals the onset of smectic order at  $T=0$ . The qualitative behavior of  $K_1$  and  $K_3$  with decreasing temperature is shown in Fig. 7.

It is interesting to contrast our results with the behavior expected in a two-dimensional superconduc-

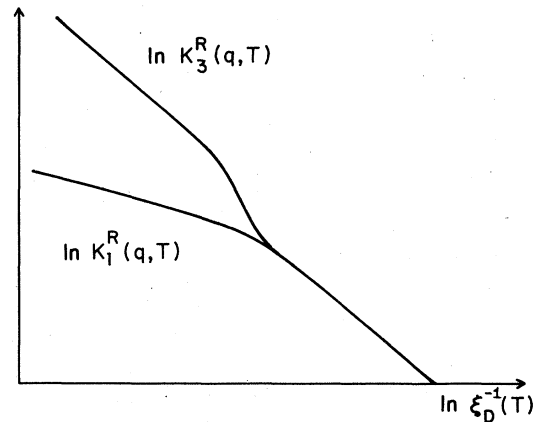


FIG. 7. Plot of the logarithm of the renormalized Frank constants  $K_1^R(q, T)$  and  $K_3^R(q, T)$  vs  $\ln \xi_D^{-1}$ , for small fixed  $q$ . These two quantities first appear to diverge in the same way, but ultimately acquire different temperature dependences.

tor,<sup>38</sup> which we discuss in Sec. IV. Here, currents screen out the effects of Abrikosov vortices exponentially fast, and isolated vortices have a finite energy  $E_v$ . A finite density of such vortices produces a normal material at any nonzero temperature. Taking over arguments of Schmid,<sup>39</sup> we find that the diamagnetic susceptibility  $\chi$  should diverge at low temperatures like the square of a vortex correlation length  $\xi_v$ ,

$$\chi \sim \xi_v^2 \sim \exp(E_v/k_B T) . \quad (1.22)$$

Since the diamagnetic susceptibility is the analog of the Frank constant  $K_3(T)$  in smectics,<sup>26</sup> this result agrees with Eqs. (1.19) and (1.20). In superconductors, however,  $K_1(T) \equiv 0$ , and there is no crossover behavior of the kind we have found for  $K_1(T)$  in smectics.

At very low temperatures and finite wavelengths, we would have to say that two-dimensional smectics are equivalent to two-dimensional superconductors, in agreement with the conclusions of Halperin and Lubensky near four dimensions.<sup>28</sup> There are sufficient differences in the detailed behavior of the two systems, however, to make us uncertain of this equivalence in  $d=3$ . If one considers only defects like dislocations and vortices,  $d=2$  is the lower critical dimensionality for both problems. "Kink" excitations enforce a lower critical dimension  $d=1$  for Ising models in a very similar fashion. As we have seen, however, the behavior of phonon excitations suggest that  $d=3$  is a lower critical dimension for smectics. Nothing special happens for superconductors in  $d=3$ . The character of the smectic- $A$ -nematic transition in  $d=3$ , and, in particular, its equivalence to the superconducting transition, seems to us an open question.

We have also studied the dynamics of the nematic phase at low temperatures, using techniques developed by Ambegaokar *et al.*<sup>40</sup> and Zippelius *et al.*<sup>41</sup> for superfluidity and melting. We find that a simple diffusive model of layer motion, coupled to a finite density of dislocations, gives rise to the characteristic relaxation frequency  $\omega(q)$  of a nematic on a substrate<sup>13</sup>

$$\omega(q) = -i\Gamma_N [K_1^R(q, T)q_x^2 + K_3^R(q, T)q_z^2] . \quad (1.23)$$

This model would be appropriate for smectics on a substrate, or for the Rayleigh-Benard problem.<sup>24</sup> We find critical slowing down at low temperatures, with a nematic kinetic coefficient  $\Gamma_N(T)$  which tends to zero,

$$\Gamma_N(T) \sim \xi_D^{-2} , \quad (1.24)$$

provided  $q\xi_D \leq 1$ . There is also a nonhydrodynamic mode in the nematic phase which exhibits critical slowing down as  $T \rightarrow 0$ . The characteristic relaxation behaves like  $D\xi_D^{-2}$ , where  $D$  is a dislocation diffusion

constant. This is just the characteristic rate for dislocations to diffuse one correlation length.

In Sec. II, we discuss the effective free energies for smectics, cholesterics, and Rayleigh-Benard convective rolls, and how to incorporate dislocations into this description. Translational and orientational order in this model is studied in Sec. III, where we also work out the renormalized nematic Frank constants  $K_1^R(T, q)$  and  $K_3^R(T, q)$ . The properties of a two-dimensional superconductor at low temperature are described in Sec. IV, for comparison. A simple relaxation model of dislocations interacting with layer displacements is constructed and solved in Sec. V.

## II. SMECTICS, CHOLESTERIC, AND CONVECTIVE ROLLS WITH DISLOCATIONS

### A. Effective free energy

In this subsection, we review the connection between standard descriptions of smectics, cholesterics, and Rayleigh-Benard convective rolls, and the two-dimensional version of the effective free energy Eq. (1.2), namely,

$$F = \frac{1}{2} B \int d^2r [(\partial_z u)^2 + \lambda^2(\partial_x^2 u)^2] . \quad (2.1)$$

Throughout this paper,  $\vec{r}$  will denote the two component position vector  $(x, z)$ .

DeGennes<sup>26</sup> has observed that the requirement that the smectic free energy remain invariant under a simultaneous rotation of the nematic molecules and the planes of constant density leads to a coupling between the director field  $\vec{n}(\vec{r})$  and the complex Fourier component of the density  $\psi(\vec{r})$  defined by Eq. (1.3). The Landau-Ginzburg free energy which exhibits this coupling is,<sup>26</sup>

$$F_s = \int d^2r \left\{ \frac{1}{2} (\partial_i + iq_0 \delta n_i) \psi^* M_{ij}^{-1} (\partial_j - iq_0 \delta n_j) \psi + \frac{1}{2} r |\psi|^2 + u |\psi|^4 + \frac{1}{2} K_1 (\vec{\nabla} \cdot \vec{n})^2 + \frac{1}{2} K_3 [\vec{n} \times (\vec{\nabla} \times \vec{n})]^2 \right\} , \quad (2.2)$$

where the twist nematic elastic constant  $K_2$  is absent in two dimensions,  $\delta \vec{n}(\vec{r})$  is the deviation of the director field from a unit vector in the  $z$  direction,

$$\delta \vec{n} = \vec{n} - \vec{z} , \quad (2.3)$$

and  $M_{ij}$  is an "effective-mass" tensor.

The smectic free energy (2.2) simplifies considerably upon making several approximations valid at low temperatures. Well below the mean-field transition temperature, we can neglect fluctuations in the amplitude of  $\psi(\vec{r})$ , and write

$$\psi(\vec{r}) = \psi_0 \exp[iq_0 u(\vec{r})] , \quad (2.4)$$

where the amplitude  $\psi_0$  is given by minimizing Eq. (2.2) with all other quantities held fixed. It is readily seen that  $u(r)$  is just the layer displacement—i.e., the amount by which a surface of constant density is displaced from its equilibrium position. Taking  $M_{ij}$  to be diagonal, with nonzero components  $M_{xx}$  and  $M_{zz}$ , Eq. (2.2) becomes

$$F_S = \int d^2r \left\{ \frac{1}{2} B (\partial_z u + \delta n_z)^2 + \frac{1}{2} D (\partial_x u + \delta n_x)^2 + \frac{1}{2} K_1 (\bar{\nabla} \cdot \bar{n})^2 + \frac{1}{2} K_3 [\bar{n} \times (\bar{\nabla} \times \bar{n})]^2 \right\}, \quad (2.5)$$

with

$$B = \psi_0^2 q_0^2 / M_{zz}, \quad D = \psi_0^2 q_0^2 / M_{xx} \quad (2.6)$$

and where we have ignored constant contributions.

At low temperatures, the director  $\bar{n}(\bar{r})$  becomes locked in a direction normal to the layering. To investigate this further, we assume layering in the  $\hat{z}$  direction, and write

$$\bar{n}(\bar{r}) = (\sin\theta, \cos\theta) \quad (2.7)$$

To quadratic order in  $\theta$ , the smectic free energy becomes

$$F_S = \int d^2r \left\{ \frac{1}{2} B (\partial_z u)^2 + \frac{1}{2} D (\partial_x u)^2 + D \theta \partial_x u + \frac{1}{2} D \theta^2 + \frac{1}{2} K_1 (\partial_x \theta)^2 + \frac{1}{2} K_3 (\partial_z \theta)^2 \right\}. \quad (2.8)$$

Fluctuations in  $\theta(\bar{r})$  cost a finite energy even at long wavelengths, due to the term  $\frac{1}{2} D \theta^2$ . It is convenient to integrate out these fluctuations, and define an effective free-energy functional  $F$  of  $u(\bar{r})$  only, by

$$\exp[-F(\{u\})/k_B T] \equiv \int \mathcal{D}\theta \exp(-F_S/k_B T) \quad (2.9)$$

The functional integral over  $\theta(\bar{r})$  is easily done in Fourier space, and to leading order in the gradients, one finds free energy of the form (2.1), with  $B$  given by Eq. (2.6), and where

$$\lambda^2 = K_1/B \quad (2.10)$$

For a given field  $u(\bar{r})$ , the integrations over  $\theta$  are dominated by those configurations with

$$\theta(\bar{r}) = -\partial_x u(\bar{r}), \quad (2.11)$$

which shows that  $\theta(\bar{r})$  is indeed locked to the layer normal on average.

An effective free energy of the form (2.1) also arises from Brazovskii's model (1.5) of a cholesteric at low temperatures in a "fixed-length" approximation. It is also instructive to see the connection with a more microscopic description of a cholesteric phase. The usual model assumes a modification of the cus-

tomary nematic free energy, namely,<sup>12</sup>

$$F_c = \frac{1}{2} \int d^3r \left\{ K_1 (\bar{\nabla} \cdot \bar{n})^2 + K_2 [\bar{n} \cdot (\bar{\nabla} \times \bar{n}) + q_0]^2 + K_3 |\bar{n} \times (\bar{\nabla} \times \bar{n})|^2 \right\}. \quad (2.12)$$

The second term favors helical distortions. Considering now a cholesteric film in the  $(x, z)$  plane of thickness  $d \sim q_0^{-1}$ , we assume for simplicity that the director  $\bar{n}(\bar{r})$  takes the form

$$\bar{n}(\bar{r}) = \bar{T}(\bar{r}) \times [\hat{z} + (\partial_x u) \hat{x}], \quad (2.13a)$$

with

$$\bar{T}(\bar{r}) = (\cos(q_0 z + q_0 u), \sin(q_0 z + q_0 u), 0), \quad (2.13b)$$

where the phase variable  $u$  varies slowly, and is a function of  $x$  and  $z$  only. Inserting Eq. (2.13) into (2.12), expanding in  $u(x, z)$ , and averaging rapidly fluctuating terms like  $\sin^4[q_0(z + u)]$ , one is led to a two-dimensional effective free energy of the form (2.1) with<sup>42</sup>

$$B = K_2 q_0^2 d, \quad \lambda^2 = \frac{3}{8} K_3 / K_2 q_0^2 \quad (2.14)$$

We have assumed that  $d$  is much greater than a nematic healing length, so that  $\bar{n}(\bar{r})$  is free to rotate independent of the boundary conditions at the substrate.

The connection between the Rayleigh-Benard problem and layered systems in equilibrium has been described by Swift and Hohenberg,<sup>24</sup> who studied the dynamics of a slowly relaxing linear combination  $w(r, t)$  of a temperature deviation and the fluid velocity. They found that the dynamics could be described by a nonlinear Langevin equation,

$$\frac{\partial w}{\partial t} = -\Gamma \frac{\delta F}{\delta w} + \zeta, \quad (2.15)$$

where the Gaussian noise source  $\zeta(\bar{r}, t)$  satisfies

$$\langle \zeta(r, t) \rangle = 0, \quad (2.16a)$$

$$\langle \zeta(\bar{r}, t) \zeta(\bar{r}', t') \rangle = 2k_B T \Gamma \delta(\bar{r} - \bar{r}') \delta(t - t'), \quad (2.16b)$$

and

$$F_{RB} = \int d^2r \left\{ w [\tau + e (\nabla^2 + q_0^2)] w + g w^4 \right\}. \quad (2.17)$$

The quantities  $e$  and  $g$  are taken to be constant near the transition, and  $\tau$  is proportional to the Rayleigh number minus its critical value in the absence of fluctuations.

As can easily be checked, a steady-state solution of the Fokker-Planck equation associated with Eq. (2.15) is a probability distribution proportional to  $\exp(-F_{RB}/k_B T)$ , where  $F_{RB}$  is the Rayleigh-Benard "free energy" (2.17). Thus, equal time correlation



functions can be calculated just as if the convective rolls were in thermal equilibrium. Well below the mean-field transition temperature ( $\tau \ll 0$ ) associated with  $F_{RB}$ , we look for condensation at wave vectors somewhere on the circle in Fourier space,  $|\vec{q}| = q_0$ . Assuming the condensation takes place in the  $z$  direction, we expand  $F_{RB}$  about this state, writing

$$w(\vec{\tau}) = 2 \operatorname{Re}[\psi(\vec{\tau}) e^{iq_0 z}] , \quad (2.18)$$

where  $\psi(\vec{\tau})$ , as usual, is complex, and slowly varying over distances of order  $q_0^{-1}$ . Neglecting fluctuations in the amplitude  $\psi_0$  of  $\psi \equiv \psi_0 \exp(iq_0 u)$ , we find, to leading order in the gradients, the ubiquitous effective free energy (2.1), with

$$B = 8eq_0^4 \psi_0^2, \quad \lambda^2 = \frac{1}{4} q_0^{-2} . \quad (2.19)$$

### B. Dislocations and layered systems

As discussed in the Introduction, the long-wavelength, low-amplitude, phonon fluctuations associated with Eq. (2.1) are sufficient to destroy translational order, but not orientational order in two dimensions. In analogy to other treatments of singularities in two-dimensional materials,<sup>3-8</sup> we would like to assess the additional effect of dislocations on the layered order implied by Eq. (2.1). We first review the standard treatments<sup>26,34</sup> of dislocations embedded in a layered medium.

Consider an isolated dislocation in a layered material. We want to determine the associated displacement field  $u_D(\vec{\tau})$ , which solves the Euler equations associated with Eq. (2.1),

$$(\partial_z^2 - \lambda^2 \partial_x^2) u_D(\vec{\tau}) = 0 , \quad (2.20)$$

subject to suitable boundary conditions. We shall also need the distortion of the layer normals produced by a dislocation,

$$\theta_D(\vec{\tau}) = -\partial_x u_D(\vec{\tau}) . \quad (2.21)$$

The strength of a dislocation is characterized in the usual way<sup>43</sup> by the integral of  $\vec{\nabla} u$  along a path drawn counterclockwise around it which traverses an equal number of layers going up and going down [see Fig. 4(a)]. For a dislocation made by removing  $m$  layers on the right, this path fails to close by  $m$  layer spacings  $d$ ,

$$\oint \vec{\nabla} u \cdot d\vec{\Gamma} = md . \quad (2.22)$$

If layers are *added* on the right,  $m$  is negative.

In order to satisfy this condition, cuts must be introduced to make the function  $u_D(\vec{\tau})$  single valued. By convention, we take this cut to run from the center of the dislocation out the positive  $x$  axis in Fig. 4(a). The function  $u_D(\vec{\tau})$  exhibits a jump discontinuity of size  $md$  across the cut. Considering the effect of the operator  $\partial_z^2 - \lambda^2 \partial_x^2$  near this cut, we see that a source term must be added to Eq. (2.20) to satisfy this boundary condition. Thus, we must solve instead the equation

$$(\partial_z^2 - \lambda^2 \partial_x^2) u_D(\vec{\tau}) = md [\partial_z \delta(z)] \Theta(x) , \quad (2.23a)$$

where  $\Theta(x)$  is the step function

$$\Theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0 \end{cases} . \quad (2.23b)$$

Equation (2.23) is readily solved by Fourier transformation to give

$$\hat{u}_D(\vec{q}) = -\frac{md}{2\pi} \frac{q_z}{q_x(q_z^2 + \lambda^2 q_x^2)} , \quad (2.24)$$

or, returning to real space,

$$u_D(\vec{\tau}) = \frac{1}{4} md \operatorname{sgn}(z) [\operatorname{erf}(x/\sqrt{4\lambda|z|}) + 1] . \quad (2.25)$$

The corresponding layer orientation field is

$$\theta_D(\vec{\tau}) = \frac{1}{4} md \frac{1}{\sqrt{\pi\lambda|z|}} \operatorname{sgn}(z) \exp\left[\frac{-x^2}{4\lambda|z|}\right] . \quad (2.26)$$

These are, of course, results for a single dislocation at the origin. We can obtain these fields for an arbitrary configuration of dislocations by superposition:

$$u_D(\vec{\tau}) = \int d^2 r' m(r') G(\vec{\tau} - \vec{\tau}') , \quad (2.27a)$$

$$\theta_D(\vec{\tau}) = -\int d^2 r' m(r') \partial_x G(\vec{\tau} - \vec{\tau}') , \quad (2.27b)$$

where  $m(\vec{\tau})$  is an integer-valued field specifying the dislocation strength at point  $\vec{\tau}$ , and

$$G(\vec{\tau} - \vec{\tau}') = \frac{1}{4} d \operatorname{sgn}(z - z') \left[ \operatorname{erf}\left[\frac{x - x'}{\sqrt{4\lambda|z - z'|}}\right] + 1 \right] . \quad (2.28)$$

To study the statistical mechanics associated with an array of interacting dislocations, we decompose  $u(\vec{\tau})$  in Eq. (2.1) into a smoothly varying part  $\phi(\vec{\tau})$  and a part due to dislocations,

$$u(\vec{\tau}) = \phi(\vec{\tau}) + u_D(\vec{\tau}) . \quad (2.29)$$

The effective free energy then breaks up into two parts

$$F = F_0 + F_D , \quad (2.30)$$

where

$$F_0 = \frac{1}{2} B \int d^2 r [(\partial_z \phi)^2 + \lambda^2 (\partial_x^2 \phi)^2] \quad (2.31)$$

and

$$F_D = \frac{1}{2} B \int d^2 r_1 \int d^2 r_2 \int d^2 r m(r_1) m(r_2) \times [\partial_z G(\vec{\tau} - \vec{\tau}_1) \partial_z G(\vec{\tau} - \vec{\tau}_2) + \lambda^2 \partial_x^2 G(\vec{\tau} - \vec{\tau}_1) \partial_x^2 G(\vec{\tau} - \vec{\tau}_2)] . \quad (2.32)$$

The dislocation part of the free energy can be simplified by a trick analogous to the use of harmonic conjugates in electrostatics. Let us define a conjugate function  $\tilde{G}(\vec{r})$  to  $G(r)$  by the relation

$$\partial_z \tilde{G}(\vec{r}) = \lambda \partial_x^2 G(\vec{r}) , \quad (2.33a)$$

$$\partial_z G(\vec{r}) = \lambda \partial_x^2 \tilde{G}(\vec{r}) . \quad (2.33b)$$

As can easily be checked, the harmonic conjugate of  $G$  is

$$\tilde{G}(\vec{r}) = \frac{1}{4} d [\operatorname{erf}(x/\sqrt{4\lambda|z|}) + 1] . \quad (2.34)$$

The relations (2.33) allow  $G(\vec{r})$  to be replaced everywhere in Eq. (2.32) by the simpler function  $G(r)$ , which satisfies

$$(\partial_z^2 - \lambda^2 \partial_x^4) \tilde{G}(\vec{r}) = \lambda d \partial_x \delta(\vec{r}) , \quad (2.35)$$

in contrast to Eq. (2.23a). Repeated integrations by parts in Eq. (2.32) then allows us to use this relation to eliminate the integration over  $\vec{r}$ , and obtain finally

$$F_D = \frac{1}{2} \int d\vec{r}_1 \int_{|\vec{r}_1 - \vec{r}_2| > a} d\vec{r}_2 U(\vec{r}_1 - \vec{r}_2) m(\vec{r}_1) m(\vec{r}_2) + E_D \int d^2\vec{r} m^2(\vec{r}) , \quad (2.36)$$

where

$$U(\vec{r}) = B \lambda d \partial_x \tilde{G}(\vec{r}) = \frac{1}{4} B d^2 \left[ \frac{\lambda}{\pi|z|} \right]^{1/2} \exp(-x^2/4\lambda|z|) . \quad (2.37)$$

Note that  $U(r)$  tends to zero for large  $r$ , so that isolated dislocations have a finite energy. We have added a term proportional to  $E_D$  in Eq. (2.36), which gives the energy of an isolated dislocation. This depends in part on microscopic details near the core region, which are not well described by continuum elastic theory. The dislocation interaction  $U(\vec{r})$  is also not well described near the core, so we have imposed the restriction  $|\vec{r}_1 - \vec{r}_2| > a$ , where  $a$  is the core diameter [ $a = O(d)$ ], in Eq. (2.36). Specializing for concreteness to the case of two dislocations with strength  $m_a$  and  $m_b$  at  $\vec{r}_a$  and  $\vec{r}_b$ ,

$$m(\vec{r}) = m_a \delta(\vec{r} - \vec{r}_a) + m_b \delta(\vec{r} - \vec{r}_b) , \quad (2.38)$$

we recover the results of DeGennes<sup>26</sup> and Pershan<sup>34</sup> for this problem.

In order to impose an ultraviolet cutoff on the statistical mechanics implied by Eq. (2.36), it is convenient to convert the integrals in Eq. (2.36) to discrete sums over, say, a square lattice of possible sites for dislocations,

$$F_D = \frac{1}{2} \sum_{\vec{r} \neq \vec{r}'} U(\vec{r} - \vec{r}') m(\vec{r}) m(\vec{r}') + E_D \sum_{\vec{r}} m^2(\vec{r}) . \quad (2.39)$$

The partition function is then,

$$Z = \int \mathfrak{D}\phi(\vec{r}) \exp(-F_0/k_B T) \times \sum_{\{m(\vec{r}) = -\infty\}^{+\infty}} \exp(-F_D/k_B T) . \quad (2.40)$$

The variables  $\{m(\vec{r})\}$  take on all possible discrete dislocation strengths from  $-\infty$  to  $+\infty$ .

### III. EQUILIBRIUM PROPERTIES

#### A. Translational and orientational order at finite temperatures

We are now in a position to study effects of phonons and dislocations on layered systems at finite temperatures. Translational order is measured directly by the Fourier-transformed density-density correlation function. Upon defining

$$\delta\rho(\vec{r}) = \rho(\vec{r}) - \rho_0 \quad (3.1)$$

we find using Eqs. (1.3) and (1.4) that

$$\langle \delta\hat{\rho}(\vec{q}) \delta\hat{\rho}(-\vec{q}) \rangle = 4\rho_0^2 \int d^2\vec{r} e^{i\vec{q}\cdot\vec{r}} \cos(\vec{q}_0 \cdot \vec{r}) \psi_0^2 \times \langle \exp\{iq_0[u(\vec{r}) - u(\vec{0})]\} \rangle . \quad (3.2)$$

Evidently, density correlations are determined by

$$C(\vec{r}) = \psi_0^2 \langle \exp\{iq_0[u(\vec{r}) - u(\vec{0})]\} \rangle , \quad (3.3)$$

and  $\psi(\vec{r}) = \psi_0 \exp[iq_0 u(\vec{r})]$  can be regarded as a kind of translational order parameter. The thermal averages in Eqs. (3.2) and (3.3) are understood to be over an ensemble specified by the free energy (2.31). If we ignore dislocations, the average over the smooth phonon field  $\phi(\vec{r})$  is easily carried out in a cumulant expansion,

$$\langle \psi^*(\vec{r}) \psi(\vec{0}) \rangle = \psi_0^2 \langle \exp\{iq_0[\phi(\vec{r}) - \phi(\vec{0})]\} \rangle \approx \psi_0^2 \exp\left\{-\frac{1}{2} q_0^2 \langle [\phi(\vec{r}) - \phi(\vec{0})]^2 \rangle\right\} . \quad (3.4)$$

The average in the exponential is conveniently evaluated in Fourier space,

$$f(\vec{r}) \equiv \frac{1}{2} \langle [\phi(\vec{r}) - \phi(\vec{0})]^2 \rangle = \int \frac{d^2q}{4\pi^2} \langle \hat{\phi}(\vec{q}) \hat{\phi}(-\vec{q}) \rangle (1 - e^{i\vec{q}\cdot\vec{r}}) . \quad (3.5)$$

where

$$\langle \hat{\phi}(\vec{q}) \hat{\phi}(-\vec{q}) \rangle = \frac{k_B T}{B(q_z^2 + \lambda^2 q_x^4)} . \quad (3.6)$$

Carrying out the integrations in Eq. (3.5), we find

$$f(\vec{r}) = \frac{k_B T}{B} \left\{ \left( \frac{|z|}{4\pi\lambda} \right)^{1/2} \exp(-x^2/4\lambda|z|) + \frac{|x|}{4\lambda} \left[ \operatorname{erf} \left( \frac{|x|}{\sqrt{4\lambda|z|}} \right) \right] \right\}, \quad (3.7)$$

which simplifies in the limits of large  $z$  and  $x$ ,

$$f(\vec{r}) = \frac{k_B T}{B} \left( \frac{|z|}{4\pi\lambda} \right)^{1/2}, \quad x^2 \ll \lambda z \\ = \frac{k_B T}{4B\lambda} |x|, \quad x^2 \gg \lambda z. \quad (3.8)$$

Substituting these expressions into (3.4), we obtain the results (1.8), first derived by Graham.<sup>23</sup>

Again ignoring dislocations, it is very easy to work out correlations in the orientational order parameter  $\vec{N}(\vec{r})$ , defined by

$$N_x(\vec{r}) + iN_z(\vec{r}) = e^{i\theta(\vec{r})} \\ = \exp[-i\partial_x u(\vec{r})]. \quad (3.9)$$

The local layer normal angle is  $\theta(\vec{r}) = -\partial_x u(\vec{r})$ . Proceeding as in the case of translational correlations, we have

$$\langle \vec{N}(\vec{r}) \cdot \vec{N}(\vec{0}) \rangle = \langle \exp[i\{\theta(\vec{r}) - \theta(\vec{0})\}] \rangle \\ \approx \exp\left\{-\frac{1}{2}\langle [\theta(\vec{r}) - \theta(\vec{0})]^2 \rangle\right\}. \quad (3.10)$$

Evaluating the average in the exponent with

$$\theta(\vec{r}) = -\partial_x \phi(\vec{r}), \quad (3.11)$$

one obtains

$$\langle \vec{N}(\vec{r}) \cdot \vec{N}(\vec{0}) \rangle \approx e^{-g(\vec{r})/2}, \quad (3.12a)$$

where

$$g(\vec{r}) = 2 \frac{k_B T}{B} \int_q \frac{d^2 q}{4\pi^2} \frac{q_x^2}{q_z^2 + \lambda^2 q_x^4} (1 - e^{i\vec{q} \cdot \vec{r}}). \quad (3.12b)$$

Since  $g(\vec{r})$  tends to a cutoff-dependent constant at large  $\vec{r}$ , we have

$$\lim_{r \rightarrow \infty} \langle \vec{N}(\vec{r}) \cdot \vec{N}(\vec{0}) \rangle = |\langle \vec{N}(\vec{r}) \rangle|^2 \\ \approx \exp(-k_B T \Lambda / 2\pi B \lambda). \quad (3.13)$$

Equation (3.12b) has been evaluated with a convenient cutoff. There is long-range orientational order in this approximation.

These results for translational and orientational

correlations cannot hold for all separation vectors  $\vec{r}$  at nonzero temperature, because of effects due to a finite density of free dislocations. Because the energy of an isolated dislocation is finite, we expect them with density

$$n_D \approx \frac{1}{a^2} \exp(-E_D/k_B T), \quad (3.14)$$

where  $E_D$  is the energy of a screened isolated dislocation, and should be the same order of magnitude as the dislocation energy appearing in Eq. (3.29). The core diameter  $a$  should be the same order of magnitude as the layer spacing  $d$ . Associated with this dislocation density, there is a correlation length  $\xi_D$  giving the separation between dislocations, which diverges exponentially rapidly at low temperatures.

$$\xi_D \equiv n_D^{-1/2} \approx a \exp(E_D/2k_B T). \quad (3.15)$$

As can be seen from Eq. (2.25), a dislocation produces a translational order parameter  $\psi_0 \exp[iq_0 u(r)]$  which is  $180^\circ$  out of phase far to the right of a dislocation from its value far to the left. The same dephasing takes place immediately above and below an isolated dislocation. For points  $\vec{r}$  and  $\vec{r}'$  separated only in the  $\hat{x}$  direction, significant dephasing of  $\langle \psi(\vec{r}) \psi^*(\vec{r}') \rangle$  will occur only from dislocations within a region centered about the line  $\vec{r} - \vec{r}'$  and bounded by two parabolas. The number of dislocations in this region is of order  $n_D |\vec{r} - \vec{r}'|^3 / \lambda$ . Thus  $\langle \psi(r) \psi^*(r') \rangle$  will begin to fall off significantly when  $|\vec{r} - \vec{r}'|$  exceeds a correlation length perpendicular to the  $\hat{z}$  direction,

$$\xi_{\perp} \approx \lambda^{1/3} n_D^{-1/3}. \quad (3.16a)$$

A similar argument shows that correlations begin to fall off for points separated in the  $\hat{z}$  direction beyond

$$\xi_{\parallel} \approx \lambda^{-1/3} n_D^{-2/3}. \quad (3.16b)$$

The length  $\xi_D$ , used throughout this paper, is just the geometric mean of  $\xi_{\perp}$  and  $\xi_{\parallel}$ ,

$$\xi_D = \sqrt{\xi_{\perp} \xi_{\parallel}}. \quad (3.16c)$$

One can be much more precise about orientational correlations. Correlations in the layer normal angle  $\theta(\vec{r}) = -\partial_x u(\vec{r})$  split into a phonon and dislocation contribution, upon making the decomposition (2.29). In terms of the Fourier-transformed field  $\hat{\theta}(\vec{q})$ , we find

$$\langle \hat{\theta}(\vec{q}) \hat{\theta}(-\vec{q}) \rangle = q_x^2 \langle \hat{\phi}(\vec{q}) \hat{\phi}(-\vec{q}) \rangle \\ + \langle \hat{\theta}_D(\vec{q}) \hat{\theta}_D(-\vec{q}) \rangle, \quad (3.17)$$

where  $\hat{\theta}_D(\vec{q})$  is the transform of Eq. (2.26b)

$$\hat{\theta}_D(\vec{q}) = -iq_x 2\pi \hat{G}(\vec{q}) \hat{m}(\vec{q}) = id \frac{q_z}{q_z^2 + \lambda^2 q_x^4} \hat{m}(q). \quad (3.18)$$

Inserting this result together with Eq. (3.6) into Eq. (3.17), we find that the orientation angle correlation function is determined by correlations in the Fourier-transformed dislocation strength field  $\hat{m}(\vec{q})$ ,

$$\begin{aligned} \langle \hat{\theta}(\vec{q}) \hat{\theta}(-\vec{q}) \rangle &= \frac{k_B T q_x^2}{B(q_z^2 + \lambda^2 q_x^4)} \\ &+ \frac{d^2 q_z^2}{(q_z^2 + \lambda^2 q_x^4)^2} \langle \hat{m}(\vec{q}) \hat{m}(-\vec{q}) \rangle . \end{aligned} \quad (3.19)$$

Because the field  $m(\vec{r})$  is constrained to take only integer values, the average  $\langle \hat{m}(\vec{q}) \hat{m}(-\vec{q}) \rangle$  is quite difficult to evaluate in general. At temperatures such that  $k_B T \gg E_D$ , however, dislocations with very high strengths will be excited, and we can integrate, rather than sum, over their possible values. This "Debye-Hückel" approximation<sup>44-46</sup> can be justified by application of the Poisson summation formula<sup>47</sup> to each summation over  $m(\vec{r})$ . A systematic high-temperature expansion can be obtained in this way, with the first term given simply by integrating, rather than summing, over the  $\{m(\vec{r})\}$ . We also expect the "Debye-Hückel" approximation to hold at long wavelengths at fixed, finite temperatures. For wave vectors  $q$  such that  $q \xi_D \ll 1$ , we imagine regions of size  $q^{-1}$  containing screened dislocations interacting weakly via temperature-dependent elastic parameters  $B(T)$  and  $\lambda(T)$ . One should be able to integrate continuously over the total charge due to the "microscopic" dislocations contained in a region of size  $q^{-1}$ . The temperature dependence of  $B(T)$  and  $\lambda(T)$  will be determined in Sec. III B.

Treating the  $\{m(\vec{r})\}$  as continuous variables, we rewrite  $F_D$  [Eq. (2.39)] in Fourier space

$$F_D = \frac{1}{2} \int d^2 q \left[ \frac{d^2 B \lambda^2 q_x^2}{q_z^2 + \lambda^2 q_x^4} + 2E_D a^2 \right] \hat{m}(\vec{q}) \hat{m}(-\vec{q}) , \quad (3.20)$$

and find immediately that

$$\langle \hat{m}(\vec{q}) \hat{m}(-\vec{q}) \rangle = \frac{k_B T (q_z^2 + \lambda^2 q_x^4)}{d^2 \lambda^2 B q_x^2 + 2E_D a^2 q_z^2 + 2E_D a^2 \lambda^2 q_x^4} . \quad (3.21)$$

Combining this result with Eq. (3.19) we find our final result, correct to lowest order in  $q_x^2$  and  $q_z^2$ ,

$$\langle \hat{\theta}(\vec{q}) \hat{\theta}(-\vec{q}) \rangle = \frac{k_B T}{B \lambda^2 q_x^2 + (2E_D a^2 / d^2) q_z^2} . \quad (3.22)$$

But this is precisely the correlation function one would expect for a two-dimensional nematic liquid crystal, aligned in the  $\hat{z}$  direction, and with Frank constants

$$K_1 = B \lambda^2, \quad K_3 = 2E_D a^2 / d^2 . \quad (3.23)$$

The long-wavelength properties, even for cholesterics and the Rayleigh-Benard problem, are described by the nematic free energy (1.14)!

When the nonlinear terms in Eq. (1.14) are taken into account, it can be shown<sup>35</sup> that the Frank constants  $K_1$  and  $K_3$  become equal at very long wavelengths to a common value  $K$ , so that one actually has

$$F_N = \frac{1}{2} K \int d^2 r (\nabla \theta)^2 \quad (3.24a)$$

and

$$\langle \hat{\theta}(\vec{q}) \hat{\theta}(-\vec{q}) \rangle = k_B T / K q^2 . \quad (3.24b)$$

There is no genuine broken orientational symmetry. Indeed, evaluating Eq. (3.10) using Eq. (3.24) we find algebraic decay of orientational order,

$$\langle e^{2i\theta(\vec{r})} e^{-2i\theta(0)} \rangle \sim r^{-\eta_2(T)} , \quad (3.25)$$

where  $\eta_2(T)$  is given by Eq. (1.17b).

Although free dislocations exist at any finite temperature, disclinations are bound into pairs with a logarithmic attraction by the nematic free energy (3.24a). We can then take over of the theory of Kostertitz and Thouless<sup>3-5</sup> for this problem, and find that disclinations unbind to produce an isotropic phase at a temperature  $T_c$  such that<sup>36</sup>

$$\eta_2(T_c^-) = \frac{1}{4} . \quad (3.26)$$

Both orientational and translational order decay exponentially in this phase.

### B. Behavior of the Frank constants at low temperatures

Strictly speaking, the estimates (3.23) for the nematic Frank constants  $K_1$  and  $K_3$  are only accurate at high temperatures and at wavelengths such that the nonlinear terms in the nematic free energy (1.14) are unimportant. More generally, one would like to determine the fully renormalized Frank constants  $K_1^R(T, q)$  and  $K_3^R(T, q)$  at long wavelengths and at low temperatures. We do this by first determining the temperature dependence of the Frank constants  $\tilde{K}_1(T)$  and  $\tilde{K}_3(T)$ , dressed only by effects due to dislocations. These will then be considered as microscopic input parameters for the renormalization-group theory of two-dimensional nematics,<sup>35</sup> which takes into account nematic nonlinearities.

To determine the temperature dependence of  $\tilde{K}_3(T)$ , we follow DeGennes<sup>26</sup> and apply simple physical arguments developed in the theory of fluctuation diamagnetism in superconductors.<sup>39</sup> We imagine layered systems at finite temperatures to be made up of smectic islands of area  $\xi_B^2$  embedded in a nematic background. Taking over arguments of Schmid,<sup>39</sup> we find that the susceptibility of such a region to bend

$[\bar{n} \times (\bar{\nabla} \times \bar{n}) \neq 0]$  goes like  $\xi_{11}\xi_1 = \xi_D^2$ . Hence, this susceptibility, which is just  $\tilde{K}_3(T)$ , is predicted to diverge,

$$\tilde{K}_3(T) \sim \xi_D^2 \sim \exp(E_D/k_B T) . \quad (3.27)$$

The temperature dependence of  $\tilde{K}_1(T)$  is readily determined from its definition,

$$\tilde{K}_1^{-1}(T) = \lim_{q_x \rightarrow 0} \lim_{q_z \rightarrow 0} q_x^2 \langle \hat{\theta}(\bar{q}) \hat{\theta}(-\bar{q}) \rangle . \quad (3.28)$$

We can see from Eq. (3.19), that the dislocation contribution to  $\tilde{K}_1(T)$  drops out in the limit  $q_z \rightarrow 0$ . Thus the splay elastic is unaffected by dislocations, as one would expect on physical grounds.

$$\tilde{K}_1(T) \sim \text{const} \quad (3.29)$$

as  $T \rightarrow 0$ .

A nematic with different bend and splay elastic constants in two dimensions has been studied using a momentum shell renormalization group by Nelson and Pelcovits.<sup>35</sup> The behavior of a nematic with microscopic Frank constants  $K_1$  and  $K_3$  is related to that of a nematic with Frank constants  $K_1(l)$  and  $K_3(l)$  after a fraction  $1 - e^{-2l}$  of the degrees of freedom have been integrated out. The effective Frank constants  $K_1(l)$  and  $K_3(l)$  satisfy differential recursion relations, namely,

$$\frac{dt(l)}{dl} = \frac{-\Delta(l)t^2(l)}{2\pi\sqrt{1+\Delta(l)}} , \quad (3.30a)$$

$$\frac{d\Delta(l)}{dl} = \frac{-\Delta(l)t(l)[2+\Delta(l)]}{2\pi\sqrt{1+\Delta(l)}} , \quad (3.30b)$$

where

$$t(l) = k_B T / K_1(l) \quad (3.31a)$$

and

$$\Delta(l) = [K_3(l) - K_1(l)] / K_1(l) > 0 . \quad (3.31b)$$

Here, we want to solve these differential equations with initial conditions,  $K_1(l=0) = \tilde{K}_1$ , and  $K_3(l=0) = \tilde{K}_3$ . It is straightforward to show that the quantity which determines  $K_1^R(T, q)$  and  $K_3^R(T, q)$ , namely,

$$f(\bar{q}, K_1, K_3) \equiv \langle \hat{\theta}(\bar{q}) \hat{\theta}(-\bar{q}) \rangle \quad (3.32)$$

transforms as

$$f(\bar{q}, K_1, K_3) = e^{2l} f(e^l \bar{q}, K_1(l), K_3(l)) , \quad (3.33)$$

under the renormalization group constructed in Ref. 35. The renormalized Frank constants are related to  $f(\bar{q}, K_1, K_3)$  by

$$\begin{aligned} k_B T / K_1^R &= q_x^2 f(\bar{q}, K_1, K_3) , \\ k_B T / K_3^R &= q_z^2 f(\bar{q}, K_1, K_3) . \end{aligned} \quad (3.34)$$

The advantage of doing calculations with the renormalized system is that the recursion relations (3.30) drive the system toward a fixed line with  $K_1^* = K_3^* \equiv K$  at low temperatures,

$$\lim_{l \rightarrow \infty} \Delta(l) = 0 . \quad (3.35)$$

The resulting system is like a two-dimensional  $XY$  model, which can be accurately treated using a simple spin-wave theory at low temperatures.<sup>47</sup> At finite wave vectors,  $e^l q$  may grow to be of order of the cut-off  $\Lambda \sim a^{-1}$  before  $\Delta(l)$  becomes very small. At this point, however, fluctuations are unimportant and we can use the linearized theory of a nematic with two Frank constants,

$$K_1^R(T, q) = K_1(l^*) , \quad (3.36a)$$

$$K_3^R(T, q) = K_3(l^*) , \quad (3.36b)$$

where

$$l^* = \ln(\Lambda/q) . \quad (3.36c)$$

This program is implemented in the Appendix, where the recursion relations (3.30) are studied in some detail. The results are summarized in Figs. 6 and 7. At sufficiently small wave vectors  $q$ ,  $K_1^R$  and  $K_3^R$  are essentially equal, and *both* appear to diverge like  $\xi_D^2$ . These Frank constants begin to separate at a locus of critical wave vectors  $q_c(T)$ . A careful solution of the recursion relations is required to determine this critical wave vector, below which nonlinearities enforce equality of the Frank constants. The result is that

$$q_c(T) \sim \frac{1}{a} \exp[-c \exp(E_D/k_B T)] , \quad (3.37)$$

where  $c$  is a numerical constant of order unity. The wavelength necessary to see equality of the Frank constants rapidly becomes of order of the size of the universe with decreasing temperature.

At low temperatures, or at wave vectors greater than this critical value,  $K_1^R$  and  $K_3^R$  diverge with different powers of  $\xi_D$ ,

$$K_1^R \sim \xi_D^{2/3} \left[ \ln \left( \frac{1}{qd} \right) \right]^{2/3} , \quad K_3^R \sim \xi_D^2 , \quad (3.38)$$

as shown in Fig. 7. Although  $K_1^R$  now diverges, the ratio  $K_1^R/K_3^R$  tends to zero

$$K_1^R/K_3^R \sim \xi_D^{-4/3} , \quad (3.39)$$

as one would expect in layered systems. At temperatures such that

$$\xi_D \gg q^{-1} , \quad (3.40)$$

the system behaves like a layered material, decorrelated only by phonon fluctuations.

#### IV. COMPARISON WITH TWO-DIMENSIONAL SUPERCONDUCTORS

As observed by DeGennes,<sup>26</sup> the Landau-Ginzburg free energy for a superconductor bears a striking resemblance to the expression appropriate for a smectic liquid crystal. For a superconductor, we have

$$F_{sc} = \int d^2r \left[ \frac{\hbar^2}{2m} \left| \nabla - \frac{2ie}{\hbar c} \vec{A} \right| \psi \right]^2 + \frac{1}{2} r |\psi|^2 + u |\psi|^4 + \frac{1}{8\pi\mu} (\nabla \times \vec{A})^2 \quad (4.1)$$

which should be compared with Eq. (2.2) for a smectic. Here,  $\psi(\vec{r})$  is a complex order parameter,  $\vec{A}(\vec{r})$  is the vector potential, and  $\mu$  is the magnetic permeability. We assume that  $\vec{A}(\vec{r})$  is a vector in the two-dimensional plane, so that the magnetic field  $\vec{H} = \nabla \times \vec{A}$  is always normal to this plane.

Just as for smectics, we assume  $r < 0$  and neglect amplitude fluctuations, writing  $\psi(\vec{r}) = \psi_0 e^{i\theta(\vec{r})}$ , with

$$\psi_0 \approx \left( \frac{-r}{4u} \right)^{1/2} = \text{const} \quad (4.2)$$

In the Coulomb gauge, ( $\nabla \cdot \vec{A} = 0$ ), the free energy (4.1) becomes, neglecting constant contributions,

$$F_{sc} = \int d^2r \left[ \frac{1}{2} K (\nabla \theta)^2 + 2 \left( \frac{e}{\hbar c} \right)^2 K |A|^2 + \frac{1}{8\pi\mu} (|\nabla \times A|^2) \right] \quad (4.3a)$$

where

$$K = \psi_0^2 \hbar^2 / m \quad (4.3b)$$

Although the phase and vector potential appear to be decoupled [in contrast to the variables appearing in the smectic free energy (2.6)], there is an indirect coupling when Abrikosov vortex solutions of the field equations are taken into account. In fact, the auxiliary condition, analogous to Eq. (2.21) for smectics, which must be satisfied is<sup>48</sup>

$$\int \left[ \nabla \theta - \frac{2e}{\hbar c} \vec{A} \right] \cdot d\vec{T} = 0 \quad (4.4)$$

for any closed contour around a vortex. Because the vector potential enters Eq. (4.4) explicitly, we cannot simply integrate it out, as was done with the layer orientation field in the case of smectics.

If vortices are ignored, the free energy (4.3a) is just what one expects for a superconductor far below the superconducting transition temperature, and one

can readily determine the correlation function which gives the susceptibility  $\chi(q)$  at finite temperatures. Upon defining

$$\chi^{-1}(q) \equiv -q^2 \left[ \delta_{ij} - \frac{q_i q_j}{q^2} \right] \langle \hat{A}_i(\vec{q}) \hat{A}_j(-\vec{q}) \rangle \quad (4.5)$$

we find that

$$\chi(q) = \frac{-1}{4\pi\mu_0 k_B T} - \frac{4(e/\hbar c)^2 K}{q^2 k_B T} \quad (4.6)$$

which diverges as  $q$  tends to zero. We now show that, if vortices are included, the properties are those of a normal material, and the susceptibility is finite at all nonzero temperatures.

Abrikosov vortices have been extensively studied in the literature,<sup>48</sup> so we only quote the necessary results. The strength of an isolated vortex at position  $\vec{r}$  is characterized by the requirement that the wave function  $\psi(\vec{r})$  be single valued,

$$\int \nabla \theta \cdot d\vec{T} = 2\pi m(\vec{r}) \quad (4.7)$$

where  $m(\vec{r})$  is an integer. Upon decomposing  $\theta$  and  $\vec{A}$  into smoothly varying parts  $\phi$  and  $a$ , and contributions due to a collection of vortices,

$$\theta(\vec{r}) = \phi(\vec{r}) + \theta_v(\vec{r}) \quad (4.8)$$

$$\vec{A}(\vec{r}) = \vec{a}(\vec{r}) + \vec{A}_v(\vec{r}) \quad (4.8)$$

where

$$\nabla \times \vec{A}_v(\vec{r}) = 2\pi m(\vec{r}) \quad (4.9)$$

the superconducting free energy  $F_{sc}$  breaks up into two parts,

$$F_{sc} = F_{sc}^{(0)} + F_{sc}^{(v)} \quad (4.10)$$

The analog of the "phonon part" in layered systems is just

$$F_{sc}^{(0)} = \int d^2r \left[ \frac{1}{2} K (\nabla \phi)^2 + 2 \left( \frac{e}{\hbar c} \right)^2 K |\vec{a}|^2 + \frac{1}{8\pi\mu} |\nabla \times \vec{a}|^2 \right] \quad (4.11)$$

while the contribution from a collection of interacting Abrikosov vortices may be written

$$F_{sc}^{(v)} = \frac{1}{2} \sum_{\vec{r} \neq \vec{r}'} U_v(|\vec{r} - \vec{r}'|) m(\vec{r}) m(\vec{r}') + E_v \sum_{\vec{r}} m^2(\vec{r}) \quad (4.12)$$

As in our discussion of layered systems, we restrict the vortices to lattice with spacing of order the core diameter  $a$ . The interaction energy between vortices

is isotropic,<sup>48</sup>

$$U_v(r) = \frac{1}{8} \left( \frac{\hbar c}{e} \right)^2 \frac{1}{\lambda_L^2} K_0 \left( \frac{r}{\lambda_L} \right), \quad (4.13)$$

where  $\lambda_L$  is the London penetration depth,

$$\lambda_L^2 = \frac{mc^2}{8\pi|\psi_0|^2 e^2} \quad (4.14)$$

and  $E_v$  is the finite energy associated with an isolated vortex. The function  $K_0(x)$  is a zero-order Hankel function of imaginary argument, and vanishes exponentially fast for large  $x$ .

We want to calculate the susceptibility, which may be written

$$-\chi^{-1}(q) = \left[ \frac{1}{4\pi\mu_0} + \frac{4}{q^2} \left( \frac{e}{\hbar c} \right)^2 K \right]^{-1} k_B T + \left( \frac{\hbar\pi c}{e} \right)^2 \langle \hat{m}(\vec{q}) \hat{m}(-\vec{q}) \rangle. \quad (4.15)$$

The first term is just the contribution (4.6), obtained neglecting vortices. As in our analysis of layered systems, we can evaluate the vortex-vortex correlation function in Eq. (4.15) with the aid of a "Debye-Hückle" approximation, valid at sufficiently high temperatures. In order to integrate rather than sum over vortex complexions  $\{m(\vec{r})\}$ , we need the vortex free energy in Fourier space, namely,

$$F_{sc}^{(v)} = \frac{1}{2} \int \frac{d^2q}{4\pi^2} \left[ \frac{(\pi\hbar c/e)^2}{8\pi^2[1+(\lambda_L q)^2]} + 2a^2 E_c \right] \times \hat{m}(\vec{q}) \hat{m}(-\vec{q}). \quad (4.16)$$

It is now straightforward to evaluate the susceptibility at small wave vectors. The first term of Eq. (4.15) vanishes as  $q \rightarrow 0$ , and the second gives

$$\chi^{-1}(\vec{q}=0) = -\lim_{q \rightarrow 0} \left( \frac{\pi\hbar c}{e} \right)^2 \langle \hat{m}(\vec{q}) \hat{m}(-\vec{q}) \rangle \quad (4.17)$$

or

$$k_B T \chi(\vec{q}=0) \approx - \left[ \frac{1}{8\pi^2} + 2a^2 E_c \left( \frac{e}{\pi\hbar c} \right)^2 \right]. \quad (4.18)$$

This is the finite, diamagnetic susceptibility one expects in a normal material with superconducting fluctuations.

Since we expect a density of vortices

$$n_v \approx \frac{1}{a^2} \exp(-E_v/k_B T), \quad (4.19)$$

the system should behave like a superconductor on scales less than

$$\xi_v \equiv n_v^{-1/2} \approx a \exp(E_v/2k_B T). \quad (4.20)$$

Applying Schmid's analysis<sup>39</sup> of fluctuation diamagnetism in superconductors, we conclude that  $\chi(\vec{q}=0)$  diverges like  $\xi_v^2$ ,

$$\chi(\vec{q}=0) \sim \exp(E_v/k_B T), \quad (4.21)$$

at low temperatures. The relation between these results, and the corresponding ones for layered systems, was discussed in the Introduction.

## V. DYNAMICS

As is well known, layered systems like smectics and cholesterics have rather different hydrodynamic excitations than nematics.<sup>12</sup> As  $T$  tends to zero, one expects that the nematic phase of these layered materials will support smecticlike excitations at wavelengths less than  $\xi_D$ . A very similar situation arises in one-dimensional Heisenberg and  $XY$  magnets,<sup>49</sup> which exhibit short-wavelength spin waves even though there is no magnetic order at finite temperatures. To study this further, we have constructed a simple model of dislocations interacting with the layer displacement field  $u(\vec{r})$ . The effect of a finite density of moving dislocations on the layer dynamics is to produce the characteristic excitations of a nematic at long wavelengths. This approach allows us to predict the temperature dependence of the kinetic coefficient which characterizes nematic hydrodynamics. We shall rely heavily on techniques developed in studies of the dynamics of superfluids<sup>40</sup> and melting<sup>41</sup> in two dimensions.

### A. Hydrodynamics with dislocations

It is impossible to define a smooth, single-valued displacement field  $u(\vec{r})$  in the presence of dislocations. To make  $u(\vec{r})$  single valued, one must introduce cuts, across which  $u(\vec{r})$  jumps discontinuously. Since following the dynamics of the cuts can be difficult, we work instead with a quantity analogous to the superfluid velocity in a helium film, namely,

$$\vec{\nabla} \equiv (\psi^* \vec{\nabla} \psi - \psi \vec{\nabla} \psi^*) / 2iq_0 \psi_0^2. \quad (5.1)$$

In contrast to  $u(\vec{r})$ ,  $\psi(\vec{r}) = \psi_0 \exp[iq_0 u(\vec{r})]$  is single valued, and only singular at the actual positions of the dislocations. By its construction,  $\vec{\nabla}(\vec{r})$  is just  $\vec{\nabla} u(\vec{r})$ , but with the  $\delta$  functions arising from the cuts excluded.

Since the integral of  $\vec{\nabla}(\vec{r})$  around any closed path is just  $d$  times the enclosed dislocation charge, we have from Eq. (2.22) that

$$\vec{\nabla} \times \vec{\nabla}(\vec{r}, t) = \hat{y} m(\vec{r}, t), \quad (5.2)$$

where  $m(\vec{r}, t)$  is a dislocation charge density,

$$m(\vec{r}, t) = d \sum_{\alpha} m_{\alpha} \delta(\vec{r} - \vec{r}^{(\alpha)}(t)), \quad (5.3)$$

and  $\hat{y}$  is a unit vector perpendicular to the  $xz$  plane. Here  $m_\alpha$  and  $\vec{r}^{(\alpha)}(t)$  are the charge and position of the  $\alpha$ th dislocation. Associated with the dislocation charge density is a dislocation current.

$$\vec{J} = d \sum_{\alpha} m_{\alpha} \frac{d\vec{r}^{(\alpha)}(t)}{dt} \delta(\vec{r} - \vec{r}^{(\alpha)}(t)) , \quad (5.4)$$

and, together, these quantities must satisfy an equation of continuity,

$$\frac{\partial m}{\partial t} + \vec{\nabla} \cdot \vec{J} = 0 . \quad (5.5)$$

Since Eqs. (5.2) and (5.5) can be combined to read

$$\vec{\nabla} \times \left( \frac{\partial \vec{v}}{\partial t} - \hat{y} \times \vec{J} \right) = 0 , \quad (5.6)$$

we must have

$$\frac{\partial \vec{v}}{\partial t} = \vec{\nabla} \Xi + \hat{y} \times \vec{J} , \quad (5.7)$$

where  $\Xi(\vec{r}, t)$  is a smooth function of position.

To complete our specification of the hydrodynamics, it is necessary to know the function  $\Xi(\vec{r}, t)$ . To determine this function, we first propose a simple model of layered hydrodynamics in the *absence* of dislocations. A particularly simple dynamical model is summarized by the equation of motion

$$\frac{\partial u}{\partial t} = -\Gamma \frac{\delta F}{\delta u} + Y , \quad (5.8)$$

where  $F$  is the free-energy functional (2.1), and  $Y(\vec{r}, t)$  is a zero-mean Gaussian Langevin noise source with autocorrelation

$$\langle Y(\vec{r}, t) Y(\vec{r}', t') \rangle = 2k_B T \Gamma \delta(\vec{r} - \vec{r}') \delta(t - t') . \quad (5.9)$$

This would be an appropriate model for a smectic on a substrate in equilibrium with its vapor pressure, so that momentum, energy, and particle number are not conserved. Moreover, the dynamical equation (2.14) of Swift and Hohenberg<sup>24</sup> for Rayleigh-Benard convective rolls reduces to this model when amplitude fluctuations are neglected.

Suppressing for simplicity the noise term in Eq. (5.8), the equation of motion for  $u$  neglecting dislocations is

$$\frac{\partial u}{\partial t} = \Gamma B \partial_z^2 u - \Gamma B \lambda^2 \partial_x^4 u , \quad (5.10a)$$

or, in terms of  $\vec{v} = \vec{\nabla} u$ ,

$$\frac{\partial \vec{v}}{\partial t} = \Gamma B \partial_z^2 \vec{v} - \Gamma B \lambda^2 \partial_x^4 \vec{v} . \quad (5.10b)$$

In order that Eq. (5.7) agrees with the layered hydrodynamics implied by Eq. (5.10) far from any disloca-

tions, we must take

$$\Xi(\vec{r}, t) = \Gamma B \partial_z v_z(\vec{r}, t) - \Gamma B \lambda^2 \partial_x^2 v_x(\vec{r}, t) . \quad (5.11)$$

Our final equation of motion for  $\vec{v}(\vec{r}, t)$  can then be written

$$\frac{d\vec{v}}{dt} = \Gamma B \partial_z^2 \vec{v} - \Gamma B \lambda^2 \partial_x^4 \vec{v} + \hat{y} \times \vec{J} . \quad (5.12)$$

### B. Solution of the model dynamics

To proceed further, we need to close the system of Eqs. (5.5) and (5.12) with an expression giving the dislocation current  $\vec{J}(\vec{r}, t)$  which appears in response to inhomogeneities in the layer spacing and dislocation density. A simple model for dislocation motion is

$$\frac{d\vec{r}^{(\alpha)}(t)}{dt} = m_{\alpha} \underline{D} \vec{f}(\vec{r}^{(\alpha)}) + \vec{\eta}^{(\alpha)}(t) , \quad (5.13)$$

where  $\underline{D}$  is a diffusion matrix and where the Langevin noise source  $\eta_i(t)$  satisfies

$$\langle \eta_i^{(\alpha)}(t) \eta_j^{(\beta)}(t') \rangle = 2\delta_{\alpha\beta} D_{ij} k_B T \delta(t - t') . \quad (5.13a)$$

The quantity  $\vec{f}(\vec{r})$  is the layered analog of the Peach-Koehler force which acts on dislocations in ordinary crystalline materials.<sup>50</sup> It can be extracted from the paper by Pershan,<sup>34</sup> or more directly, by asking for the force on a dislocation at  $\vec{r}^{(\alpha)}$  with strength  $m_{\alpha}$  in the presence of specified layer displacement gradients  $\vec{v}$ . The requirement that this force gives the correct energy of a dislocation pair leads to a force with components

$$f_x(\vec{r}) = B d v_z(\vec{r}) , \quad (5.14a)$$

$$f_z(\vec{r}) = B \lambda^2 d \partial_x^2 v_x(\vec{r}) . \quad (5.14b)$$

The diffusion matrix  $\underline{D}$  should be diagonal in a coordinate system aligned with layers,

$$\underline{D} = \begin{pmatrix} D_x & 0 \\ 0 & D_z \end{pmatrix} . \quad (5.15)$$

By studying the Fokker-Planck equation for the dislocation charge density associated with Eq. (5.13), we easily find that the conserved current density for small inhomogeneities is

$$\vec{J}(\vec{r}, t) = n_D \underline{D} \vec{f}(\vec{r}, t) + k_B T \underline{D} \vec{\nabla} m(\vec{r}, t) , \quad (5.16)$$

where  $n_D \sim \exp(-E_D/k_B T)$  is the equilibrium density of dislocations. That  $\vec{J}$  must have this form is clear on physical grounds. The ratio of the coefficients of  $\vec{f}$  and  $\vec{\nabla} m$  is fixed by the requirement that the current in the presence of a uniform, time-independent force, i.e., when  $m(\vec{r}, t) = n_D \exp(-\vec{f} \cdot \vec{r}/k_B T)$ ,



vanish to lowest order in  $\bar{\Gamma}$ . Equation (5.16) reflects a kind of Einstein relation for the dislocation charges.

Using Eq. (5.16) to eliminate  $\bar{\Gamma}$  from the equation of continuity (5.5) and from Eq. (5.12), it is straightforward to determine the eigenfrequencies of this coupled system of equations,

$$\omega_1(q) = -iD_z(\lambda^2 B dn_D q_x^2 + k_B T q_z^2) , \quad (5.17a)$$

$$\omega_2(q) = -iD_x B dn_D . \quad (5.17b)$$

The first eigenfrequency is exactly what we would expect for a purely dissipative nematic with no conservation laws. To see this, we take as our nematic free energy (1.14) linearized in  $\theta(\bar{\Gamma})$ , with a local alignment in the  $\hat{z}$  direction,

$$F_N = \frac{1}{2} \int d^2r [K_1(\partial_x \theta)^2 + K_3(\partial_z \theta)^2] . \quad (5.18)$$

The simplest relaxational model is

$$\frac{\partial \theta}{\partial t} = -\Gamma_N \frac{\delta F}{\delta \theta} + \dots , \quad (5.19)$$

where the ellipsis represents a noise term and  $\Gamma_N$  is a nematic kinetic coefficient, and the noise brings the system into equilibrium. The characteristic nematic frequency is

$$\omega_N(q) = -i\Gamma_N(K_1 q_x^2 + K_3 q_z^2) , \quad (5.20)$$

which, when compared with Eq. (5.17a), gives the identification

$$\Gamma_N K_1 = D_z B dn_D \lambda^2 , \quad (5.21a)$$

$$\Gamma_N K_3 = D_x k_B T . \quad (5.21b)$$

Taking the ratio of these equations, we find

$$\frac{K_1}{K_3} = \frac{B dn_D \lambda^2}{k_B T} \sim \xi_D^{-2} , \quad (5.22)$$

which checks with our equilibrium results (3.27) and (3.29). Equations (5.21) can only be completely consistent if the nematic kinetic coefficient shows critical slowing down,

$$\Gamma_N \sim \xi_D^{-2} \sim \exp(-E_D/k_B T) \quad (5.23)$$

at very low temperatures.

These results neglect effects of nonlinearities in the nematic free energy (1.4). As discussed in Sec. III B, these drive  $K_1$  and  $K_3$  toward equality at long wavelengths, and cause  $K_1$  to ultimately diverge like  $\xi_B^{2/3}$  at finite wave vectors. We have considered the effects of these nonlinearities on the dynamical model (5.19), and find no significant renormalization of the kinetic coefficient  $\Gamma_N$ . Thus, we conclude that the characteristic frequency  $\omega_N(q)$  is well approximated by

$$\omega_N(q) = -i\Gamma_N [K_1^R(T, q) q_x^2 + K_3^R(T, q) q_z^2] , \quad (5.24)$$

where  $K_1^R$  and  $K_3^R$  were determined in Sec. III B and

$\Gamma_N$  behaves as in Eq. (5.23).

The second eigenfrequency (5.17b) has a very simple physical interpretation. It is associated with the dislocation density  $m(\bar{\Gamma}, t)$ , and is just the rate at which a dislocation diffuses one correlation length.

*Note added in proof.* After this manuscript was submitted, we learned of a number of references which draw attention to defects in the Rayleigh-Benard problem. Graham emphasized the analogy with smectic-*A* liquid crystals in the last part of Ref. 23. A discussion of defects in real experiments has been given by P. Bergé, in *Lecture Notes in Physics: Dynamic Critical Phenomena and Related Topics*, edited by C. P. Enz (Springer, New York, 1979). See also P. Bergé and M. Dubois, in Proceedings of the Symposium: "Systems Far from Equilibrium," Sitges, Spain, June, 1980 (unpublished). The breakup of a square lattice of convective structures in a nematic has been described in a recent preprint by J. M. Dreyfus and E. Guyon. These authors suggest a connection with two-dimensional melting theories.

#### ACKNOWLEDGMENTS

It is a pleasure to acknowledge informative conversations with B. I. Halperin, T. C. Lubensky, P. C. Martin, S. Meiboom, P. Pershan, R. Pindak, and S. Ostlund. The possibility of a connection between the melting theory of Ref. 7 and the Rayleigh-Benard problem was pointed out to us by E. Guyon and R. Graham. This work was supported in part by the NSF under Grant No. DMR77-10210 and through the Materials Research Laboratory. One of us (D.R.N.) acknowledges the receipt of a grant from the Alfred P. Sloan Foundation.

#### APPENDIX: RECURSION-RELATION ANALYSIS OF FRANK CONSTANTS

In this Appendix we calculate the renormalized Frank constants from the recursion relations (3.30):

$$\frac{dt(l)}{dl} = \frac{-\Delta(l)t^2(l)}{2\pi\sqrt{1+\Delta(l)}} , \quad (A1a)$$

$$\frac{d\Delta(l)}{dl} = -\frac{\Delta(l)t(l)[2+\Delta(l)]}{2\pi\sqrt{1+\Delta(l)}} , \quad (A1b)$$

with

$$t(l) \equiv \frac{k_B T}{K_3(l)} , \quad \Delta(l) = \frac{K_3(l) - K_1(l)}{K_1(l)} > 0 ,$$

and the initial conditions

$$K_1(l=0) = \bar{K}_1 , \quad K_3(l=0) = \bar{K}_3 . \quad (A1c)$$

We begin by noting that

$$[\Delta(l) + 2] \frac{dt(l)}{dl} - t(l) \frac{d\Delta(l)}{dl} = 0 , \quad (A2)$$

from which it follows that:

$$\frac{t(l)}{\Delta(l) + 2} = \text{const} \quad (\text{A3})$$

or equivalently,

$$K_1(l) + K_3(l) = \text{const} = 2K_\infty \quad (\text{A4})$$

The reason for this notation is that as  $l \rightarrow \infty$ ,  $\Delta(l) \rightarrow 0$  and hence  $K_1(l = \infty) = K_3(l = \infty) = K_\infty$ . The value of  $K_\infty$  can be evaluated from the initial conditions

$$K_\infty = \frac{1}{2}(\bar{K}_1 + \bar{K}_3) \approx \frac{1}{2}\bar{K}_3 \propto \xi_D^2 \text{ as } T \rightarrow 0 \quad (\text{A5})$$

Thus, at wavelengths such that  $l = \ln(\Lambda/q)$  is large enough that the Frank constants are renormalized to equality, both Frank constants diverge as  $\xi_D^2$  as  $T \rightarrow 0$ . We also have

$$\frac{t}{\Delta + 2} = \frac{k_B T}{2K_\infty} \approx \frac{k_B T}{\bar{K}_3} \quad (\text{A6})$$

Using this relation one can easily solve the recursion relations (A1) when  $\Delta(l) \gg 1$  or  $K_3(l) \gg K_1(l)$ —limits that are certainly satisfied by the initial conditions (A1c). In this limit it follows from Eqs. (A1b) and (A6) that

$$\frac{d\Delta}{dl} = -\frac{\Delta^{5/2}}{2\pi(\bar{K}_3/k_B T)} \quad (\text{A7})$$

which is readily solved for  $\Delta(l)$

$$\Delta(l) = \left[ \Delta^{-3/2}(0) + \frac{3l}{4\pi(\bar{K}_3/k_B T)} \right]^{-2/3} \quad (\text{A8})$$

In the long wavelength ( $l \rightarrow \infty$ ) limit we thus have

$$\Delta(l) \approx \left[ \frac{3l}{4\pi(\bar{K}_3/k_B T)} \right]^{-2/3} \quad (\text{A9})$$

Combining this with Eqs. (A4) and (A5) we can solve for  $K_1(l)$  and  $K_3(l)$ :

$$K_1(l) = \bar{K}_3^{1/3} \left[ \frac{3l k_B T}{4\pi} \right]^{2/3} \propto \xi_D^{2/3} l^{2/3}, \quad (\text{A10a})$$

$$K_3(l) \approx \bar{K}_3 \propto \xi_D^2, \quad (\text{A10b})$$

which gives us the results quoted in Sec. III, upon setting  $l = \ln(\Lambda/q)$ .

The results (A10) were based upon the approximation  $\Delta(l) \gg 1$ , which according to Eq. (A9) clearly breaks down when  $l = l_c \approx \bar{K}_3/k_B T$ . Recalling that  $\bar{K}_3 \propto \exp(E_c/k_B T)$  and  $l = \ln(\Lambda/q)$  we see that this condition is equivalent to  $q_c(l) \approx (1/d) \times \exp[-C \exp(E_c/k_B T)]$ , which is the result quoted in Sec. III. For wave vectors smaller than this, since  $\Delta(l)$  is small, the two Frank constants should both equal  $K_\infty$  and diverge like  $\xi_D^2$ , whereas for  $q \gg q_c(l)$  the results (A10) should hold.

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