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Dislocation-mediated melting of anisotropic layers

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Using the ideas of Kosterlitz and Thouless to describe dislocation-mediated melting of two-dimensional (2D) crystals, we consider the melting of anisotropic layers of molecules. Depending on the symmetry of the Burgers vector of the dislocation most prone to unbind, new types of melting behavior occur. In the most interesting case, the properties of the melted phase are described by three characteristic lengths. There are crossovers between regimes of 2D solidlike, 2D smecticlike, 2D nematiclike, and quasi-isotropic behavior. At the melting temperature, there are divergences in the anisotropic properties of the crystal due to one type of dislocation being free, but the other type being effectively bound. In the presence of an incommensurate crystalline substrate, the 2D smectic properties may be stabilized at large distances giving rise to a distinct smectic phase. Similarly, 2D smectic order may be stabilized by the interactions between the layers of a 3D smectic giving rise to a distinct "bismectic" phase, intermediate between the smectic-*C* and -*H* phases. Consequences of these results for various scattering experiments have been calculated. The general theory of dislocations in an anisotropic 2D solid is worked out in detail in Appendix A with explicit calculations for the interactions between dislocations and the stress and displacement fields associated with them.

I. INTRODUCTION

A. Purpose

The theory of dislocation-mediated melting of two-dimensional solids has recently made much progress based on ideas due to Kosterlitz and Thouless.[1–3] The theory has been developed in greatest detail for the melting of a regular triangular crystal where the elastic properties are the same as for an isotropic, two-dimensional solid.[4–6] In the present paper, we consider the melting of two-dimensional (2D) crystals of lower symmetry, where the elastic properties are anisotropic. We analyze properties of the system just above melting, and find behavior which differs in many important ways from that of the regular, triangular solid.

Phase transitions in isolated layers of smectic liquid crystals are an important potential application of two-dimensional melting theory. Many such systems, however, will be more anisotropic than the regular lattice. In particular, smectic layers may be formed of rodlike molecules, whose axes are aligned along a vector at an angle away from the normal to the layer.[7] The molecular tilt will lead to a distortion of the lattice even if the molecules would otherwise tend to form a regular, triangular lattice.[8] The projection of the orientation vector onto the plane of the layer will generally have a preferred direction relative to the bonds in the solid. In the simplest case which we consider in detail, the molecules align either along or halfway between the bond directions and the solid retains a rectangular symmetry with two perpendicular symmetry axes (see Fig. 1).

A layer of nonspherical molecules adsorbed on a crystalline surface may form an anisotropic 2D solid.[9] If the adsorbate lattice is incommensurate with the substrate,[10, 11] its melting may be described by the theory of the present paper, with some modifications discussed below.

Anisotropic solids have the possiblity of very interesting behavior, since all elementary dislocations[12] are not equivalent, as they are in the regular triangular solid. In the uniaxial solid, two equivalent dislocations, hereafter labeled type I, have their Burgers vector along a reflection symmetry axis and four dislocations (type II), equivalent with each other, but inequivalent with the first type, lie at angles of $\pm\phi_0$ from the reflection axis. The x axis is taken to be the reflection axis coincident with the elementary lattice vector (see Figs. 2 and 3).

The solid phase has dislocations which are tightly bound in pairs. When the temperature is raised, the pairs unbind and destroy the crystalline order. The entropy associated with the creation of a dislocation is $\Delta S = k_B \ln(R^2/a^2)$ where a^2 is the core area and R^2 is the system area. The energy increase of the system is $\Delta U = \frac{1}{2}K \ln(R/a)$, where K is determined by the lattice constant and the elastic constants. Thus the free energy $\Delta F = \Delta U - T\Delta S$ favors the creation

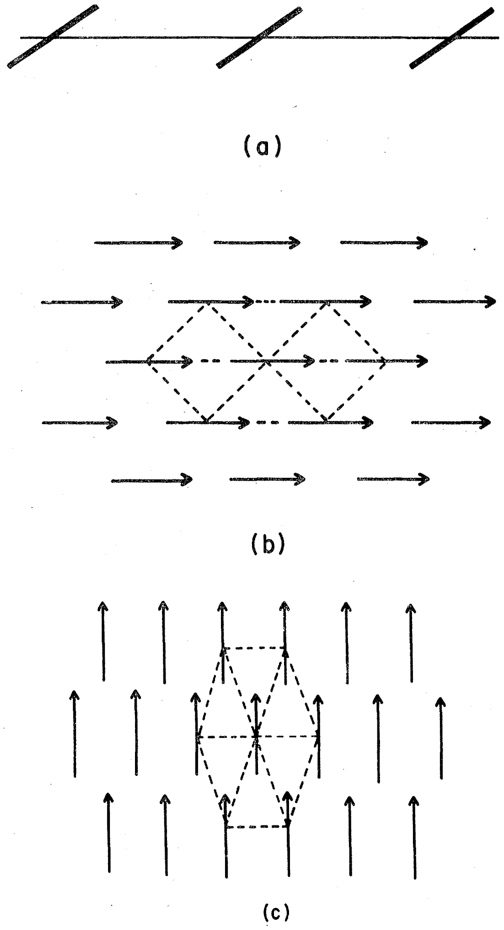

FIG. 1. (a) Side view of a layer of tilted molecules is shown. (b) Top view of the 2D solid phase (smectic-H layer) is shown. The arrow heads indicate the upper end of the rodlike molecule. We have assumed here that the molecular axis projection on the xy plane tend to point along one of the six nearest-neighbor bond directions, so that the arrows form a chain, lying head to tail. Dotted lines indicate bonds of the triangular lattice formed by the centers of the molecules. (c) Same as (b), but here the molecular axis projection lies intermediate between two nearest-neighbor bonds. The arrows line up side by side in rows. In this case, as in (b) there is one bond direction which lies in the relfection plane through the x axis. In this case the molecular axis projection lies halfway between nearest-neighbor bonds, but the reflection symmetry of y remains for elastic properties.

of dislocations above the temperature determined by $k_B T = \frac{1}{4}K$ For the anisotropic solid, the coefficient K depends on the dislocation type, and we shall use the symbols $K_{\rm I}$ and $K_{\rm II}$ for type I and type II. [Formulas for $K_{\rm I}$ and $K_{\rm II}$, in terms of the lattice constants and elastic moduli are given in Eqs. (2.14) and (A29).]

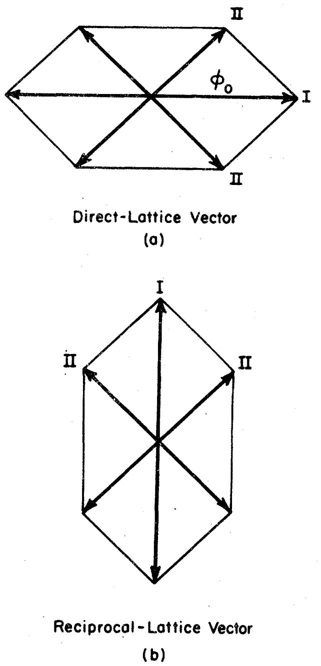

FIG. 2. Six elementary Burgers vectors for the lattice in Fig. 1(b). The type-I lattice vector lies along the x axis, and the type-II dislocation Burgers vector at angles of $\pm\phi_0$ with the x axis. (b) The reciprocal-lattice vectors are shown.

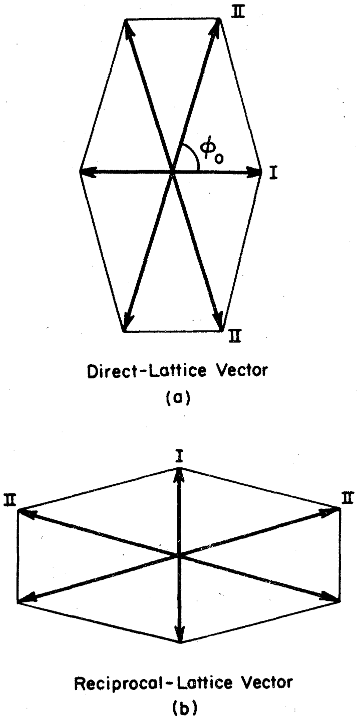

FIG. 3. (a) and (b) are the same as Figs. 2(a) and 2(b), but for the lattice in Fig. 1(c).

Applying the entropy argument of the previous paragraph, either type-I or type-II dislocations would unbind at lower temperature, depending on the relative magnitude of the K_α. Thus, if K_{II} is less than K_{I}, *a priori* type-II dislocations should unbind at a lower temperature than type I. But since a pair of type-II dislcoations oriented at angles of $\pm\phi_0$ from the positive x axis, is indistinguishable from a single type-I dislocation when observed with a resolution large compared to their separation, it follows that type-I dislocations will also be unbound. We call this "type-II" melting. If K_{I} is less than K_{II}, a more complicated situation arises. This is called "type-I melting." Over a large range of lengths, type-I dislocations are free, while type-II dislocations are bound. Nevertheless, the presence of type-I dislocations screens the logarithmic interaction between a pair of type-II dislocations, such that both types of dislocations are free at sufficiently long lengths.

If the molecules in a liquid-crystal layer lie side by side as in Fig. 1(c), the type-I Burgers vector is the short lattice vector. It seems particularly likely that type-I melting will occur in this case.

For both type-I and type-II melitng, the phase just above T_m is characterized by algebraic decay (quasi-long-range order) of orientational correlations, in the limit of large lengths. The melted phase may be described loosely as a two-dimensional nematic[13] where the role of the director in a nematic is taken by the projection $\vec{n}$ of the molecular axis onto the xy plane. (Unlike a true nematic, the orientations $\vec{n}$ and $-\vec{n}$ are distinguishable in the present case. Since the orientation of tilted molecules defines a unique direction in the plane, rather than an axis with two equivalent ends as in a true nematic, the elementary disclination is 360° in the present case, rather than 180° for a true nematic. However, the elastic properties of the two systems are identical.)

In the case of type-I melting, on the intermediate length scale where only type-I dislocations are free, we may describe the system as a *two-dimensional smectic*. The centers of the molecules are arranged in "rows" parallel to the x axis, and it is meaningful to discuss displacements perpendicular to the rows. Properties of a two-dimensional smectic have been discussed recently by Toner and Nelson.[14] At fixed lengths, the smecticlike behavior goes smoothly over to nematiclike behavior without a phase transition as the temperature is raised further above T_m.

If the temperature is raised sufficiently, one will eventually reach a point where *disclinations* appear in the molecular orientation and bond orientation fields, and the quasi-long-range orientational order is lost.[4,5,8] This second transition will not be discussed here; rather we shall concentrate on the properties of the nematic phase, at various intermediate length scales close to the melting temperature T_m. (See however, the discussion in Sec. III C below.)

It should be remarked that an alternative to the dislocation-mediated melting theory, discussed here, is that melting may proceed via a first-order transition, directly from a solid to a fluid. Various computer experiments have been performed to study the melting of simple 2D crystals, made by point particles interacting with r^{-n} and Lennard-Jones potentials and first-order transitions have been claimed in many cases. There is still controversy regarding this point, however.[15–17]

This paper is divided into four major sections. The results of the research are summarized in the remaining section of the Introduction. In Sec. II, we present the details of the investigation of the anisotropic melting analysis as applied to the uniaxial solid. The application of the theory to general anisotropic systems, as well as extensions to 2D layers on substrates and to layers stacked in a three-dimensional smectic is discussed in Sec. III. Section IV contains a discussion of the problems involved in using x-ray or neutron scattering data to investigate the phase transition.

The equations determining the effect of dislocations in a general 2D anisotropic medium have to our knowledge never been worked out in detail.[18,19] The energy between dislocations and the stress and displacement fields generated is calculated in Appendix A using a very simple approach based on Fourier transforms. In Appendix B we calculate the properties of the nematiclike regime by considering it as a solid with free type-I and -II dislocations. In Appendix C, the results of Toner and Nelson[14] are used to calculate properties of the 2D smectic and the 2D smectic-to-nematic crossover, using the smectic Hamiltonian as a starting point.

B. Results for type-I melting

As the temperature approaches the melting temperature T_m from below, all elastic constants remain finite. For the case of type-I melting, the two compliance coefficients S_{1111} and S_{1212} (see Appendix A), approach their melting-point values with a square-root singularity, while the other compliances have dominant regular behavior with very weak singularities which will not be detectable experimentally. The constant K_{I}, defined above, is a relatively complicated function of the compliances, but approaches the universal constant 4, when measured in units of $k_B T$.[20]

Above melting, there are three characteristic lengths, ξ_I, ξ_N, and ξ_S. These obey

$$\xi_S \propto \exp(t^{-1/2}) \quad , \tag{1.1}$$

$$\xi_N \propto \xi_S^{p+1} \quad , \tag{1.2}$$

$$\xi_I \propto \exp(\text{const}\,\xi_S^2) \quad , \tag{1.3}$$

where $t \propto (T - T_m)$ and p is a nonuniversal number greater than zero defined in Eq. (2.37). On a length scale L smaller than ξ_S, the system retains the properties of the two-dimensional solid. When $\xi_S < L < \xi_N$, the system may be described by a smecticlike Hamiltonian, with molecules arranged in rows parallel to the x axis[13, 14]:

$$\frac{H_0^S}{k_B T} = \frac{1}{2} B \int d^2r \left[\left(\frac{\partial u}{\partial y} \right)^2 + \lambda^2 \left(\frac{\partial^2 u}{\partial x^2} \right)^2 \right] . \tag{1.4}$$

Here $u \equiv u_y$ is the displacement of the rows in the y direction. Dislocations with Burgers vector in the x direction are unbound, but there is a vanishingly small density of dislocations with Burgers vector components along the y direction, corresponding to the occurrence of incomplete rows (see Fig. 4). The length λ in Eq. (1.4) diverges as ξ_S^2, while the elastic constant B remains finite, when $T \to T_m^+$. The constants B and λ are computed in Sec. II.

On a length scale $L >> \xi_N$, all types of dislocations are free, and the system is nematiclike, with effective Hamiltonian[13, 14]

$$\frac{H_N}{k_B T} = \frac{1}{2} \int d^2r \left[K_x \left(\frac{\partial \phi}{\partial x} \right)^2 + K_y \left(\frac{\partial \phi}{\partial y} \right)^2 \right] , \tag{1.5}$$

where $\phi(r)$ is the angle between the x axis and the projection of the molecular axis in the xy plane. (The local orientation of nearest-neighbor bonds will be locked to the molecular orientation, so that ϕ may also be interpreted as a fluctuation in the bond orientation field.) For molecules aligned side by side, as in Fig. 1(a), K_x is the Frank constant for *splay* in the molecular orientation, and K_y is the Frank constant for *bend*. The definition of splay and bend is reversed for the end-to-end orientation shown in Fig. 1(b).

Close to T_m, for type-I melting, the "bare" Frank constants K_x^0 and K_y^0, measured on a length scale $L \simeq \xi_N$ will be very anisotropic, with $K_x^0 >> K_y^0$. In particular as $T \to T_m$

$$K_x^0 \propto \xi_S^2 , \tag{1.6a}$$

$$K_y^0 \propto \xi_N^2 , \tag{1.6b}$$

$$K_y^0 / K_x^0 \propto \xi_S^{2p} \to \infty . \tag{1.6c}$$

Fluctuations in the orientation field renormalize K_x and K_y in such a way that they become equal at very long lengths, $L > \xi_I$. The mechanism for this effect is discussed by Nelson and Pelcovits.[21] The value of ξ_I may be enormous for moderate values of t, and this quasi-isotropic regime may be very difficult to observe in practice.

If observations are made at a fixed length scale L, large compared to the molecular spacing, one may pass through all of the above regimes with increasing temperature. Solidlike behavior would occur for temperatures slightly above T_m, smecticlike behavior when $\xi_S(T) < L < \xi_N(T)$ and nematiclike behavior when $\xi_S(T)$ becomes less than L. The quasi-isotropic behavior may be observed if one can reach a regime with $\xi_I(T) < L$. This behavior is summarized in Fig. 5. Of course, these different regimes are not

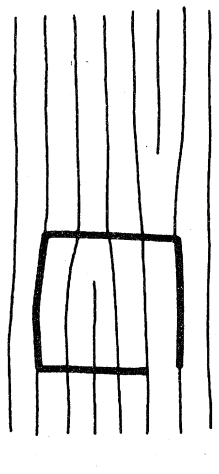

FIG. 4. Schematic diagram of a 2D smectic. There is short-range translational order within a row and longer-range order between the rows. An elementary dislocation in the smectic has a Burgers vector component pointing in the y direction equal to the amount by which the contour (heavy line) fails to close. The x component of the Burgers vector has no significance in the smectic.

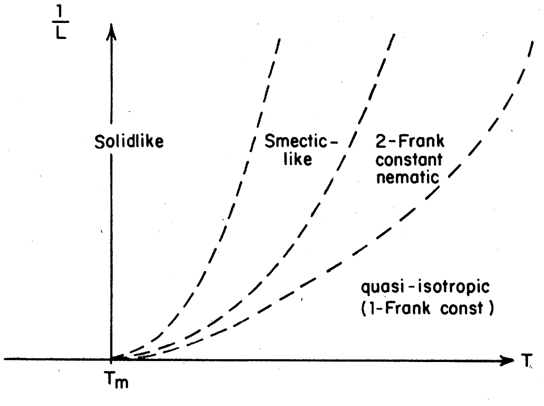

FIG. 5. Four regimes relevant for type-I melting are shown as a function of temperature and $1/L$, the inverse of the experimental length scale. For high temperatures, the system is quasi-isotropic, with one Frank constant. When the temperature is lowered, L falls below the isotropic length scale ξ_I and behavior can be described by a 2D nematic, if $L > \xi_N$. When the temperature is lowered further, there is a crossover to a smecticlike phase and finally when $L < \xi_S$, we see behavior appropriate to a 2D solid. The temperature T_m is the melting temperature which is observed by an experiment on an infinite-length scale.

separated by sharp phase transitions and represent different regimes of the same 2D liquid-crystal phase with short-range translational order and quasi-long-range algebraic decay of orientational order.

It is a peculiarity of two-dimensional smectics that phononlike fluctuations in the displacement of the molecular rows are large enough to destroy correlations in the translational order parameters $e^{i\vec{G}\cdot\vec{u}(\vec{r})}$ for separations larger than a length ξ_p, which we term the phonon correlation length of the smectic. It turns out, however, that ξ_p is not very different in magnitude from the correlation length ξ_S, which determines the crossover from solidlike to 2D smecticlike behavior.

The x-ray structure factor[22] above T_m will have a series of diffuse Bragg rings having a width in reciprocal space comparable to $1/\xi_S$;

$$\delta_q \propto \xi_S^{-1} \ . \tag{1.7}$$

C. Type-II melting

In the case $K_{\text{II}} < K_{\text{I}}$, type-II dislocations are more likely to unbind that those of type I. But since a type-I dislocation can be constructed by adding two type-II dislocations, it follows that the renormalized core energies of the type-I dislocations are roughly twice the type-II core energy. Although some anisotropy remains, there are no real divergences in anisotropic behavior as the temperature approaches the melting temperature. The behavior for this type of melting is summarized in Fig. 6. In particular, there is no smecticlike phase, and the Frank constants obey

$$K_x^0 \propto K_y^0 \propto \xi_S^2 \tag{1.8}$$

as T approaches T_m. The ratio K_x^0/K_y^0 approaches a nonuniversal constant. The nonzero elastic constants all display weak singularities of the type $t^{\bar{\nu}}$, with $\bar{\nu}=\frac{1}{2}$. The coefficient K_{II}, again a relatively complicated function of the compliances, approaches the universal constant 4, and the structure factor $S(q)$ diverges with a half-width which scales like ξ_S^{-1} at all Bragg points.

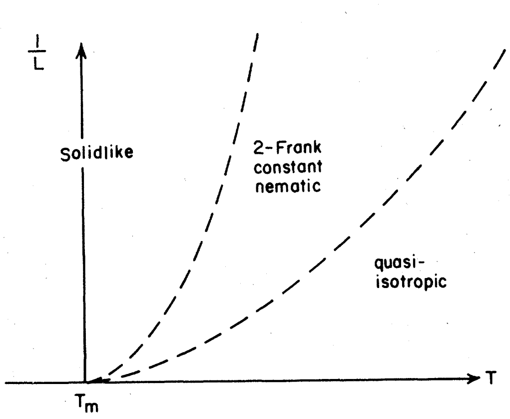

FIG. 6. Three regimes relevant to type-II melting. The crossovers are similar to that for type I, except now there is no intermediate smectic regime.

The only 2D solid for which the dislocation picture give $\bar{\nu}$ not equal to $\frac{1}{2}$ is the regular, triangular solid.[5,6,23] General anisotropic lattices, square, and rectangular lattices all have $\bar{\nu}=\frac{1}{2}$. Only in the isotropic triangular solid do interacting triplets of dislocations affect the behavior at the melting temperature, and give the anomalous value to $\bar{\nu}=0.369\cdots$. For all lattices without a reflection symmetry, the dislocation melting picture gives behavior consistent with type I as discussed in Sec. III B.

D. Anisotropic solid

The study of dislocations in a general anisotropic medium is very complicated, compared to that of isotropic media.[18,24] Considerable simplifications occur in the elasticity theory, when the dimensionality is reduced from 3 to 2, however. The number of elastic constants for a general anisotropic solid in d dimensions is $\frac{1}{8}d(d+1)(d^2+d+2)$, so reducing the dimensionality from 3 to 2 reduces the number of independent elastic constants from 21 to 6. Many of the Green's functions associated with dislocations can be calculated explicitly. The details of these calculations are presented in Appendix A. The results, particularly in the Fourier-transform representation, are surprisingly simple, even for the most general anisotropy. For the uniaxial solid, the reflection symmetry causes all odd elastic constants to be zero and only S_{1111}, S_{1212}, S_{1122}, and S_{2222} remain nonzero.

It is well known that a 2D solid cannot support long-range positional order although the phase can be well described by continuum elasticity theory.[25] The absence of long-range order in the displacement field shows up in the structure factor $S(\vec{q})$ and the Debye-Waller correlation function $C_{\vec{G}}(\vec{R})$. In the absence of dislocations, these are defined by[26]

$$C_{\vec{G}}(\vec{R}) = \langle \exp\{i\vec{G}\cdot[\vec{u}(R)-\vec{u}(\vec{0})]\}\rangle \ , \tag{1.9}$$

$$S(\vec{q}) = \langle |\rho_{\vec{q}}|^2\rangle \approx \sum_{\vec{R}}{}' \exp[i(\vec{q}-\vec{G})\cdot\vec{R}]C_{\vec{G}}(\vec{R}) \ , \tag{1.10}$$

where $\vec{u}(\vec{R})$ is the displacement field at the lattice site $\vec{R}$, while $\vec{G}$ is a reciprocal-lattice vector, and $\rho_{\vec{q}}$ is the density at wave vector $\vec{q}$.

The large distance behavior of $C_{\vec{G}}(R)$ is

$$C_{\vec{G}}(\vec{R}) \simeq (|R|/a)^{-\eta_{ij}G_iG_j} \tag{1.11}$$

$$\equiv (|R|/a)^{-\eta(\vec{G})} \; . \tag{1.12}$$

(Here and henceforth, the convention of summing over repeated Latin indices is implied.) The tensor η_{ij} is a function of the temperature and compliance matrix of the solid and reduces to a function times the unit tensor for the isotropic solid. There is an algebraic decay of the order-parameter correlation function $C_{\vec{G}}(\vec{R})$ which depends strongly on the reciprocal-lattice vector $\vec{G}$ and very weakly on direction of $\vec{R}$ in the lattice. The structure factor near a reciprocal-lattice vector $\vec{G}$ is given by

$$S(\vec{q}) \propto |\vec{q}-\vec{G}|^{-[2-\eta(\vec{G})]} \; , \tag{1.13}$$

showing sharp peaks at the reciprocal-lattice points instead of the δ-function peaks of a conventional solid with long-range order. Note that $S(\vec{q})$ has either a finite cusp or a divergence, depending on the magnitude of $2-\eta(\vec{G})$.

We can define a bond-angle order parameter $\Psi_n(\vec{R}) = e^{ni\phi(R)}$ by considering the orientation $\phi(\vec{R})$ of the lattice relative to a fixed coordinate system. For a solid with only a reflection axis, n is 2, if the local symmetry includes rotations of π; otherwise, $n=1$. For the triangular isotropic solid, $n=6$, and $n=4$ for the square lattice. The solid displays true long-range orientational order, so that the correlation function $C_n(\vec{R})$, defined by

$$C_n(\vec{R}) \equiv \langle \Psi_n(\vec{R}) \Psi_n^*(0) \rangle \tag{1.14}$$

approaches a nonzero constant as $\vec{R} \rightarrow \infty$.

E. Relation to other work

Halperin and Nelson[4,5] and Young[6] have studied in detail the melting of a regular triangular lattice. The sixfold symmetry of the regular case leads to isotropic elastic constants and to six equivalent elementary dislocations. The renormalization group equations for the regular lattice form a singular limit of most of the present equations. In particular the term of order y^2 in the renormalization for the dislocation fugacity y causes the value of the exponent $\bar{\nu}$ in the regular lattice to differ from $\frac{1}{2}$. The angular dependence of the interaction energies between dislocations is simpler than in the present case.

Nelson and Halperin have also discussed many features of the possible phase diagrams for a layer of tilted molecules in Ref. 8, hereafter called (NH). They describe three possible phases in which there is long-range order, or quasi-long-range order in the molecular tilt orientation. One of these phases, labeled H in the phase diagram in NH, is an anisotropic solid with long-range orientational order. This corresponds to a single layer of a (three-dimensional) smectic-H liquid crystal, and is identical to the anisotropic solid of the present paper. A second phase, described as a locked tilted hexatic phase, and labeled C in the phase diagram, is identical to the "nematic-like" melted phase of the present paper, and may be identified with a single layer of a smectic-C liquid crystal. This phase has quasi-long-range order in bond orientations as well as in the molecular tilt orientations, and the two orientations are locked in the sense that the low-energy long-wavelength fluctuations require equal simultaneous fluctuations in both orientations. The melting in the present paper describes the phase transition between the phases H and C. The Frank constants K_x and K_y of the present paper are the principal values of the Frank constant tensor, denoted K_R^+ in NH. The tensor character of the Frank constants was ignored in most of the discussion in NH, partly in order to simplify the discussion, and partly because the two principal values are expected to become equal in the limit of extremely long wavelengths.

In addition to the anisotropic solid H and the nematiclike locked tilted hexatic phase C, there is another possible tilted phase, called the unlocked tilted hexactic, or C^* phase, in NH, for which there is independent quasi-long-range order in the tilt and bond orientations. Here there are three Frank constants (denoted K_1, K_6, and g, in NH) describing, respectively, the energies of gradients in the tilt orientation and bond directions, and the coupling between the two gradients. Each of these Frank constants is itself a tensor with two principal values, if the wavelength is not too large. The C^* phase has no counterpart in the present work.

The phase diagram of NH suggested that a transition of unknown character may occur directly from the solid H phase to the unlocked tilted hexatic C^* phase for a certain range of material parameters. Our present analysis suggests, however, that at least for the case of a dislocation-mediated continuous phase transition, one cannot melt directly from the H to a C^* phase. It was argued in NH that a solid phase with order in the tilt directions will always have true long-range order because of coupling to the shear modes of the crystal, and that the tilt direction is accordingly locked relative to the bond orientation in the solid. A generalization of that argument suggests that when a small number of free dislocations is added to the solid (i.e., the situation is just above melting), the effective Frank constant K_1 for the tilt-orientation fluctuations on the length scale of the dislocation spacing, will be very large, as will the coupling between the bond and tilt orientations. This places the system in the range of parameters where the C^* phase is unstable, and we see that a locked C phase results. The details of the above argument will not be given here.

As the temperature is raised above T_m, a point may be reached where the nematiclike C phase is connected to the unlocked C^* phase. Further temperature increase may then bring about a disclination unbinding transition which converts the C^* into an isotropic 2D liquid (denoted A in NH) with only short-range orientational correlations. Alternatively, there may be a preliminary disclination unbinding transition which converts the C^* to a nontilted hexatic phase, or there may be a disclination unbinding transition directly from the locked C phase to the isotropic 2D liquid-phase A. These various possibilities are discussed in NH.

II. DISLOCATIONS IN THE SOLID

A. Contributions to the compliance matrix

It is convenient to write the elastic constants in terms of a_0^2 and k_BT, where a_0^2 is the area of the unit cell in the solid. Thus

$$S_{ijkl}=(k_BT/a_0^2)\bar{S}_{ijkl} \ . \tag{2.1}$$

$\bar{S}_{ijkl}$ is the compliance in standard units, i.e., area/energy. The reduced Hamiltonian can be written as

$$\frac{H_B}{k_BT}=\frac{1}{2}\int\frac{d^2r}{a_0^2}\,u_{ij}(\vec{r})C^0_{ijkl}u_{kl}(\vec{r}) \ . \tag{2.2}$$

The full strain field, including dislocations is u_{ij} and C^0_{ijkl} is the bare (microscopic) elasticity tensor which is the inverse to the bare compliance S^0_{ijkl} [see Eq. (A2c)]. In the absence of dislocations, the fluctuations in u_{ij} are related to the bare compliance by

$$\int d^2r\,d^2r'\,\langle u_{ij}(\vec{r})u_{kl}(\vec{r}\,')\rangle=S^0_{ijkl}a_0^2\,\Omega \ , \tag{2.3}$$

where Ω is the area of the system. When dislocations pairs are present, the renormalized (macroscopic) compliance tensor S^R_{ijkl} is computed using[5]

$$S^R_{ijkl}=\Omega^{-1}\langle U_{ij}U_{kl}\rangle \ , \tag{2.4}$$

and

$$U_{ij}\equiv-\frac{1}{2}\int_B(u_in_j+u_jn_i)\,dl \ . \tag{2.5}$$

The integral is over the boundary of the solid with free boundary conditions, while $\vec{n}$ is the normal and $\vec{u}$ is the displacement field at the boundary. Ambiquity due to the multivaluedness of $\vec{u}$ is resolved by placing cuts between members of a dislocation pair, or equivalently, by defining cuts from each dislocation to the origin.

Because u_{ij} can be written as the derivative of the displacement field, Eq. (A1b), we find that $S^0_{ijkl}=S^R_{ijkl}$ in the absence of dislocations. This can be checked by using Green's theorem on the displacement field in Eq. (2.3) to convert the interior integral to a boundary integral. Thus the macroscopic compliance is equivalent to the microscopic compliance if there are no dislocations present. In the presence of dislocations pairs, Eq. (2.4) is also a convenient definition for the compliances, because it defines the macroscopic compliance in terms of fluctuations at the perimeter of the solid and is therefore the compliance which is measured in an elasticity experiment. The purpose of this calculation is to find out how S^R_{ijkl} is modified from the bare value when the effects of dislocations are included.

Assume that there are dislocations with Burgers vectors $\vec{b}^1, \vec{b}^2, \ldots, \vec{b}^n$ present in the sample at $\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_n$, and that the average particle density of the system remains constant. Then u_{ij} can be decomposed into

$$u_{ij}=u^D_{ij}+\phi_{ij} \ , \tag{2.6}$$

where u^D_{ij} is the strain which minimizes the energy subject to having the dislocations present [Eq. (A8)] and ϕ_{ij} is the deviation from this minimum. We insert Eq. (2.6) into Eq. (2.2) and add the core energy contribution by the matrix E^c_{ij}, defined so that

$$b_i^\alpha E^c_{ij}b_j^\alpha=E_{\text{core}}(\vec{b}^\alpha)/k_BT \tag{2.7}$$

gives the correct temperature-reduced core energy for the elementary dislocations α. The Hamiltonian takes the form

$$H(\vec{r}_1,\ldots,\vec{r}_n)=H_E+H_D \ , \tag{2.8a}$$

$$\frac{H_E}{k_BT}=\frac{1}{2}\int\frac{d^2r}{a_0^2}\,\phi_{ij}C_{ijkl}\phi_{kl} \ , \tag{2.8b}$$

$$\frac{H_D}{k_BT}=\frac{1}{2}\sum_{u\neq\nu}b_i^\mu b_j^\nu E^{ij}(\vec{r}^\mu-\vec{r}^\nu)+\sum_\mu E^c_{ij}b_i^\mu b_i^\mu \ . \tag{2.8c}$$

The interaction energy $E^{ij}(\vec{R})$ between dislocations is given by Eqs. (A18) and (A28). The cross terms between ϕ_{ij} and u^D_{ij} are zero because we have assumed that ϕ_{ij} is the fluctuation about the minimum u^D_{ij}.

The complete partition function can be calculated by summing over all possible dislocation configurations which preserve vector charge neutrality

$$\sum_\mu b_i^\mu=0 \ . \tag{2.9}$$

This is necessary to avoid infinite dislocation energies. Thus the partition function Z is calculated using

$$Z=\text{Tr}\exp[-(H_E+H_D)/k_BT] \ ,$$

where

$$\mathrm{Tr}=\prod_{\vec{\mathrm{R}}}\int d\phi_{ij}(\vec{\mathrm{R}})\prod_{\alpha=1}^{6}\sum_{n_\alpha=0}^{\infty}\frac{1}{n_\alpha!}\int d^2r_1^\alpha\cdots\int d^2r_{n_\alpha}^\alpha \tag{2.10}$$

subject to the restriction Eq. (2.9), and α ranges over the (six) types of elementary dislocations of the (triangular) lattice. The free energy and compliances are calculated as power series in the fugacities y_α

$$y_\alpha=\exp(-b_i^\alpha b_j^\alpha E_{ij}^c) \tag{2.11}$$

of each type of dislocation α.

To calculate S_{ijkl}^R in the presence of dislocations, the effect of the dislocation on U_{ij} must be considered. By introducing a cut from the origin to each dislocation site $\vec{\mathrm{r}}^\mu$, the full strain field u_{ij} including dislocations can be written as the derivative of a displacement field. Using Green's theorem in this cut plane, using the fact that for the dislocation part $\int_\Omega u_{ij}^D(r)=0$, and the fact that the discontinuity of $\vec{\mathrm{u}}$ across the cut to $\vec{\mathrm{r}}^\mu$ is just $\vec{\mathrm{b}}^\mu$, one finds

$$U_{ij}=U_{ij}^0+U_{ij}^D\ , \tag{2.12a}$$

$$U_{ij}^0=\int d^2r\ \phi_{ij}(r)\ , \tag{2.12b}$$

$$U_{ij}^D=\tfrac{1}{2}a_0\sum_\mu(b_i^\mu r_{\hat{j}}^\mu+b_j^\mu r_{\hat{i}}^\mu)\ . \tag{2.12c}$$

The definition $r_{\hat{j}}^\mu=\epsilon_{ji}r_i^\mu$ has been used where ϵ_{ij} is the antisymmetric tensor. Thus

$$S_{ijkl}^R=S_{ijkl}^0+\Omega^{-1}\langle U_{ij}^DU_{kl}^D\rangle\ . \tag{2.13}$$

The fact that U_{ij}^0 describes fluctuations about the minimum in energy causes the cross term $\langle U_{ij}^DU_{kl}^0\rangle$ to vanish. We define

$$V_\alpha(\theta)=b_i^\alpha b_j^\alpha V_{ij}(\theta)\ , \tag{2.14a}$$

$$K_\alpha=b_i^\alpha b_j^\alpha K_{ij}\ . \tag{2.14b}$$

With the definitions of V_{ij} and K_{ij} given in Eq. (A28), the interaction energy between a ± pair of dislocation of type α at separation $\vec{\mathrm{r}}$ is given by

$$E_\alpha(\vec{\mathrm{r}})=K_\alpha\ln(r/a)+V_\alpha(\hat{r})\ . \tag{2.14c}$$

Equations (2.12) and (2.13) are used to expand the trance to second order in the fugacities:

$$S_{ijkl}=S_{ijkl}^0+\tfrac{1}{4}\sum_{\alpha=1}^{3}y_\alpha^2\int_0^{2\pi}e^{-V_\alpha(\theta)}d\theta\,(b_i^\alpha\hat{r}_{\hat{j}}+b_j^\alpha\hat{r}_{\hat{i}})(b_k^\alpha\hat{r}_{\hat{l}}+b_l^\alpha\hat{r}_{\hat{k}})\int_a^\infty\frac{dr}{a}\left(\frac{r}{a}\right)^{3-K_\alpha}\ . \tag{2.15}$$

Here a is the core radius and $\hat{r}$ is the unit vector determined by θ. The ith component of the vector $\vec{\mathrm{r}}$ rotated by 90° is $\vec{\mathrm{r}}_{\hat{i}}$ [see Eq. (A21)]. The second-order term diverges if any of the K_α are less than 4, and this occurs for the same condition on K_α as for the phase transition predicted by the entropy argument of Kosterlitz and Thouless.

B. Recursion relations

To study the limit as K_α approaches 4, we use the renormalization group ideas of Kosterlitz and Thouless.[1] The integral Eq. (2.15) can be broken into two parts:

$$\int_a^\infty\frac{dR}{a}=\int_a^{ae^\delta}\frac{dR}{a}+\int_{ae^\delta}^\infty\frac{dR}{a}\ . \tag{2.16}$$

Here δ is infinitesimal. The first part is a shell integral which is absorbed into a redefinition of S_{ijkl}^0. The volume integral which remains contributes to a redefinition of y_α^2, after rescaling the length so that the volume integral ranges from a to ∞ again. The core size is effectively increased from a to ae^δ.

There is also another contribution to the redefinition of y_α. Consider the three dislocations $\tilde{a}$, $\tilde{b}$, and $\tilde{c}$ in Fig. 7. When two of the dislocations ($\tilde{b}$ and $\tilde{c}$) coalesce into $\tilde{a}$ as the effective core size is increased, the pair probability of finding a $\pm\tilde{a}$ pair changes. This effectively renormalizes the fugacity of $\tilde{a}$. These ideas lead to recursion relations for S_{ijkl}. We define the following quantities:

$$F_\alpha^{ij}=|\vec{\mathrm{b}}^\alpha|^2\int_0^{2\pi}d\theta\,\hat{r}_i\hat{r}_je^{-V_\alpha(\theta)}\ , \tag{2.17a}$$

$$A_{\alpha\beta}=\int_0^{2\pi}d\theta\exp[b_i^\alpha b_j^\beta V_{ij}(\theta)]\ . \tag{2.17b}$$

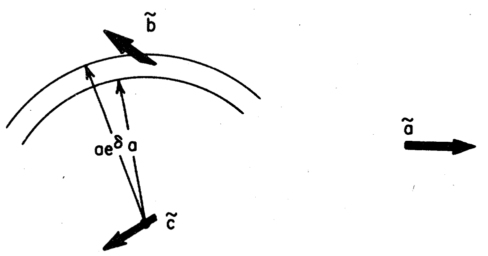

FIG. 7. When the core size is rescaled from a to ae^l, the dislocations labeled $\tilde{b}$ and $\tilde{c}$ effectively coalesce to an $\tilde{a}$ dislocation. This renormalizes the fugacity of the $\tilde{a}$-type dislocations.

The three elementary lattice vectors are $\vec{b}^{\alpha}$, and $\hat{r}$ is determined by θ. The renormalization group takes the form

$$\frac{dS_{1111}}{dl}=y_{\rm I}^2F_{\rm I}^{22}+2y_{\rm II}^2\cos^2\phi_0F_2^{22} \ , \tag{2.18a}$$

$$\frac{dS_{2222}}{dl}=y_{\rm II}^2 2\sin^2\phi_0F_2^{11} \ , \tag{2.18b}$$

$$\frac{dS_{1122}}{dl}=y_{\rm II}^2 2\sin\phi_0\cos\phi_0F_2^{12} \ , \tag{2.18c}$$

$$\frac{dS_{1212}}{dl}=\tfrac{1}{4}y_{\rm I}^2F_{\rm I}^{11}+\tfrac{1}{2}y_{\rm II}^2(\cos^2\phi_0F_2^{11}+\sin^2\phi_0F_2^{22}-2\sin\phi_0\cos\phi_0F_2^{12}) \ , \tag{2.18d}$$

$$\frac{dy_{\rm I}}{dl}=y_{\rm I}(2-\tfrac{1}{2}K_{\rm I})+2y_{\rm II}^2A_{23} \ , \tag{2.18e}$$

$$\frac{dy_{\rm II}}{dl}=y_{\rm II}(2-\tfrac{1}{2}K_{\rm II})+2y_{\rm I}y_{\rm II}A_{12} \ . \tag{2.18f}$$

The vector $b^2=b^{\rm II}$ is determined by ϕ_0 and b^3 is oriented at the angle $\pi-\phi_0$ from the positive x axis and has the same length as b^2. These equations describe fugacities and compliance tensors as function of the rescaling variable l.

It is important to analyze the stability of the resultant equations. A possible mechanism for a dislocation-driven structural transition occurs if the compliances renormalize to their stability limit without the dislocations unbinding. For the uniaxial solid, this would occur if any of the following stability conditions were violated[18]

$$S_{1111}>0, \ \ S_{2222}>0, \ \ S_{1212}>0 \ , \tag{2.19}$$

$$\tilde{D}\equiv S_{1111}S_{2222}-S_{1122}^2>0 \ . \tag{2.20}$$

If λ and μ are real it is easy to check that Eq. (2.19) is preserved since $F_{\alpha}^{ii}>0$ and

$$\lambda^2F_2^{22}+\mu^2F_2^{11}-2\lambda\mu F_2^{12}\geqslant 0 \ . \tag{2.21}$$

We can also show that if $\tilde{D}>0$, then $d\tilde{D}/dl>0$. Thus $\tilde{D}$ is never driven to zero by dislocations, and any singular behavior contributed by the dislocations must be an unbinding transition of the type studied in subsequent sections. The renormalization group does not introduce any divergences in the compliances. From the explicit expression for K_{α}, we find that K_{α} is monotonically decreasing along the trajectory. It follows that all compliances remain finite since K_{α} is bounded below by 4. This, together with the stability conditions is sufficient to assure

$$\lim_{T\to T_m} S_{ijkl}(T)<\infty \ . \tag{2.22}$$

C. Type-I melting

1. Below T_m

Consider the case when $K_{\rm II}>4$, but $K_{\rm I}\simeq 4$. The fixed point for Eq. (2.18) will be determined by $K_{\rm II}>4$ and $K_{\rm I}=4$. Because the term $\frac{1}{2}(K_{\rm II}-2)>0$, the fugacity $y_{\rm II}$ is driven exponentially to zero along a renormalization group trajectory so that the recursions involving $y_{\rm I}$ and $y_{\rm II}$ decouple. The renormalization equations involving $y_{\rm I}$ simplify to

$$\frac{dS_{1111}}{dl}=y_{\rm I}^2F_{\rm I}^{22} \ , \tag{2.23a}$$

$$\frac{dS_{1212}}{dl}=\tfrac{1}{4}y_{\rm I}^2F_{\rm I}^{11} \ , \tag{2.23b}$$

$$\frac{dy_{\rm I}}{dl}=(2-\tfrac{1}{2}K_{\rm I})y_{\rm I} \ . \tag{2.23c}$$

The renormalization group trajectories look like those shown in Fig. 8. The fugacities $y_{\rm I}$ and $y_{\rm II}$ are plotted schematically as functions of

$$S(l)=\frac{S_{2222}(l)}{S_{2222}^*}-\frac{S_{1111}^*}{S_{1111}(l)} \ .$$

The superscript * means evaluated at the fixed point. The quantities $F_{\rm I}^{11}$, $F_{\rm I}^{22}$, and $K_{\rm II}$ are functions of the compliances. Sufficiently close to T_m they may be replaced by the values at T_m, so they are treated as constants in the subsequent discussion. Figure 8 indicates trajectories starting from the initial conditions $y_{\rm I}^0=y_{\rm II}^0$.

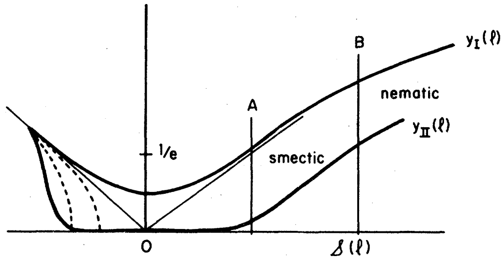

FIG. 8. Dotted renormalization group trajectories show the fugacity $y_{\rm I}$ as a function of $S(l)=S_{2222}(l)/S_{2222}^*-S_{1111}^*/S_{1111}(l)$, chosen with initial conditions in the solid. The heavy trajectories show $y_{\rm II}$ and $y_{\rm I}$ as a function of S for initial condition $y_{\rm I}(0)=y_{\rm II}(0)$ at a temperature just above melting. The upper trajectory is $y_{\rm I}$ and $y_{\rm II}$ is the lower. The number of iterations required to renormalize $y_{\rm I}$ from its starting value to the position A is given by $l_1^*+l_2^*$ and another $p(l_1^*+l_2^*)$ iterations renormalize the fugacity $y_{\rm II}$ so it is finite at B. The type-I dislocations are effectively unbound at A, and all dislocations are unbound at B, so that between the length scales $\exp[(l_1^*+l_2^*)]$ and $\exp[(l_1^*+l_2^*)]$ the system is described as a 2D smectic.

Dividing Eq. (2.23b) by Eq. (2.23a), we find

$$\frac{dS_{1212}}{dS_{1111}}=\frac{1}{4}\frac{F_{\mathrm{I}}^{11}}{F_{\mathrm{I}}^{22}} \quad . \tag{2.24}$$

This immediately determines some properties of the transition. Since the fugacity y_{I} is absent in the equations renormalizing S_{1122} and S_{2222}, the analytic terms in temperature close to T_m will dominate the behavior of these macroscopic elastic constants. The other two compliances, S_{1111} and S_{1212}, exhibit dominant nonanalytic behavior. The ratio

$$\frac{S_{1212}^{R}(t)-S_{1212}^{R}(0)}{S_{1111}^{R}(t)-S_{1111}^{R}(0)}=\frac{1}{4}\frac{F_{\mathrm{I}}^{11}}{F_{\mathrm{I}}^{22}} \tag{2.25}$$

is a well defined, but nonuniversal quantity. [The variable t is proportional to $(T_m-T)/T_m$.]

We expand the renormalization group equations for S_{ijkl} as a function of length scale e^{l} near the fixed point in terms of y_{I} and D, where

$$S_{1111}(l)=S_{1111}^{*}+m(y_{\mathrm{I}}+D) \quad . \tag{2.26}$$

Since S_{ijkl}^{*} is the fixed point value of S_{ijkl}, it coincides with the value of this quantity at the melting temperature. The constant m is to be determined, and D is the deviation from the critical separatrix determined by $D(l)=0$. The quantity $D(l=0)$ is proportional to t since the renormalization group trajectory flows to the fixed point for $D=0$. We find

$$m\frac{dy_{\mathrm{I}}}{dl}+m\frac{dD}{dl}=y_{\mathrm{I}}^{2}F_{\mathrm{I}}^{22} \quad , \tag{2.27a}$$

$$\frac{dy_{\mathrm{I}}}{dl}=m\left[-\frac{1}{2}\left(\left.\frac{\partial K_{\mathrm{I}}}{\partial S_{1111}}\right|_{*}+\frac{1}{4}\frac{F_{\mathrm{I}}^{11}}{F_{\mathrm{I}}^{22}}\left.\frac{\partial K_{\mathrm{I}}}{\partial S_{1212}}\right|_{*}\right)\right] \times y_{\mathrm{I}}(y_{\mathrm{I}}+D) \quad , \tag{2.27b}$$

when the lowest-order terms in y_{I} and D near the fixed point are kept. (An asterisk means evaluated at $S_{ijkl}=S_{ijkl}^{*}$.) Then, setting $D=0$, we find

$$m_{\pm}=\pm\left[-8(F_{\mathrm{I}}^{22})^{2}\Big/\left(4F_{\mathrm{I}}^{22}\left.\frac{\partial K_{\mathrm{I}}}{\partial S_{1111}}\right|_{*}+F_{\mathrm{I}}^{11}\left.\frac{\partial K_{\mathrm{I}}}{\partial S_{1212}}\right|_{*}\right)\right]^{1/2} . \tag{2.28}$$

Since $\partial K_{ij}/\partial S_{mnop}<0$, the constant m^{2} is positive. Below T_m, $m=m_{-}$. Equations (2.27) then simplify to

$$\frac{dD}{dl}=-\frac{F_{\mathrm{I}}^{22}}{m_{-}}y_{\mathrm{I}}D \quad , \tag{2.29a}$$

$$\frac{dy_{\mathrm{I}}}{dl}=\frac{F_{\mathrm{I}}^{22}}{m_{-}}y_{\mathrm{I}}^{2} \quad . \tag{2.29b}$$

Near the melting temperature

$$y_{\mathrm{I}}(l)=\frac{y_{\mathrm{I}}^{0}}{1+\mathrm{const}\,l}\sim l^{-1} \tag{2.30}$$

for large l. For small D, the deviation from the separatrix obeys

$$\frac{dD}{dy_{\mathrm{I}}}=-\frac{D}{y_{\mathrm{I}}} \quad , \tag{2.31a}$$

$$D(l)=D(0)y_{\mathrm{I}}^{0}/y_{\mathrm{I}}(l) \quad . \tag{2.31b}$$

The trajectory breaks away from the incident separatrix and goes rapidly to zero when $D(l^{*})\approx y_{\mathrm{I}}(l^{*})$. Substituting for $y_{\mathrm{I}}(l)$ and $D(l)$ we find that

$$t\propto D(0)\propto(l^{*})^{-2} \quad . \tag{3.32}$$

Since $D(l=0)$ is proportional to t, we have that $l^{*}\propto t^{-1/2}$. We therefore find that at length scales $L>ae^{l^{*}}$, the system behaves like a 2D solid, since there are almost no dislocations present at these lengths. The correlation length is therefore finite in terms of the rescaled core size ae^{l}, so that

$$\xi_{-}\propto\exp(t^{-1/2}) \quad . \tag{2.33}$$

Note that for S_{1111} and S_{1212}

$$[S_{ijkl}^{R}(t)-S_{ijkl}^{*}]\propto t^{1/2} \quad . \tag{2.34}$$

There are cusped singularities in these compliances.

Weak singularities occur in the remaining compliances. The equations which renormalize these are

$$\frac{dS_{2222}}{dl}=y_{\mathrm{II}}^{2}F_{2}^{11} \quad , \tag{2.35a}$$

$$\frac{dy_{\mathrm{II}}}{dl}=y_{\mathrm{II}}(2-\tfrac{1}{2}K_{\mathrm{II}}) \quad . \tag{2.35b}$$

From the second of these equations, we see

$$y_{\mathrm{II}}(l^{*})=y_{\mathrm{II}}^{0}e^{-pl^{*}} \quad , \tag{2.36}$$

where $p=\frac{1}{2}K_{\mathrm{II}}-2$. Using the explicit form for K_{II} [Eqs. (2.14) and (A33)], and the fact that $K_{\mathrm{I}}=4$ at the melting temperature, one obtains

$$-p=2\left[1-\frac{|b^{\mathrm{II}}|^{2}}{|b^{\mathrm{I}}|}\left(\cos^{2}\phi_{0}+\frac{S_{2222}^{*}}{S_{1111}^{*}}\sin^{2}\phi_{0}\right)\right] \quad . \tag{2.37}$$

From Eqs. (2.35a) and (2.35b)

$$\frac{dS_{2222}}{dy_{\mathrm{II}}}\propto y_{\mathrm{II}} \quad . \tag{2.38}$$

Similar equations hold for S_{1122}. Thus the nonanalytic contributions to S_{1122} and S_{2222} take the form

$$S_{ijkl}^{R}(t)-S_{ijkl}^{*}\propto\xi_{-}^{-2p} \quad , \tag{2.39a}$$

where

$$\xi_{-}\equiv a_{0}e^{l^{*}}\propto\exp(t^{-1/2}) \quad . \tag{2.39b}$$

The singularity Eq. (2.39a) is extremely weak, and will not be detected experimentally. Various relations between $\eta(\vec{G})$ [Eq. (A43)] for different $\vec{G}$ can be derived at the melting temperature by using $K_{\rm I}=4$, $K_{\rm II}=4+2p$, and Eq. (A40).

2. *Above T_m*

For initial conditions corresponding to a temperature above T_m, renormalization group trajectories follow the incident separatrix until $l=l_1^*$, break away and join the outgoing separatrix determined by $y_{\rm I}=m_+[S_{1111}(l)-S_{1111}^*]$ for another l_2^* iteration. Here $y_{\rm I}$ is again small but of order unity. The length $\xi_S \simeq a_0 \exp(l_1^*+l_2^*)$ is therefore the characteristic separation between free type-I dislocations. The fugacity $y_{\rm II}$ decreases exponentially, however, even as $y_{\rm I}$ is increasing on the outgoing separatrix because the second $y_{\rm I}y_{\rm II}$ term renormalizing $y_{\rm II}$ in Eq. (2.18f) is not sufficient to overcome the first term (see Fig. 8). At the length scale ξ_S it is appropriate to make a continuum approximation for the type-I dislocations and we treat them in a Debye-Huckel approximation as a gas which effectively screens the remaining type of dislocation. At this length, the fugacity $y_{\rm II}$ is very small, and is given by

$$y_{\rm II}=y_{\rm II}^0 \exp[-p(l_1^*+l_2^*)] \ . \qquad (2.40)$$

To analyze the phase just above melting we generate an effective Hamiltonian for the remaining dislocations.

We decompose the original dislocation Hamiltonian into interactions between x- and y-component Burgers vectors. In Fourier space, this is the transform of Eq. (2.8c), and is given by

$$\frac{H_D}{k_BT}=\frac{1}{2}\int d^2k \left[\frac{|k_x b_y(\vec{k})-k_y b_x(\vec{k})|^2}{k^4 Q(\vec{k})} + 2a^2 E_{ij}^c b_i(\vec{k}) b_j(\vec{k}) \right] \ . \qquad (2.41)$$

$Q(k)$ is defined in Eq. (A21c) and is a quartic polynomial in $(k_i/|k|)$. In the Debye-Huckel approximation the variable $b_x(k)$ may be integrated over freely. After completing the square in b_x, there is an effective interaction between dislocations with Burgers vector components in the $\hat{y}$ direction given by

$$\frac{H_D^S}{k_BT}=\frac{1}{2}\int d^2k \left[\frac{2a^2 k_x^2 E_{11}^c}{k_y^2+2a^2E_{11}^c k^4 Q(\vec{k})} + 2a^2E_{22}^c \right] \times |b_y(\vec{k})|^2 \ , \qquad (2.42)$$

where a^2, and E_{ij}^c, are the values of the renormalized quantities at $l=l_1^*+l_2^*$;

$$E_{11}^c=1 \ , \qquad (2.43a)$$

$$E_{22}^c=-\ln(y_{\rm II})=p(l_1^*+l_2^*) \ , \qquad (2.43b)$$

$$a=\xi_S \ , \qquad (2.43c)$$

and $Q(\vec{k})$ may be evaluated using the elastic constants at T_m. For small values of the wave vector k, the term involving k^4Q is important only when k is close to the x direction. Then, using the definition Eq. (A21c), one finds $k^4Q \simeq k_x^4 S_{2222}^*$. Equation (2.42) takes on a form appropriate for the dislocation Hamiltonian of a 2D smectic[27]:

$$\frac{H_D^S}{k_BT}=\frac{1}{2}B\int d^2k \left[\frac{(\lambda k_x)^2}{k_y^2+\lambda^2 k_x^4} + \frac{2a^2E_s}{B} \right] |b_y(\vec{k})|^2 \ , \qquad (2.44)$$

where

$$B=(S_{2222}^*)^{-1}, \ \lambda^2=2a^2E_{11}^c S_{2222}^*=2\xi_S^2 S_{2222}^* \ ,$$

$$E_s=E_{22}^c=p(l_1^*+l_2^*) \ . \qquad (2.45)$$

This Hamiltonian is discussed in the Appendix C, and in more detail in Ref. 14. The potential energy between dislocations is short ranged and highly anisotropic.

If we were to use Eq. (2.41) at the stage where the length scale equals ξ_S, ignore the discreteness of the Burgers vectors and integrate over them in the Debye-Huckel approximation, we would find (see Appendix B)

$$\langle \phi(\vec{k})\phi(-\vec{k}) \rangle = (2a^2E_{ij}^c k_i k_j)^{-1}\Omega \ . \qquad (2.46)$$

Using this, we would identify the Frank constants in Eq. (1.5) as

$$K_x=2a^2E_{11}^c \ ,$$
$$K_y=2a^2E_{22}^c \ , \qquad (2.47)$$

where a and E_{ij}^c are given in Eq. (2.43). This procedure is not correct, however, unless E_{ij}^c is $\lesssim 1$. It is necessary to take the discreteness of b_y into account. Following the procedure of TN, we work with the smectic Hamiltonian in Eq. (2.44).

Further length rescaling, rescales $y_{\rm II}$ by the area, so that after l_3^* more iterations, $y_{\rm II}$ is also finite and of the order 1. This can be written

$$1=\exp(l_3^*)\exp[-p(l_1^*+l_2^*)]$$

so that $l_3=p(l_1^*+l_2^*)$. We can now apply the Debye-Huckel approximation to the remaining Burgers vectors, and describe the system by a gas of free, interaction dislocations of all types. The length at which this is done determines the mean distance ξ_N between dislocations with Burgers vectors components in the y direction.

We then find the result that at these lengths the bare values of K_x and K_y obey

$$K_x^0 \propto \xi_S^2, \quad K_y^0 \propto \xi_N^2 >> K_x^0 \ . \tag{2.48}$$

The higher-order terms in the Hamiltonian [terms such as $(\nabla \cdot \vec{n})^4$], renormalize the Frank constants to equality[21] at very large length scales $L > \xi_1$ given by Eq. (1.3). For smaller length scales, the dislocation-renormalized Frank constants K_x^0 and K_y^0 are measured.

For any fixed length scale, as the temperature approaches the melting temperature from above, the inequality $L > \xi_N(T)$ will cease to be valid. The continuum approximation for the b_2 dislocations is then invalid and the system is effectively described by the smectic Hamiltonian Eq. (2.44) when $L > \xi_S$. When $L < \xi_S$, behavior appropriate to a 2D solid occurs.

There is an important difference between the smecticlike phase considered here, and the smectic considered in Ref. 14. That smectic occurs only at zero temperature and as the temperature is lowered toward zero, the phonons with displacements along the y directon disappear simultaneously with the fugacities of the dislocations. In the smectic considered in the present work, the renormalized fugacity vanishes as the transition is approached, but the phonons remain since the temperature is finite at the transition.

The structure factor $S(\vec{q})$ shows interesting critical behavior. Using the formula[5]

$$S(\vec{G}) = \exp\left(2l - \int_0^l dl' \, \eta_{\vec{G}}(l')\right) S(\vec{G})|_l \tag{2.49}$$

we find that

$$S(\vec{G}) \propto \xi_S^{2-\eta(\vec{G})} S(\vec{G})|_{l_1^* + l_2^*} \ . \tag{2.50}$$

Since $S(\vec{G})$ is finite for a smectic for $\vec{G}$ both parallel and perpendicular to the rows, we find

$$S(\vec{G}) \propto \xi_S^{2-\eta(\vec{G})} \ . \tag{2.51}$$

There are longer-range correlations in the y direction, and although the ratio $S(\vec{G}_x = 0)/S(G_x \neq 0)$ may be quite large, all true divergences should be accounted for by the value of $\eta(\vec{G})$. The width across the Bragg peak in the y direction is complicated by the existence of the two length scales ξ_N and ξ_P, for dislocations and phonons, respectively. The shape of the structure factor is discussed in more detail in Sec. IV.

The free energy scales like ξ_S^{-2}, so there are only essential singularities in the specific heat which cannot be detected in experiments, although in analogy with the xy model, there may be a broad specific-heat maximum just above T_m.[28]

It is worth digressing to discuss the consistency of the picture of the 2D smectic regime above T_m. This regime can either be though of as a solid, with phonons and free type-I dislocations via the Hamiltonian Eqs. (2.8b) and (2.8c), or as a 2D smectic. We define the distance between the rows of the smectic to be u. The Hamiltonian for the smectic must have the form:

$$\frac{H}{k_B T} = \frac{1}{2} B \int d^2r \left[\left(\frac{\partial u}{\partial y} \right)^2 + \lambda^2 \left(\frac{\partial^2 u}{\partial x^2} \right)^2 \right] \ . \tag{2.52}$$

We have shown that the type-I dislocated solid gives the effective energy Eq. (2.44) between type-II dislocations, and Pershan[27] has shown that the smectic Hamiltonian Eq. (2.52) leads directly to the same energy between y dislocations. For consistency, it is necessary to verify that the dislocated-solid picture indeed gives fluctuations in the y position of the molecules in accord with Eq. (2.52).

In the dislocated solid there are two contributions to the fluctuations in the y displacements: $u = \phi_y + u_y^D$. The smooth "phonon" part ϕ_y is determined directly by Eq. (2.2) via the elastic tensor, and the dislocation part u_y^D is determined in Eqs. (A22) and (A25) by b^1 dislocations. The y- displacement correlation function $C_{yy}(\vec{k})$ is defined as

$$C_{yy}(\vec{k}) = \frac{1}{\Omega} \langle u_y(\vec{k}) u_y(-\vec{k}) \rangle \ . \tag{2.53}$$

It is given as the sum of C_{yy}^D due to dislocations and C_{yy}^P due to ϕ_y:

$$C_{yy}(\vec{k}) = C_{yy}^D + C_{yy}^P \ . \tag{2.54}$$

The quantity C_{yy}^P is calculated in Eq. (A38) as

$$C_{yy}^P = (\tilde{V}^{-1})_{22} \ . \tag{2.55}$$

The dislocation part requires a bit more work.

The correlation $B_{11}(\vec{k})$ between type-I dislocations in the absence of type-II dislocations is given by the $E_{22} \rightarrow \infty$ limit of Eq. (B2). Using this, together with the formula (A25) of the y displacement generated by a type-I dislocation it can be shown that

$$C_{yy}^D = \frac{S_{2222}}{k_y^2 + E_{11} S_{2222} k_x^4} - (V^{-1})_{22} \ . \tag{2.56}$$

(For convenience, the notation $E_{ij} = 2a^2 E_{ij}^c$ has been used.) The last term in the above expression exactly cancels the contribution C_{yy}^P in the expression for C_{yy} so that

$$C_{yy}(k) = \frac{S_{2222}}{k_y^2 + E_{11} S_{2222} k_y^4} \ . \tag{2.57}$$

This is precisely the correlation function one obtains from the smectic Hamiltonian Eq. (2.52) after the identification $B=(S_{2222})^{-1}$, and $B\lambda^2=E_{11}$. Note that type-I dislocations do not affect the single valuedness of the y displacements, so there are no ambiguities in writing the Hamiltonian in terms of gradients of a displacement.

D. Type-II melting

Type-II melting occurs when $K_{\rm II}<K_{\rm I}$. The fixed point for the renormalization group is determined by $K_{\rm II}=4$, and $K_{\rm I}>4$. The analysis is similar to that in the previous section when $T<T_m$. For all pairs of compliances, the relationships analogous to Eq. (2.25) hold. The ratio, which of course depends on the particular pair of compliances, is a well defined but nonuniversal quantity. The singularities in all compliances obey Eq. (2.34), so that again $\bar{\nu}=\frac{1}{2}$. Furthermore, a special combination

$$2S_{1212}+S_{1122}-\tfrac{1}{2}[\cot^2(\phi_0)S_{2222}+\tan^2(\phi_0)S_{1111}] \tag{2.58}$$

has a weaker nonanalyticity of the form $t^{3/2}$. This is obtained by using $y_{\rm I}\approx y_{\rm II}^2$, apparent from Eq. (2.18f) and the recursion relation for this linear combination which depends only on $y_{\rm I}^2$.[29] The relation $y_{\rm I}\approx y_{\rm II}^2$ must hold throughout the renormalization group trajectory and is a direct consequence of the fact that two type-I dislocations add to form a type II. Thus $y_{\rm I}$ is not driven to zero and both types of dislocations unbind at the same length scale. No smecticlike phase occurs and we find $\xi_N=\xi_S\propto\exp(t^{-1/2})$. Two Frank constants are measured on the length scale $\xi_S\lesssim L<<\xi_I$, and both Frank constants diverge like ξ_S^2 at T_m. The width of the peaks in the structure factor diverges as $1/\xi_S$ as the temperature approaches that of melting. There are essential singularities in the free energy and specific heat.

III. GENERALIZATIONS TO OTHER SYSTEMS

A. Melting of square lattices

Square lattices exhibit type-II melting, and most of the results discussed in the previous section remain valid. In this case $S_{1111}=S_{2222}$, and $y_{\rm I}=y_{\rm II}$. Since there are no canceling triplets of elementary dislocations, $\bar{\nu}=\frac{1}{2}$. Equations (2.25) and (2.34) hold for all compliances except S_{1122}. This compliance exhibits a $t^{3/2}$ singularity, which is weaker than the analytic term proportional to t since the first term renormalizing S_{1122} is of order $y_{\rm I}^4$. Equation (2.51) remains valid for all $\vec{G}$.

B. Melting of an anisotropic lattice without reflection symmetry

Except for the square lattice, type-II melting can only occur in a lattice where two elementary dislocations, equivalent under a symmetry operation, add to form a third elementary lattice vector. If there is no reflection symmetry axis for the underlying lattice, the dislocation-mediated melting must be of type I.

For such a system, the scattering at the reciprocal-lattice vectors perpendicular to the axis whose dislocations unbinds at lowest temperature, will be most intense and narrow. The ratio of scattering intensities and widths of this scattering is given by Eqs. (1.7) and (2.51). The constant p is again a nonuniversal number of order unity. Furthermore, all compliances, including the odd ones, will exhibit cusped singularities of the type $t^{1/2}$. Special linear combinations of the compliances will exhibit essential singularities, analogous to S_{1122} and S_{2222} for type-I melting combinations, but these linear combinations now depend on the lattice structure. The Frank constants again diverge according to Eq. (2.38), and the appropriate phase diagram is given in Fig. 5.

C. Effects of a substrate

Nelson and Halperin have considered in some detail the effect of a substrate on the melting of an adsorbed layer when the adsorbate lattice has hexagonal symmetry. If the substrate periodicity is incommensurate with the adsorbate or if it is commensurate at a sufficiently high order, the most important effect of the substrate is to introduce a discrete set of preferred directions for the adsorbate structure. By expanding about one of the preferred orientations, one may represent the effect of the substrate by a term in the Hamiltonian of the form

$$\frac{H_A}{k_BT}=2\gamma\int\theta^2(r)\frac{d^2r}{a_0^2} \tag{3.1a}$$

$$=\tfrac{1}{2}\gamma\int(\vec{\nabla}\times\vec{u})^2\frac{d^2r}{a_0^2}\ , \tag{3.1b}$$

where the angle $\theta(\vec{r})$ describes the deviation of the bond orientations from the favored direction and γ is a new effective elastic constant.

The new elastic term Eq. (3.1) modifies the interactions between dislocations in the regular solid by changing the ratio between the coefficients of the logarithmic and angular terms. This modification has relatively little effect on the melting transition at the temperature T_m where free dislocations appear, but the coupling to the substrate does affect the nature of the orientational order in the melted phase. There should now be true long-range order, instead of the quasi-long-range order predicted for the hexatic phase in the absence of a substrate. The disclination unbinding transition between the hexatic and isotropic liquid phases which occurs at a temperature T_i (higher than T_m) in the absence of a substrate, may be suppressed entirely or will be modified substantially, according to whether there exists one or several distinguishable favored orientations for the adsorbate relative to substrate, at temperatures just above T_m.

If the adsorbate consists of molecules whose axes are tilted away from the normal to the substrate, the substrate anisotropy will lead to a set of favored directions for the tilt orientation as well as for the orientations of bonds in the adsorbate. Since we consider the tilt orientation to be locked to the bond orientation, however, we may simply identify the bond orientation angle $\theta(\vec{r})$ in Eq. (3.1a), with the tilt orientation $\phi(\vec{r})$, and use this equation to describe the effect of the substrate. To generalize many of the formulas of the present paper we use an asymmetric bare elasticity tensor C^A_{ijkl},

$$C^A_{ijkl}=C^0_{ijkl}+\gamma\epsilon_{ij}\epsilon_{kl} \ , \tag{3.2}$$

where the symmetric part C^0_{ijkl} will be roughly the elasticity tensor of the unperturbed adsorbate. The interchange symmetry for ij and kl is no longer valid, and this is reflected in the inverse tensor S^A_{ijkl} being determined by

$$C^A_{ijkl}S^A_{klmn}=\delta_{im}\delta_{jn} \ . \tag{3.3}$$

Note the difference with Eq. (A2c). Care must be taken when attempting to understand the singular $\gamma\rightarrow 0$ limit.

It is possible to work out in detail the effects of term Eq. (3.1) on the interaction between two dislocations separated by a vector $\vec{R}=[R\cos(\theta), R\sin(\theta)]$ in an anisotropic medium.[30] As in the isotropic case, one finds a change in the form of the angular term $V_{ij}(\theta)$ relative to the logarithmic term $K_{ij}\ln(r/a)$ appearing in Eq. (A28).

Due to broken rotational invariance, the presence of a small density of free dislocations with Burgers vector in the x direction, treated in the Debye-Huckel approximation, does not now provide screening sufficient to eliminate the logarithmic interaction between dislocations with $b_y\neq 0$. It is plausible that the latter dislocations remain bound above the first melting temperature T_m, until a second transition temperature T'_m is reached where the coefficient of the logarithm falls below the critical value $4k_BT$. In the temperature range $T_m<T<T'_m$, one predicts quasi-long-range order for the correlation functions $C_{\vec{G}}(\vec{R})$ provided that $\vec{G}$ has no component in the x direction, so the system may be properly described as a 2D smectic.

The stabilizing effect of the substrate interaction may be readily understood if we consider the smectic Hamiltonian Eq. (2.52). The orienting forces lead to a modified Hamiltonian, of the form

$$\frac{H^S_0}{k_BT}=\frac{1}{2}\int\left[B\left(\frac{\partial u}{\partial y}\right)^2+B\lambda^2\left(\frac{\partial^2 u}{\partial x^2}\right)^2+4\gamma\left(\frac{\partial u}{\partial x}\right)^2\right]d^2r \ . \tag{3.4}$$

At sufficiently long wavelengths, the term proportional to $(\partial^2u/\partial x^2)^2$ may be neglected and the Hamiltonian has the same form as for a two-dimensional planar spin model (xy model). It is clear that the interaction between dislocations remains logarithmic at large distances and that there should be quasi-long-range order for the ordering variables e^{iG_yu}. By analogy with the xy model, one can readily estabish the necessary condition for stability of the 2D smectic phase

$$(\gamma_RB_R)^{1/2}\gtrsim 4\pi/d_y^2 \ , \tag{3.5}$$

where γ_R and B_R are the macroscopic (renormalized) values of the elastic constants and d_y is the layer spacing.

The effect of substrate potentials which lock the solid into a commensurate layer has been considered in a separate work.[30] Many different phases occur in this system. True long-range positional order is now possible, and the phases involve all combinations of short-range, quasi-long-range, and long-range order in the two perpendicular displacement variables. The "floating" solid is identical in its large-distance properties to the continuum solid studied in the present research. Reference 30 investigates the properties of a simple lattice gas which incorporates the central features of the solid, including dislocations. It is found that if the ratio of the lattice spacing of the solid divided by the lattice spacing of the substrate is less than a minimum value $p_{\min}$, the harmonic floating solid phase does not exist. The value of $p_{\min}$ is $2\sqrt{3}$ for a triangular lattice, and $p_{\min}=4$ for a square lattice.

D. Three-dimensional stack of smectic layers

The interaction between layers in a bulk liquid crystal may also stabilize the partial translational order characteristic of the 2D smectic regime. In particular, the interlayer coupling will tend to lock the displacements in one layer to those in its neighbor. One could obtain a bulk phase with broken translational symmetry in the y direction parallel to the layers, as well as in the z direction, perpendicular to the layers. We may call such a system a three-dimensional bismectic. The x-ray structures factor of the bismectic will have Bragg peaks on a two-dimensional lattice of points, laying in the yz plane.

The leading terms in the energy associated with displacements $\vec{u}$ in the bismectic may be written as

$$\frac{H_B}{k_B T}=\frac{1}{2}\int d^3r\left[M_{ijkl}\frac{\partial u_i}{\partial r_j}\frac{\partial u_k}{\partial r_l}+N_{ij}\frac{\partial^2 u_i}{\partial x^2}\frac{\partial^2 u_j}{\partial y^2}\right], \tag{3.6}$$

where indices are restricted to the values y and z, and M and N are tensor coefficients.

An analysis of the effects of long-wavelength thermal fluctuations predicts a finite root-mean-square displacement in the bismectic, so that true long-range order exists, and the Bragg peaks should be δ functions in reciprocal space.[31] This contrasts with the situation for an ordinary smectic-A or smectic-C phase, where quasi-long-range order is found in three dimensions. Of course, the bismectic phase will also have long-range order in the orientations of the molecules.

We may note that the proposed bismectic phase is identical in its properties to an anisotropic version of the H_1 mesophase of disklike molecules proposed by Chandrasekhar[32] and theoretically investigated by Kats.[31] The effect of interlayer coupling may also be understood by considering the energy of an isolated dislocation in a single layer, at a temperature slightly above the melting temperature T_m. If the layer melting is of type I, then there is an intermediate length scale on which the layer may be described as a 2D smectic and the energy of the point dislocation is found to be large but finite. A point dislocation in one layer which does not occur in the neighboring layers requires a mismatch betwen the displacements, at least along a line stretching from the dislocation point to the boundary of the sample. Thus, if there is any coupling between the layers, the energy of a point dislocation becomes infinite in the limit of an infinite sample, and isolated point dislocations will not exist in equilibrium. If a dislocation occurs at approximately the same point in every layer, then no mismatch occurs, a dislocation line is formed, and the energy in each layer is again finite. The total energy is proportional to the length of the line, however, so that an isolated dislocation line will again have infinite energy in an infinite sample.

If a finite density of dislocation points is present in each layer, screening effects lead to a finite energy per dislocation. At a certain temperature it will be favorable to have free dislocations, and the bismectic phase will be converted into the ordinary smectic-C phase. Conversely, if the coupling between layers is sufficiently strong, there may be induced translational order in all three directions, and the bismectic will be converted to a three-dimensional solid (smectic-H) phase.

IV. STRUCTURE FACTOR IN EXPERIMENTAL SYSTEMS

The structure factor measured in an x-ray or neutron scattering experiment is a direct probe of the translational correlation function $C_{\vec{G}}(\vec{R})$. We discuss here the expected results of a scattering experiment for a film at a temperature slightly above the melting temperature T_m. We shall concentrate on the case of type-I melting.

We first discuss the case of a multidomain ("powder") sample. If the domain size is sufficiently large so that finite-size-effect broadening is negligible, the experimental structure factor is given by

$$\bar{S}(q)=(2\pi q)^{-1}\int S(\vec{q}\,')\delta(q-q')\,d^2q' , \tag{4.1}$$

where $S(\vec{q}\,')$ is the structure factor of an oriented domain. If $S(\vec{q})$ is dominated by scattering near a reciprocal-lattice vector $\vec{G}$, then $S(\vec{q})$ can be approximated by

$$\begin{aligned}\bar{S}_{\vec{G}}(\vec{q})&\equiv(2\pi q)^{-1}\int S(\vec{q}\,')\delta(q-\vec{q}\,'\cdot\hat{G})\,d^2q\\&\approx q^{-1}\int_{-\infty}^{\infty}ds\,C_{\vec{G}}(s\hat{G})e^{iqs} ,\end{aligned} \tag{4.2}$$

where $C_{\vec{G}}(s\hat{G})$ is the correlation function in real space, for a separation $\vec{R}=s\hat{G}$ parallel to $\vec{G}$, computed for a domain aligned with its symmetry axis parallel to the x axis and sufficiently small so that angular fluctuations are $<<1$. In practice, we may choose this domain size L to be of order of a few times the correlation length ξ_S.

When $G_x\neq 0$, the correlations in $C_{\vec{G}}(\vec{R})$ decay with a characteristic length given by ξ_S, due to both type-I dislocations and phonons, so that the width δ_q of the structure factor $S_{\vec{G}}(q)$ obeys

$$\delta_q(S_{\vec{G}})\propto\xi_S^{-1} . \tag{4.3}$$

The situation is more complicated when $G_x=0$. In this case, there are two competing lengths, ξ_P which describes the decay in the y direction of the displacement order parameter due to phonons in the smectic, and ξ_Y, the decay due to type-II dislocations. The length ξ_Y is given by $\xi_N^{4/3}/\xi_S^{1/3}$ (see Ref. 14). The decay of C_{G_y} due to phonons is given by the exponential of a square root at large distances along the y axis[14]:

$$C_{G_y}^{\text{phonon}}(y)\propto\exp[-(y/\xi_P)^{1/2}] . \tag{4.4}$$

The length ξ_P is proportional to ξ_S, and is obtained from Eqs. (C11), (C5), and (2.45) with[33]

$$\xi_P\simeq\frac{4\sqrt{2}\pi}{(d_yG_y)^4(S_{2222}^{*})^{3/2}}\xi_S , \tag{4.5}$$

where d_y is the layer spacing. There is also an exponential decay of correlations provided by the dislocations

$$C^D_{G_y} \propto e^{-y/\xi_Y} \ . \tag{4.6}$$

The total order-parameter correlation function is therefore given by

$$C_{G_y}(y) = C^D_{G_y}(y) C^{\text{phonon}}_{G_y}(y) \ . \tag{4.7}$$

In Fig. 9, we have plotted $S_{\vec{G}}(q)$ for several values of (ξ_Y/ξ_P). The sequence of graphs from upper right to lower left represents the lowering temperature. The structure factor reaches the limiting form for the smectic with a half-width of $\frac{1}{4}\xi_P^{-1}$ when $\xi_Y/\xi_P \gtrsim 16$. Since $\xi_N \propto \xi_S^{1+p}$ and $\xi_P \propto \xi_S$, this condition will always be satisfied unless $\xi_P >> \xi_S$, and in fact, Eq. (4.3) will usually hold for all $\vec{G}$. By estimating K_{11}^{-1} by

$$2\pi (S^*_{1111})^{1/4} (S^*_{2222})^{3/4}$$

[Eq. (A33)], we find that the ratio ξ_P/ξ_S is given approximately by

$$\left(\frac{\xi_P}{\xi_S}\right) \simeq \frac{8}{\pi^{3/2}} \frac{1}{n^4} \left(\frac{d_y}{d_x}\right)^{3/2} \left(\frac{S^*_{1111}}{S^*_{2222}}\right)^{3/8} , \tag{4.8}$$

where d_y is the average layer separation, d_x is the average distance between atoms along the x axis, and n is the order of the Bragg point along the y axis. In general, this number is of order unity. If $d_y >> d_x$, the phonon correlation length may be sufficiently large to see the width of $\delta_q(S_{G_y})$ determined by ξ_Y. Only in this exceptional case, and then only in a range of temperature when $\xi_P >> \xi_N$ will the width of $\delta_q(S_{G_y})$ be given by ξ_Y^{-1}. We are forced to conclude that x-ray scattering experiments are a weak probe of 2D smectic order, at least for polydomain samples. The only signature of the smectic order which is likely to be observed is the relatively narrow width of the y-component scattering, and this width still scales with ξ_S.

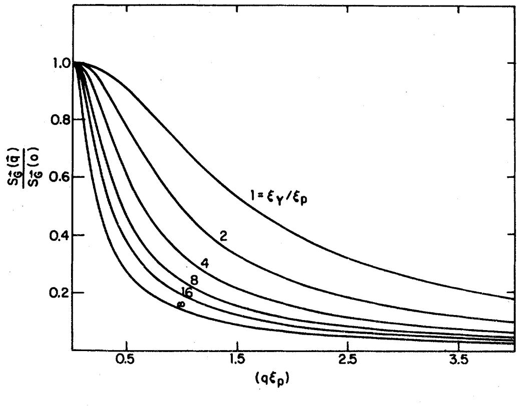

FIG. 9. Reduced structure factor $S_{\vec{G}}(q)/S_{\vec{G}}(0)$ is plotted vs the quantity $(q\xi_P)$ for various values of the ratio of phonon correlation length ξ_P to the dislocation correlation length ξ_Y. The function becomes very weakly dependent on (ξ_Y/ξ_P) when this ratio is greater than 16. The vector $\vec{G}$ is parallel to $\hat{y}$.

For a monodomain sample, there is a distinguishable angular spread to the Bragg pattern, which sharpens as the melting transition is approached from above (see Fig. 10). The width radially across the ring is given by Eq. (4.3), while the angular width is given by the angle fluctuations at the experimental length scale. Thus

$$(\delta\theta)^2 \propto (K_x K_y)^{-1/2} \ln(L/a) \ . \tag{4.9}$$

The angular width of the scattering vanishes at T_m according to

$$\delta\theta \propto (\xi_N \xi_S)^{-1/2} \ . \tag{4.10}$$

In contrast to x-ray and neutron experiments, *light scattering experiments* give a direct measure of orientational correlations. The divergence of $K_x K_y$ may be measured in this way.

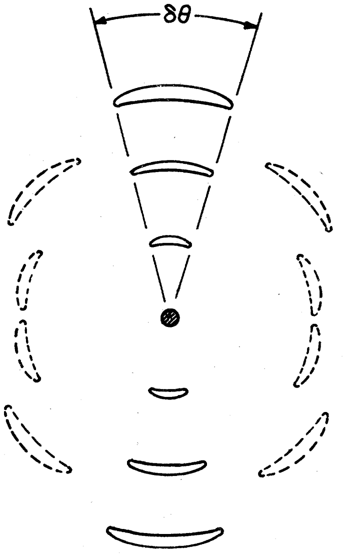

FIG. 10. Bragg pattern is shown corresponding to the lattice geometry in Fig. 1(c) for a monodomain sample in the nematiclike regime. The angular width $\delta\theta$ is a function of system size, and for a given L, it decreases $\propto \exp[-\text{const}(T-T_m)^{-1/2}]$, as $T \rightarrow T_m^+$. If the two-dimensional smectic order were stabilized by substrate anisotropy or an applied field, the spots indicated by solid curves would become power-law Bragg peaks, while the other spots remain diffuse. In the absence of orienting perturbations, all spots are diffuse.

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APPENDIX A: DISLOCATIONS IN AN ANISOTROPIC SOLID

1. Anisotropic elasticity

Each molecule in the solid is located at a position $\vec{r} = \vec{u}(\vec{R}) + \vec{R}$. The vector displacement field $\vec{r}$ is a function of lattice position $\vec{R}$, and measures the deviation of the molecule from the position it would occupy in the perfect crystal. In the presence of dislocations, $\vec{u}$ is a multivalued function of position.

We construct the following quantities from the displacement field:

$$w_{ij} = \partial u_i / \partial x_j \ , \tag{A1a}$$

$$u_{ij} = \tfrac{1}{2}(w_{ij} + w_{ji}) \ , \tag{A1b}$$

$$v_{ij} = \tfrac{1}{2}(w_{ij} - w_{ji}) \ . \tag{A1c}$$

The derivative of the displacement field is w_{ij}, and u_{ij} and v_{ij} are the symmetric and antisymmetric tensors formed from the differential displacements.[18,24] The stress tensor σ_{ij} is related to the strain u_{ij} by the elastic tensor C_{ijkl}, and the compliance tensor S_{ijkl} by

$$\sigma_{ij} = C_{ijkl} u_{kl} \ , \tag{A2a}$$

$$u_{ij} = S_{ijkl} \sigma_{kl} \ , \tag{A2b}$$

$$S_{ijkl} C_{klmn} = \tfrac{1}{2}(\delta_{im}\delta_{jn} + \delta_{in}\delta_{jm}) \ . \tag{A2c}$$

(The summation convention of summing over repeated latin indices is used.) The elastic energy per unit area is given by E, where

$$E = \tfrac{1}{2} u_{ij} \sigma_{ij} = \tfrac{1}{2} \sigma_{ij} S_{ijkl} \sigma_{kl} \ , \tag{A3}$$

and the net force per unit area is given by

$$F_i = \frac{\partial \sigma_{ij}}{\partial x_j} = 0 \ . \tag{A4}$$

2. Theory of dislocations

We now calculate the displacement field, stress and energy fields associated with a dislocation of Burgers vector $\vec{b}$. According to standard theory[12]

$$b_k = -\oint w_{kj}\, dx_j \ , \tag{A5}$$

where the path integral is chosen to be counter clockwise once around the dislocation core. Note that w_{kj} is single valued while $\vec{u}$ is multivalued.

Equation (A5) can be rewritten using the antisymmetric tensor ϵ_{ij}, with $\epsilon_{12} = 1 = -\epsilon_{21}$:

$$b_k = -\oint w_{kj} \epsilon_{jn} \epsilon_{nl}\, dx_l \ , \tag{A6}$$

where $\epsilon_{jn}\epsilon_{nl} = -\delta_{jl}$ has been used. Since $\epsilon_{nl} dx_l = dn_n$ is the normal differential to the path, the rest of the term inside the integral must have a gradient equal to a δ function, i.e.,

$$-b_k \delta(\vec{r}) = \epsilon_{jn} \frac{\partial w_{kj}}{\partial x_n} \ . \tag{A7}$$

In linear elasticity theory, we use superposition to calculate properties associated with a collection of dislocations. It is therefore convenient to calculate $\tilde{u}_{ij}^n$ and $\tilde{w}_{ij}^n$, the Fourier transforms of the differential displacements and stress fields generated by a dislocation at the origin of unit magnitude and direction along the nth axis. In the following discussion, a tilde over an expression indicates the Fourier-transform representation of that quantity.

The conditions (A4) and (A7) in terms of the Fourier-transform variable $\vec{k}$ become:

$$i k_j \tilde{\sigma}_{ij}^m = 0 \ , \tag{A8a}$$

$$i k_n \tilde{w}_{kj}^m \epsilon_{jn} = \delta_k^m \ . \tag{A8b}$$

The Kronecker δ is denoted by δ_i^n. These equations are sufficient to solve for $\tilde{u}_{ij}^n$ and $\tilde{\sigma}_{ij}^n$, as well as for E_{ij}, the Fourier transform of the interaction energy between two Burgers vectors. Condition (A8a) above, enables us to write

$$\tilde{\sigma}_{ij}^n = T_{ij} \tilde{A}^n \ , \tag{A9}$$

$$T_{ij} = \left(\delta_{ij} - \frac{k_i k_j}{k^2} \right) \ . \tag{A10}$$

$\tilde{A}^n$ is a function of $\vec{k}$ to be determined, and T_{ij} is the transverse projection operator. The quantity w_{ij} can be decomposed into symmetric and antisymmetric parts

$$\tilde{w}_{ij} = \tilde{u}_{ij} + \tilde{v}_{ij} \ . \tag{A11}$$

Using the fact that the antisymmetric part must be proportional to ϵ_{ij}, we find

$$\tilde{v}_{ij}^l = \tilde{B}^l \epsilon_{ij} \ , \tag{A12}$$

where $\tilde{B}$ is another function of $\vec{k}$ to be determined. Substitution of Eqs. (A9)–(A12) into Eq. (A8b) leads to

$$k_n \epsilon_{nm} \tilde{u}^l_{im} + \tilde{B}^l k_i = i\delta^l_i \ . \tag{A13}$$

We now substitute for $\tilde{u}^l_{ij}$, using the compliance matrix, to find

$$\tilde{R}_i \tilde{A}^n + k_i \tilde{B}^n = i\delta^n_i \ , \tag{A14a}$$

$$\tilde{R}_i \equiv k_n \epsilon_{nm} S_{imrt} T_{rt} \ . \tag{A14b}$$

Multiplying Eq. (A14a) by $\epsilon_{li} k_l$, we obtain

$$\tilde{A}^m = \frac{i}{k^2} \frac{k_n \epsilon_{nm}}{Q(\vec{k})} \ , \tag{A15}$$

where

$$Q(\vec{k}) = T_{ij} S_{ijkl} T_{kl} \ . \tag{A16}$$

The stress field can be written

$$\tilde{\sigma}^m_{ij} = \frac{i}{k^2} \frac{k_n \epsilon_{nm}}{Q(\vec{k})} T_{ij} \ . \tag{A17}$$

The interaction between dislocations $b^n(\vec{r}_1)$ and $b^m(\vec{r}_2)$ is given by

$$E^{nm}(\vec{r}_1 - \vec{r}_2) = \int d^2r \, \sigma^n_{ij}(\vec{r} - \vec{r}_1) S_{ijkl} \sigma^m_{kl}(\vec{r} - \vec{r}_2) \ , \tag{A18a}$$

or equivalently

$$E^{nm}(\vec{r}_1 - \vec{r}_2) = \int d^2r \, u^n_{ij}(\vec{r} - \vec{r}_1) C_{ijkl} u^m_{kl}(\vec{r} - \vec{r}_2) \ . \tag{A18b}$$

Using the convolution theorem for Fourier transforms, we find that

$$\tilde{E}^{nm} = \tilde{\sigma}^n_{ij}(-\vec{k}) S_{ijkl} \tilde{\sigma}^m_{kl}(\vec{k}) \ . \tag{A19}$$

This is easily calculated as

$$\tilde{E}^{nm} = \frac{T^{nm}(\vec{k})}{k^2 Q(\vec{k})} \ . \tag{A20}$$

To find the displacement field we need to find B^l, which is obtained by multiplying Eq. (A14a) by $\epsilon_{ni}\tilde{R}_n$. We make a further definition to simplify the notation, henceforth. The subscript j, with a circumflex over it ($\hat{j}$) will mean to multiply that subscript by ϵ_{ij} and relabel i to j again, i.e.,

$$k_{\hat{n}} = \epsilon_{nl} k_l \ , \tag{A21a}$$

$$T_{ij} = \frac{1}{k^2} k_{\hat{i}} k_{\hat{j}} \ , \tag{A21b}$$

$$Q(\vec{k}) = \frac{1}{k^4} k_{\hat{i}} k_{\hat{j}} k_{\hat{n}} k_{\hat{m}} S_{ijnm} \ . \tag{A21c}$$

We find that the differential displacements are given by

$$\tilde{w}^l_{ij} = \frac{i}{k^4 Q(\vec{k})} \left(S_{ijmn} k_{\hat{l}} + \epsilon_{ij} k_{\hat{s}} S_{\hat{l}smn} \right) k_{\hat{m}} k_{\hat{n}} \ , \tag{A22a}$$

$$\tilde{B}^n = \frac{i\tilde{R}_{\hat{n}}}{k^2 Q(\vec{k})} \ . \tag{A22b}$$

It is often convenient to define a single-valued displacement field $\vec{u}^n$ around a dislocation of unit magnitude and Burgers vector along the direction $\hat{r}_n$ at the origin by introducing a cut along an arbitrary but specified direction $\vec{r}_0$. This single-valued displacement field is obtained by adding a lattice displacement equal to $\vec{b}^n$ to the integral of the differential displacements every time the cut is traversed in the clockwise direction. Thus $\vec{u}^n = \vec{u}^n_s + \vec{u}^n_c$, where $\vec{u}^n_s$ is the multivalued smooth part of the displacement field, obtained by integrating w_{ij}, and $\vec{u}^n_c$ is the multivalued discontinuous part obtained by considering the cut. The demand that $\vec{u}^n_c$ increase by $\vec{b}^n$ when the cut is traversed can be written as

$$[(\hat{r}^\perp_0 \cdot \vec{\nabla}) \vec{u}^n_c]_l = -\delta^n_l \int_0^\infty ds \, \delta(\vec{r} - \hat{r}_0 s) \ . \tag{A23}$$

Here $(\hat{r}^\perp_0)_j \equiv -\epsilon_{jk}(\hat{r}_0)_k$, the vector perpendicular to $\hat{r}_0$. Equation (A23) is easily checked by integrating across the cut. The demand that $(\vec{r}_0 \cdot \vec{\nabla})\vec{u}_c = 0$ is necessary, so that the value of $\vec{u}^n$ is not altered in a direction along the cut. Taking the Fourier transform of Eq. (A23) above, and using the above considerations, one finds

$$\mathfrak{F}\left[\frac{\partial (u^n_c)_l}{\partial x_i} \right] = -\frac{\delta^n_l (r^\perp_0)_i}{\vec{k} \cdot \hat{r}_0 - i\epsilon} \ , \tag{A24}$$

where $\mathfrak{F}$ means the Fourier transform of the expression in brackets with $\vec{k}$ being the transform variable. Finally, the Fourier transform of the (singular) single-valued displacement field is found to be

$$\begin{aligned} \tilde{u}^j_n &= \frac{1}{ik_m} \tilde{w}^j_{nm} - \frac{\delta^j_n (\hat{r}^\perp_0)_m}{k_m(\hat{r}_0 \cdot \hat{k} - i\epsilon)} \ \text{(where } m = 1 \text{ or } 2) \\ &\equiv (u^j_s)_n + (u^j_c)_n \ . \end{aligned} \tag{A25}$$

One can check that u^j_n is indeed independent of the choice of the index m. This expression is used to calculate correlations in the smecticlike and nematiclike phases.

The quartic expression $Q(\vec{k})$ appears in all of the denominators which occur in the Fourier transform of the tensor fields, and to analyze these expressions in real space, we need to investigate the zeros of Q. We define quartic polynomial $\bar{Q}(z)$ by

$$\bar{Q}(z) = S_{ijkl} z_i z_j z_k z_l \ , \tag{A26}$$

with $z_1 = z$, $z_2 = 1$. Thus, $\bar{Q}(z)$ is a quartic polynomial in z. Since the coefficients are real, the roots occur as complex conjugate pairs. Denote these roots by α_1, α^*_1 and α_2, α^*_2. The polynomial $Q(\vec{k})$ factors into the fourfold product

$$Q(\vec{k})=\frac{S_{1111}}{k^4}|(k_x-\alpha_1 k_y)(k_x-\alpha_2 k_y)|^2 \tag{A27}$$

[see Eq. (2.19)]. Stability requires that $\mathrm{Im}(\alpha_i)\neq 0$, which is equivalent to the requirement that S_{ijkl} be positive definite. It is no restriction to choose $\mathrm{Im}\alpha_i > 0$, since the roots occur in pairs.

3. Interaction energy between dislocations

To perform the renormalization group analysis, we must Fourier-transform Eq. (A20) to find the energy between dislocatons in real space. Using the factorization, we can perform these integrals using contour integration techniques to find

$$E^{nm}(\vec{r})=K_{nm}\ln\left(\frac{r}{a}\right)+V_{nm}(\theta)\ , \tag{A28}$$

$$K_{11}=\frac{1}{2\pi}\frac{\mathrm{Im}\alpha_1+\mathrm{Im}\alpha_2}{S_{1111}(\mathrm{Im}\alpha_1)(\mathrm{Im}\alpha_2)|\alpha_1-\alpha_2^*|^2}\ , \tag{A29a}$$

$$K_{22}=\frac{1}{2\pi}\frac{\mathrm{Im}(\alpha_1^{-1})+\mathrm{Im}(\alpha_2^{-1})}{S_{2222}(\mathrm{Im}\alpha_1^{-1})(\mathrm{Im}\alpha_2^{-1})|\alpha_1^{-1}-(\alpha_2^{-1})^*|^2}\ , \tag{A29b}$$

$$K_{12}=\frac{1}{2\pi}\frac{\mathrm{Im}(\alpha_1\alpha_2)}{S_{1111}(\mathrm{Im}\alpha_1)(\mathrm{Im}\alpha_2)|\alpha_1-\alpha_2|^2}\ , \tag{A29c}$$

$$V_{nm}(\theta)=\frac{1}{2\pi}\,\mathrm{Re}\left(\frac{\alpha_1{}^{n+m-2}\ln(\alpha_1\cos\theta+\sin\theta)}{(\mathrm{Im}\alpha_1)|\alpha_1-\alpha_2^*|^2}\right)+\langle\text{interchange 1 and 2}\rangle\ . \tag{A29d}$$

The second equation (A29b) is analogous to Eq. (A29a), with the indices 1 and 2, and α_i and α_i^{-1} interchanged. For appropriate choice of axes, K_{12} can be made equal to zero since K_{nm} is a symmetric tensor.

4. Crystal symmetry

Considerable simplifications occur in the formulas when there is a symmetry in the crystal. For the problem at hand, the reflection symmetry $y\rightarrow -y$ is valid and every component of the compliance or elastic tensor with an odd number of equal indices vanishes. There are therefore four nonzero compliances: S_{1111}, S_{2222}, S_{1212}, and S_{1122}. The quartic expression $\bar{Q}(z)$ can then be reduced to

$$Q(z)=S_{1111}z^4+2(S_{1122}+2S_{1212})z^2+S_{2222}\ . \tag{A30}$$

This can be solved to find the following expression for the roots of $\bar{Q}(z)$:

$$\alpha^2_{\left\{1 \atop 2\right\}}=\frac{-(S_{1122}+2S_{1212})\pm[(S_{1122}+2S_{1212})^2-S_{1111}S_{2222}]^{1/2}}{S_{1111}}\ . \tag{A31}$$

Two cases now present themselves. In the first case (i), the argument of the square root is positive, giving two imaginary, independent roots. The second case (ii) occurs when the argument of the square root is negative, giving roots of equal modulus but complementary phase. The isotropic case gives degenerate roots. In all these cases

$$\alpha_1^2\alpha_2^2=S_{2222}/S_{1111}\ , \tag{A32a}$$

$$\alpha_1^2+\alpha_2^2=-(2S_{1111}+4S_{1212})/S_{1111}\ , \tag{A32b}$$

and

$$\begin{aligned}\alpha_j&=i|\alpha_j|\ ,\quad \text{for case (i)}\ ,\\ \alpha_1&=-\alpha_2^*\ ,\quad \text{for case (ii)}\ .\end{aligned} \tag{A32c}$$

The conditions (i) and (ii) are obtained by inspection and are a consequence of the reflection invariance which gives $\bar{Q}(z)$ as a polynomial in z^2. In this case we compute K_{ij} explicitly as

$$K_{11}=\frac{1}{2\pi}(2S_{2222})^{-1/2}[(S_{1111}S_{2222})^{1/2}+(S_{1122}+2S_{1212})]^{-1/2}\ , \tag{A33a}$$

$$K_{22}=K_{11}\left(\frac{S_{2222}}{S_{1111}}\right)^{1/2}\ , \tag{A33b}$$

$$K_{12}=K_{21}=0\ . \tag{A33c}$$

No real simplification for V_{ij} occurs over Eq. (A29), and the explicit form for this interaction will not be needed.

We now compute the correlation for the translational order parameter $C_{\vec{G}}(\vec{R})$ in the solid phase where the cumulant expansion is valid:

$$C_{\vec{G}}(\vec{R}) = \exp[-G_iG_jf_{ij}(\vec{R})] \ , \tag{A34a}$$

$$f_{ij}(\vec{R}) \equiv \tfrac{1}{2}\langle [u_i(\vec{R}) - u_i(\vec{0})][u_j(\vec{R}) - u_j(\vec{0})]\rangle \ . \tag{A34b}$$

The Hamiltonian for the solid is given by Eq. (2.2) so that the Hamiltonian for the Fourier-transformed fields is given by

$$\frac{H_0}{k_BT} = \frac{1}{2}\int d^2k\, k_jk_mC_{ijmn}\tilde{u}_i(\vec{k})\tilde{u}_n(-\vec{k}) \ . \tag{A35}$$

The interchange symmetry $i \leftrightarrow j$ of C_{ijmn} has been used. The expectation $\langle \tilde{u}_i(\vec{k})\tilde{u}_j(-\vec{k})\rangle$ is therefore given by $(\tilde{V}^{-1})_{ij}$, where

$$\tilde{V}_{ij}(\vec{k}) = C_{imnj}k_mk_n \ . \tag{A36}$$

Writing this explicitly in our case, we have

$$\tilde{V}_{ij} = \begin{bmatrix} C_{1111}k_1^2 + C_{1212}k_2^2 & (C_{1122}+C_{1212})k_1k_2 \\ (C_{1122}+C_{1212})k_1k_2 & C_{1212}k_1^2 + C_{2222}k_2^2 \end{bmatrix} . \tag{A37}$$

The inverse matrix is given by

$$(\tilde{V}^{-1})_{ij} = \frac{1}{k^4Q(\vec{k})}(S_{1111}S_{2222} - S_{1122}^2)\begin{bmatrix} k_1^2 & -k_1k_2 \\ -k_1k_2 & k_2^2 \end{bmatrix} + 4S_{1212}\begin{bmatrix} S_{1111}k_1^2 & S_{1122}k_1k_2 \\ S_{1122}k_1k_2 & S_{2222}k_2^2 \end{bmatrix} . \tag{A38}$$

The identities, valid for a uniaxial solid,

$$C_{1111}C_{2222} - C_{1122}^2 = (S_{1111}S_{2222} - S_{1122}^2)^{-1} \ , \tag{A39a}$$

$$C_{1212} = \tfrac{1}{4}S_{1212}^{-1} \ , \tag{A39b}$$

have been used. We can compute the large-distance behavior of the logarithm of the order-parameter correlation function, using contour integration techniques. The result is

$$f_{ij}(\vec{R}) \simeq n_{ij}\ln(|R|/a) \ , \tag{A40a}$$

where

$$n_{ij} = (S_{1111}S_{2222} - S_{1122}^2)K_{\tilde{i}\tilde{j}} + 4S_{1212}S_{ijij}K_{ij} \ , \tag{A40b}$$

and K_{ij} are the coefficients of the logarithmic term in the energy defined in Eq. (A29). No summation over indices in Eq. (A40b) is to be performed. Formulas (A20) and (A28) have been used and only the divergence as $R \to \infty$ has been kept. The order-parameter correlation function is given by

$$C_{\vec{G}}(\vec{R}) \cong (R/a)^{-\eta_{ij}G_iG_j}f_a(\vec{G},\hat{R}) \ . \tag{A41}$$

The structure factor can then be computed. The coefficient $f_a(G,R)$, which we do not explicitly calculate, couples $\vec{G}$ and $\hat{R}$ and is related to the angular term in the dislocation interaction Eq. (A29). The exponent which determines the decay of correlations, however, does not couple these variables. Taking the Fourier transform of Eq. (A41), one finds that the Bragg δ functions in the structure factor of a crystal with long-range order become cusped singularities, either remaining finite or diverging depending on the sign of $2-\eta(G)$ for a given Bragg peak.

The orientational correlation function $C_n(\vec{R})$ Eq. (1.13) can be calculated similarly, using the fact that the orientation field generated by an isolated dislocation at the origin is given by

$$\theta(r) = \tfrac{1}{2}\epsilon_{ij}w_{ij} \ . \tag{A42}$$

We find

$$\lim_{R\to\infty} C_n(\vec{R}) \to \text{const} \ , \tag{A43}$$

indicating long-range order of orientations.

APPENDIX B: PROPERTIES OF THE NEMATICLIKE REGIME CALCULATED USING THE SOLID HAMILTONIAN

The nematiclike regime may be described by a gas of free interacting dislocations added to the solid. At long wavelengths, the nematic should be described by two Frank constants, using the Hamiltonian Eq. (1.4). We compute the Frank constants by calculating the bond orientation fluctuations in the dislocation ensemble and then comparing with what we would find using Eq. (1.5).

We define the quantity

$$B_{ij}(\vec{k}) = \langle b_i(\vec{k})b_j(-\vec{k})\rangle \tag{B1}$$

as the correlation between dislocations in the Fourier-transformed variable $\vec{k}$. When the core energies are added to the dislocation Hamiltonian, we find

$$B_{ij}(\vec{k}) = \Omega\frac{k^4Q(\vec{k})E_{\tilde{i}\tilde{j}} + k_ik_j}{k^4Q(\vec{k})\det(E_{ij}) + k_ik_jE_{ij}} \ , \tag{B2}$$

where Ω is the system area, E_{ij} is the core energy matrix $2a^2E_{ij}^c$ and $\det(E_{ij})$ is the determinant. The matrix E_{ij} is of course diagonal when there is a reflection symmetry about the x or y axis. In the nematiclike regime, both eigenvalues of E_{ij} are finite, although one may be much larger than the other. Equation (B2) is used to calculate the correlations in the bond orientation field. The Fourier transform of the bond orientation field induced by a dislocation at the origin with Burgers vector $\vec{b}^n$ is given by

$$\tilde{\phi}^n(\tilde{k}) = \tfrac{1}{2}\epsilon_{ij}\tilde{w}^n \ . \tag{B3}$$

The right-hand side is just the antisymmetric part of the differential displacements. Using Eqs. (A22) we find

$$\begin{aligned}\tilde{g}(\vec{k}) &= \langle \tilde{\phi}(k)\tilde{\phi}(-k)\rangle \\ &\sim [k_i k_j E_{ij} + k^4 Q(\vec{k})\det(E)]^{-1} \ ,\end{aligned} \tag{B4}$$

for small k. Using the fact that E_{ij} is diagonal for the solid with reflection symmetry, we make the identification Eq. (2.47). The real-space angle-angle correlation function is then given by

$$\begin{aligned}\langle[\phi(R)-\phi(0)]^2\rangle &\cong \frac{1}{2\pi}(K_x^0 K_y^0)^{-1/2} \\ &\quad\times \ln\left(\frac{R_i R_j E_{\tilde{ij}}}{S_{ijkl}\hat{R}_i\hat{R}_j\hat{R}_k\hat{R}_l}\right) \equiv g(\vec{R}) \ .\end{aligned} \tag{B5}$$

In a system where the local rotational symmetry is n fold, the relevant orientational order parameter is $\psi_n(\vec{R}) = e^{ni\phi(\vec{R})}$. We can calculate the correlation function C_n by using the cumulant expansion. In this approximation

$$C_n(\vec{R}) = \exp[-\tfrac{1}{2}n^2 g(\vec{R})] \ . \tag{B6}$$

Using Eq. (B5) one can show

$$C_n(\vec{R}) = F(\hat{R})R^{-\eta} \ , \tag{B7}$$

where

$$\eta = \frac{1}{2\pi}(K_x K_y)^{-1/2} n^2 \ , \tag{B8a}$$

$$F(\hat{R}) = \left(\frac{\hat{R}_i\hat{R}_j E_{\tilde{ij}}}{S_{ijkl}\hat{R}_i\hat{R}_j\hat{R}_i\hat{R}_l}\right)^{\eta} \ . \tag{B8b}$$

The calculation of the displacement correlation functions is more difficult due to the multivaluedness of the displacements around a dislocation. It will be noticed that B_{ij} is composed of two parts:

$$B_{ij} = B_{ij}^{\parallel} + B_{ij}^{\perp} \ , \tag{B9}$$

where $B_{ij}^{\perp}$ is the part proportional to $k_i k_j$ in Eq. (B2). In real space, this correlation can be written as

$$B_{ij}^{\perp} = -\frac{\partial}{\partial r_i}\frac{\partial}{\partial r_j}g(\vec{r}) \ , \tag{B10}$$

where $g(\vec{r})$ is just the angle-angle correlation function. This term dominates fluctuations in the displacements perpendicular to the direction between locations in the lattice and this is the reason it is so closely related to angular fluctuations.

Let us define the function

$$\vec{\Delta}_m(\vec{R},\vec{R}') = \vec{u}_s^{\,m}(\vec{R}'-\vec{R}) - \vec{u}_s^{\,m}(R') \ , \tag{B11}$$

where $\vec{u}_s^{\,m}(\vec{R}')$ is the (multivalued) displacement field at the origin introduced by a unit dislocation at $\vec{R}'$ with Burgers vectors along the mth axis. Thus $\vec{\Delta}^m$ is the difference in the displacement field between the origin and the observation point $\vec{R}$, generated by a dislocation at $\vec{R}'$. We shall define the function $\vec{\Delta}^m(\vec{R},\vec{R}')$ to have a cut as a function of $\vec{R}'$ from the origin to the point $\vec{R}$. There is then no cut necessary to the dislocation itself; if the dislocation makes a closed path in the cut plane, it must loop around the origin and $\vec{R}$ an equal number of times. Hence $\vec{\Delta}(\vec{R},\vec{R}')$ will be a single-valued function of $\vec{R}'$ with just a cut between 0 and $\vec{R}$. With this convention the function

$$\vec{\Delta}(\vec{R}) = \int d^2R'\, b_m(\vec{R}')\vec{\Delta}^m(\vec{R},\vec{R}') \tag{B12}$$

is the contribution from the dislocations to the difference in displacements $[\vec{u}(\vec{R}) - \vec{u}(0)]$ and the correlation function

$$G_{ij}(\vec{R}) = \langle \Delta_i(\vec{R})\Delta_j(\vec{R})\rangle \tag{B13a}$$

can be calculated.

The decomposition of B_{ij} results in a corresponding decomposition of $G_{ij}(\vec{R})$:

$$G_{ij}(\vec{R}) \equiv G_{ij}^{\perp}(\vec{R}) + G_{ij}^{\parallel}(\vec{R}) \ , \tag{B13b}$$

with

$$\begin{aligned}G_{ij}^{\perp}(\vec{R}) &= \int d^2R'\, d^2R''\, \Delta_i^m(\vec{R},\vec{R}') \\ &\quad\times B_{mn}^{\perp}(\vec{R}'-\vec{R}'')\Delta_j^m(\vec{R},\vec{R}'') \ .\end{aligned} \tag{B14}$$

The integral extends over the entire space excluding the cut from the origin to $\vec{R}$. Using the form Eq. (B10) for G_{ij}, we see that

$$\begin{aligned}G_{ij}^{\perp}(R) &= \int d^2R'\, d^2R''\, \Delta_i^m(\vec{R},\vec{R}')\frac{\partial}{\partial R_m'}\frac{\partial}{\partial R_n''} \\ &\quad\times g(\vec{R}'-\vec{R}'')\Delta_j^n(\vec{R}',\vec{R}'') \ .\end{aligned} \tag{B15}$$

Using the fact that

$$\sum_n \frac{\partial}{\partial x_n}u_i^n = 0 \ ,$$

derived from Eq. (A22a), and using Green's theorem to rewrite the area integral into a double path integral over $\vec{R}'$ and $\vec{R}''$, we find

$$\begin{aligned}G_{ij}^{\perp}(\vec{R}) &= \oint\!\!\oint dl'\, dl''\, n_m \Delta_i^m(\vec{R},\vec{R}') \\ &\quad\times g(\vec{R}'-\vec{R}'')n_n\Delta_j^n(\vec{R},\vec{R}'') \ .\end{aligned} \tag{B16}$$

Each path integral surrounds the cut once in a counter-clockwise direction and the boundary of the surface (at $R = L$) once in the opposite sense; n_j is the ith component of the normal to the boundary.

Using the fact that the discontinuity across the cut is δ_n^i, we can reduce the cut integral to

$$G_{ij}^{\text{cut}}(\vec{R}) = \oiint dR'\, dR''\, n_i(\vec{R}')\, n_j(R'')\, g(\vec{R}' - \vec{R}'') \;. \tag{B17}$$

The double surface integral at the boundary still remains. Whether or not this surface integral is important depends on the large distance properties of g.

In the presence of a crystalline substrate which induces long-range order in the orienting parameter $e^{i\phi(r)}$, the correlation function g decreases exponentially at large distances. There is then only a contribution to G_{ij} proportional to R due to the cut. If the cumulant expansion is valid, it then follows that

$$C_{\vec{G}}(\vec{R}) \equiv \langle \exp[i\vec{G}\cdot\vec{u}(\vec{R})]\exp[-i\vec{G}\cdot\vec{u}(0)]\rangle$$

is exponential at large distances in the nematiclike phase,[34] for any direction of $\vec{R}$.

For a smooth substrate, g diverges as a logarithm, and the dominant contribution to G_{ij} has the form

$$G_{ij}(\vec{R}) \propto \tfrac{1}{2} R_i R_j (K_x^0 K_y^0)^{-1/2} \ln(\Omega/a^2) \;, \tag{B18}$$

where Ω is the system size.

The presence of free dislocations at very large length scales causes a drift in the overall angular orientation of a relatively small region in the interior of a sample. There will therefore be a displacement generated between location $\vec{R}$ and 0 which will be proportional to the separtion $\vec{R}$ since the entire region is rotating by an angle which is of order

$$\delta\theta \propto (K_x^0 K_y^0)^{-1/4} \tfrac{1}{2} \ln(\Omega/a)$$

(see the discussion in Sec. IV). The angular fluctuations become less severe as $T \to T_m$.

The large angular fluctuations also induce a differential displacement parallel to R which is proportional to $R\,(\delta\theta)^2$. The effect of this displacement on the correlation function $C_{\vec{G}}(\vec{R})$ contributes a factor

$$\approx [1 - 2iGR\,\langle(\delta\theta)^2\rangle]^{1/2} \;, \tag{B19}$$

if $\delta\theta$ is a Gaussian variable. If both R and the "system size" are of the order of the correlation length ξ_S, as is required for example in the structure-factor calculation of Sec. IV, the term $GR\,\langle(\delta\theta)^2\rangle$ is small compared to unity.

There is a second contribution to G_{ij} which is independent of the volume and which is important for the separations of interest. This term is given by Eq. (B14) when $B_{ij}^{\perp}$ is replaced by $B_{ij}^{\parallel}$. We analyze $G_{ij}^{\parallel}(R)$ by working directly in Fourier space using the single-valued, discontinuous displacement field calculated in Eqs. (A24) and (A25). The cut is chosen along the line between 0 and R. Thus

$$G_{ij}^{\parallel}(R) = \int \frac{d^2\vec{q}}{2\pi}\,(e^{i\vec{q}\cdot\vec{r}} - 1)\,\tilde{u}_i^n(\vec{q})\,B_{nm}^{\parallel}(\vec{q})\cdot\tilde{u}_j^m(-\vec{q}) \;. \tag{B20}$$

By rotating the integration variables, one finds a pole with a residue proportional to R. After considerable algebraic manipulation it can be shown that

$$G_{ij}^{\parallel}(R) = |R|\,\frac{E_{\tilde{i}\tilde{j}}}{(E_{11}E_{22})}\,F_{\parallel}(\theta) \;, \tag{B21a}$$

where

$$\begin{aligned} F_{\parallel}(\theta) = [\,&(S_{1111} + S_{2222} + \sin(2\theta)(S_{1111} - S_{2222}) \\ &+ \sin(4\theta)(S_{1111} + S_{2222} - 2S_{1122} - 4S_{1212})\,]^2 \\ &\times (E_{mn}\hat{R}_{\hat{m}}\hat{R}_{\hat{n}})^{-1/2}(S_{ijkl}\hat{R}_i\hat{R}_j\hat{R}_k\hat{R}_l)^{-3/2}(E_{11}E_{22})^{1/2} \end{aligned} \tag{B21b}$$

$$\hat{R} = (\cos\theta, \sin\theta) \;, \tag{B21c}$$

and

$$\begin{aligned} E_{11} &= K_x^0 \;, \\ E_{22} &= K_y^0 \;. \end{aligned} \tag{B21d}$$

The function $F(\theta)$ reduces to a constant for a regular triangular lattice. Collecting these results, we find that

$$C_{\vec{G}}(\vec{R}) \propto (\Omega)^{-(\vec{R}\times\vec{G})^2 (K_x^0 K_y^0)^{-1/2}\text{const}} \times \exp[-(G_x^2/K_x^0 + G_y^2/K_y^0)\,|R|\,F_{\parallel}(\theta)] \;. \tag{B22}$$

We note that this form for the correlation function is valid also for the hexatic phase above melting of the regular triangular solid and only when $\vec{G}\times\vec{R} \cong 0$ is there a well-defined exponential falloff of $C_{\vec{G}}(\vec{R})$.

APPENDIX C: CALCULATIONS BASED ON THE SMECTIC HAMILTONIAN

The Hamiltonian Eq. (2.44) for the interaction of dislocations in the smectic regime, with Burgers vectors in the y direction, can be Fourier transformed to give the following expression for the interaction of a pair of separation $\vec{r}$:

$$\epsilon_s(\vec{r}) = \tfrac{1}{4} B \left[\frac{\lambda}{\pi|y|}\right]^{1/2} \exp\left[\frac{-x^2}{4\lambda|y|}\right] \;. \tag{C1}$$

This is a highly anisotropic interaction. Note that for fixed x, ϵ_s actually decreases as y gets smaller. This is because the dislocations act on each other by compressing the intermediate layers (see Fig. 4). This mechanism becomes extremely weak when the dislocations have the same y coordinate.

The interaction energy can be derived from a smectic free energy which, in the absence of dislocations, takes the form of Eq. (2.52). The consequences of this interaction on the properties of a two-dimensional smectic have been studied by Toner and Nelson in Ref. 14, here called TN.

The potential in Eq. (C1) is quite complicated, but it is finite at large separations. A finite density of dislocations must therefore be unbound, and the length ξ_N is equal to the mean distance between dislocations. Thus

$$\xi_N \propto n_f^{-1/2} \propto a e^{E_s} = \xi_S^{1+p} \ , \tag{C2}$$

where n_f is the density of free dislocations.[35] The phase is actually a nematic above the length scale ξ_N. This crossover occurs without a transition according to the analysis in TN.

A correlation $(1/B) f(r/\lambda)$ is defined by

$$\frac{1}{B} f\left(\frac{\vec{R}}{\lambda}\right) = \frac{1}{2}\langle [u(\vec{R}) - u(0)]^2 \rangle \ . \tag{C3}$$

This is the Fourier transform of the inverse Hamiltonian in Eq. (C1) and is given in real space by

$$f(\vec{r}) = \left(\frac{|y|}{2\pi}\right)^{1/2} \exp\left(-\frac{x^2}{4|y|}\right) + \frac{1}{4}|x| \operatorname{erf}\left(\frac{|x|}{2|y|^{1/2}}\right) \ . \tag{C4}$$

This simplifies to

$$\frac{1}{B} f\left(\frac{\vec{r}}{\lambda}\right) \simeq \frac{1}{B}\left(\frac{|y|}{4\pi\lambda}\right)^{1/2}, \quad x^2 << \lambda |y| \ ;$$
$$\frac{1}{B} f\left(\frac{\vec{r}}{\lambda}\right) \simeq \frac{1}{B}\frac{|x|}{4\lambda}, \quad x^2 >> \lambda |y| \ . \tag{C5}$$

Thus, if we use the cumulant expansion on

$$C_{G_y}(\vec{R}) = \langle \exp\{iG_y[u(\vec{R}) - u(0)]\}\rangle \ , \tag{C6}$$

we find exponential decay in the x direction and exponential of a square root in the y direction.

Above the length scale ξ_N, the dislocations become important. The angle-angle correlation function can be calculated in the presence of dislocations to find K_x and K_y. We find

$$K_x \propto B\lambda^2 \propto \xi_S^2 \ , \quad K_y \propto 2E_s a^2 \ , \tag{C7}$$

well above the transition temperature. Since the energy of bending the rows (splaying the director field), is not dependent upon dislocations, K_x does not change as the temperature is lowered toward the transition. Splay of the rows requires dislocations, and it is shown in TN and Ref. 36 that K_y scales like n_f^{-1}. Therefore

$$K_x \propto \xi_S^2, \quad K_y \propto \xi_N^2 \ , \tag{C8}$$

for a vanishingly small density of dislocations with Burgers vector along the y direction. To relate this theory to the anisotropic melting problem, we use quantitites renormalized by the type-I dislocations as bare parameters for this calculation.

The correlation function $C_{G_y}(\vec{R})$ can be computed in the cumulant approximation as

$$C_{G_y}(\vec{R}) = \exp\left[-G_y^2 \frac{1}{B} f\left(\frac{\vec{R}}{\lambda}\right)\right] \ . \tag{C9}$$

The structure factor near a reciprocal-lattice vector $\vec{G}$ for a smectic takes the form

$$S(\vec{q} - \vec{G}_y) = S\left(\lambda\vec{q}, \frac{G_y^2}{B}\right) \ , \tag{C10}$$

where $S(\vec{q}, g)$ is the universal function

$$S(\vec{q}, g) = \int d^2r \, e^{i\vec{q}\cdot\vec{r}} e^{-g f(\vec{r})} \ . \tag{C11}$$

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[19] The most explicit derivation of the energy between dislocations is found in Ref. 18. However, the method of calculation in this reference gives a cut-dependent result and cannot be correct. The method described in Appendix A does not need the introduction of a cut to calculate this quantity.

[20] $K_{\rm I}$ reduces to $K_R/4\pi$, defined in Ref. 4, as the isotropic limit is taken. From this point on we incorporate a factor of T^{-1} in $K_{\rm I}$ and $K_{\rm II}$, so these quantities are dimensionless.

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[35] *Note added in proof.* The correlation length ξ_N is equivalent to the length ξ_D defined in TN, Ref. 14. This length is actually the geometric mean of two lengths, $\xi_Y \propto (\xi_N/\xi_S)^{1/3}\xi_N$ and $\xi_X \propto (\xi_N/\xi_S)^{-1/3}\xi_N$, denoted $\xi_\parallel$ and $\xi_\perp$ respectively by TN. These two lengths describe the different effects of dislocations on smectic translational correlations for points separated parallel to and perpendicular to the rows.

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