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Theory of the S_{A_1}-S_{A_2} phase transition in liquid crystals

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We present a phenomenological model for the phase transition between the monolayer (S_{A_1}) and the bilayer (S_{A_2}) phases of smectic liquid crystals. This model contains all relevant symmetries and Goldstone modes. We study the transition using the ϵ expansion and find it to be in the same universality class as the Ising model to first order in ϵ. In three dimensions, the physical correlation function, however, exhibits nonuniversal power-law behavior leading to a nonuniversal susceptibility exponent γ.

I. INTRODUCTION

In the smectic-*A* (S_A) phase of liquid crystals,[1] oriented barlike molecules of length l segregate into stacks of structureless two-dimensional planes. It is now clear that there are several types of S_A phases [2,3] characterized by the ratio of the interplanar spacing d to l. Conceptually, the simplest phase is the monolayer phase with $d=l$ denoted by S_{A_1} and depicted schematically in Fig. 1(a). In systems composed of polar molecules, a bilayer phase with $d=2l$ and an incommensurate phase with $d=sl$ with $1<s<2$ can occur as well. These phases are depicted schematically in Figs. 1(b) and 1(c). Phase transitions between all pairs of the above phases have been observed,[2] indicating that they are indeed distinct phases.

In this paper, we will be concerned with the S_{A_1}-S_{A_2} transition. The x-ray diffusion pattern for these two phases is shown in Fig. 2. In the S_{A_1} phase, there is a quasi-Bragg peak at wave number $q=2q_0=2\pi/l$ and a diffuse spot at wave number $q_0=2\pi/2l$. In the S_{A_2} phase, there are quasi-Bragg peaks at both q_0 and $2q_0$. The order parameter for these two phases can be constructed by expanding the center-of-mass density ρ in a Fourier series

$$\rho = \rho_0 + \sum(\psi_n e^{inq_0 z} + \text{c.c.}) . \tag{1.1}$$

The order parameter of the S_{A_1} phase is ψ_2, the complex amplitude of the mass-density wave at $2q_0$. The S_{A_2} phase has an additional order parameter ψ_1, the complex amplitude of the mass-density wave at q_0. Thus to study the S_{A_1}-S_{A_2} transition, we need to study the fluctuations of ψ_1 in the presence of a nonvanishing $\langle\psi_2\rangle$.

It is clear that there is no symmetry argument that would indicate that the S_{A_1}-S_{A_2} transition has to be first order, and our primary concern will be to identify the universality class of this transition when it is second order. Since ψ_2 is a complex order parameter, a naive argument would predict the universality class of the *xy* model. This, however, neglects the important coupling between ψ_1 and ψ_2. There is a preferred relative phase of the two order parameters so that only the amplitude of ψ_1 is critical once ψ_2 has ordered, indicating as pointed out by Prost [4] that the universality class should be that of the Ising model. This argument is again incomplete because it neglects the coupling between ψ_1 and the hydrodynamic phase mode (Goldstone boson) associated with the nonzero ψ_2 of the S_{A_1} phase. In this paper, we will develop a model which takes into account all of these couplings.

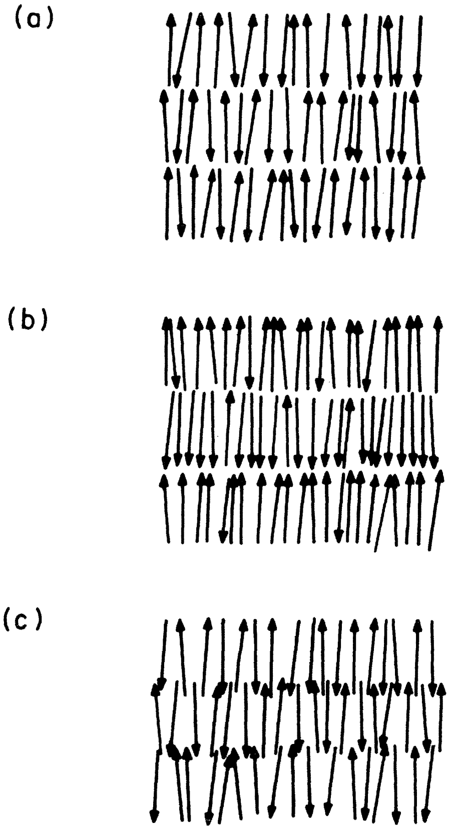

FIG. 1. Schematic representation of the three types of smectic-*A* phases: (a) the monolayer S_{A_1} phase, (b) the bilayer S_{A_2} phase, and (c) the S_{A_d} phase with layer spacing intermediate between one and two molecular lengths.

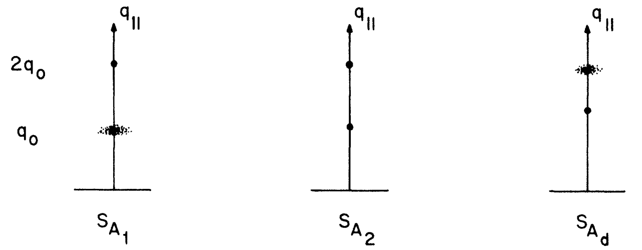

FIG. 2. X-ray diffraction patterns for the three smectic-A phases: (a) the S_{A_1} phase with a quasi-Bragg peak at $2q_0$ and a diffuse spot at q_0, (b) the S_{A_2} phase with quasi-Bragg peaks at both q_0 and $2q_0$, and (c) the S_{A_d} phase with a quasi-Bragg peak at a wave number between q_0 and $2q_0$ and a diffuse spot in the vicinity of $2q_0$.

Our conclusion is that the S_{A_1}-S_{A_2} transition is in the Ising universality class (at least near four dimensions) with isotropic correlation length critical exponents in agreement with the simple argument of Prost.[4] The physical correlation function $G(\vec{x},0)$ does not, however, behave simply as the spin correlation function in the Ising model. Interactions between the order parameter and the director lead to nonuniversal power-law behavior in $G(\vec{x},0)$ at the critical point and a resulting nonuniversal susceptibility exponent γ. This nonuniversality is simply a reflection of the well-known[5] lack of long-range order in ψ_2 in the S_{A_2} phase.

The outline of this paper is as follows. In Sec. II, we formulate an isotropic model for the S_{A_1}-S_{A_2} transition that neglects fluctuations of the Frank director, and we discuss its symmetries and associated Ward identities. In Sec. III, we develop momentum-shell recursion relations and study this model using the ϵ expansion. In Sec. IV, we formulate the full model for the S_{A_1}-S_{A_2} transition including anisotropy and couplings to the director and show that it is in the same universality class as the isotropic model of Sec. II. We then discuss the physical correlation function and derive its nonuniversal power-law behavior. Finally, there are two appendices presenting a derivation of the fundamental Ward identity and calculations of vertex functions to one-loop order in perturbation theory.

II. ISOTROPIC MODEL

The simplest model Hamiltonian $\bar{H}$ capable of describing the nematic (N), S_{A_1}, and S_{A_2} phases is a functional of the fields ψ_1 and ψ_2 only. In general, of course, all ψ_n are needed, but they can be expressed as functions of ψ_1 and ψ_2. The Hamiltonian must be invariant under uniform translations of the system. As can be seen from Eq. (1.1), a uniform translation by z along the z axis changes ψ_n to $\psi_n e^{inq_0 z}$. Thus, $\bar{H}$ must be invariant under $\psi_1 \rightarrow \psi_1 e^{i\phi}$, $\psi_2 \rightarrow \psi_2 e^{2i\phi}$. The simplest Hamiltonian[6] incorporating this invariance is

$$\bar{H} = \bar{H}_0 + \bar{H}_{\text{int}} \,, \tag{2.1}$$

where

$$\bar{H}_0 = \int d^d x \, \tfrac{1}{2}[r_1 |\psi_1|^2 + r_2 |\psi_2|^2 + |\nabla\psi_1|^2 + |\nabla\psi_2|^2] \tag{2.2}$$

is the noninteracting part and

$$\bar{H}_{\text{int}} = \int d^d x \left[\frac{u_1}{4!} |\psi_1|^4 + \frac{u_2}{4!} |\psi_2|^4 + \frac{u_{12}}{12} |\psi_1|^2 |\psi_2|^2 - \tfrac{1}{2}\bar{w} \, \text{Re}(\psi_1^2 \psi_2^*) \right] . \tag{2.3}$$

In the above, $r_1 \sim (T-T_1)$ and $r_2 \sim (T-T_2)$ where T is the temperature and T_1 and T_2 are, respectively, the mean-field N-S_{A_1} and N-S_{A_2} transition temperatures. Couplings of ψ_1 and ψ_2 to the Frank director $\vec{n}$ and spatial anisotropies are not included in this equation. They will be treated in Sec. IV. The phases of ψ_1 and ψ_2 have been chosen so that the potential $\bar{w}$ is real and a relative phase of zero is favored.

The Hamiltonian Eq. (2.1) has been used to study the N-S_{A_1}, N-S_{A_2} and S_{A_1}-S_{A_2} transitions in mean-field theory.[3,4,6] A renormalized perturbation theory and renormalization-group analysis can be applied directly to this model to study the S_{A_1}-S_{A_2} transition. Such an analysis is complicated, however, by the requirement that the equation of state for $\langle \psi_2 \rangle$ be calculated consistently at each order in perturbation theory. Near the S_{A_1}-S_{A_2} transition, fluctuations in the amplitude of ψ_2 are unimportant compared to those of the phase of ψ_2. We, therefore, replace ψ_2 by $|\psi_2| e^{i\phi}$ and treat $|\psi_2|$ as a constant to obtain the modified model

$$H = H_0 + H_{\text{int}} \,, \tag{2.4}$$

where

$$H_0 = \int d^d x \left[\tfrac{1}{2} r |\psi_1|^2 + \tfrac{1}{2} |\nabla\psi_1|^2 + \frac{K}{2} |\nabla\phi|^2 \right] , \tag{2.5}$$

and

$$H_{\text{int}} = \int d^d x \left[\frac{u}{4!} |\psi_1|^4 - \frac{w}{2} \text{Re}(e^{-i\phi}\psi_1^2) \right] , \tag{2.6}$$

where $r = r_1 + u_{12} |\psi_2|^2/6$, $K = |\psi_2|^2$, and $w = \bar{w} |\psi_2|$. In what follows, we will find it convenient to express H in terms of the variables $\psi_x = \text{Re}\psi_1$ and $\psi_y = \text{Im}\psi_1$:

$$H = \int d^d x \left[\tfrac{1}{2} r (\psi_x^2 + \psi_y^2) + \tfrac{1}{2} K (\nabla\phi)^2 + \tfrac{1}{2} (\nabla\psi_x)^2 + \tfrac{1}{2} (\nabla\psi_y)^2 - w [\sin\phi \, \psi_x \psi_y + \tfrac{1}{2} \cos\phi (\psi_x^2 - \psi_y^2)] + \frac{u}{4!} (\psi_x^2 + \psi_y^2)^2 \right] . \tag{2.7}$$

The phase translational invariance of Eq. (2.1) now takes the form of an invariance of Eq. (2.7) with respect to the transformations

$$\phi \to \phi + 2\theta\,, \quad \begin{bmatrix} \psi_x \\ \psi_y \end{bmatrix} \to \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} \psi_x \\ \psi_y \end{bmatrix} . \tag{2.8}$$

This invariance leads to a series of Ward identities for the vertex functions

$$\Gamma^{(n)}_{a_1 \cdots a_n}(x_1, \ldots, x_n) = \frac{\delta^n \Gamma}{\delta a_1(x_1) \cdots \delta a_n(x_n)}\,,$$

where Γ is the Legendre-transformed free energy and $a_i(x)$ can be $\psi_x(x)$, $\psi_y(x)$, or $\phi(x)$. The general form for these Ward identities is derived in Appendix A. Of particular interest in what follows are the relations,valid in the S_{A_1} phase,

$$\lim_{q\to 0} \Gamma^{(2)}_{\phi\phi}(\vec{q}) = 0\,, \tag{2.9a}$$

$$\lim_{q\to 0} [\,\Gamma^{(2)}_{xx}(\vec{q}) - \Gamma^{(2)}_{yy}(\vec{q})\,] = \lim_{q\to 0} 2\Gamma^{(3)}_{\phi xy}(\vec{q},\vec{q},0)\,, \tag{2.9b}$$

$$\lim_{q\to 0} \Gamma^{(4)}_{\phi\phi xx}(\vec{q},\vec{q},0,0) = \lim_{q\to 0} -2\Gamma^{(3)}_{\phi xy}(\vec{q},\vec{q},0)\,, \tag{2.9c}$$

where it is understood that x and y stand for ψ_x and ψ_y. Equation (2.9a) states the obvious that ϕ is a hydrodynamical variable in the S_{A_1} phase.

In order to develop a systematic loop expansion and renormalization-group recursion relations for functions arising from Eq. (2.7), it is convenient to expand in a power series in ϕ and to introduce a more general space of potentials. We, therefore, write

$$\begin{aligned} H = \int d^d x \Big[& \tfrac{1}{2} r_x \psi_x^2 + \tfrac{1}{2}\psi_y^2 + \tfrac{1}{2} c_x (\nabla\psi_x)^2 + \tfrac{1}{2} c_y (\nabla\psi_y)^2 + \tfrac{1}{2} K (\nabla\phi)^2 + \frac{1}{4!} u_x \psi_x^4 + \tfrac{1}{12} u_{xy} \psi_x^2 \psi_y^2 + \frac{1}{4!} u_y \psi_y^4 \\ & - w_1 \phi \psi_x \psi_y + \frac{1}{3!} w_3 \phi^3 \psi_x \psi_y + \tfrac{1}{4} w_{2x} \phi^2 \psi_x^2 - w_{2y} \phi^2 \psi_y^2 - \frac{w_{4x}}{2\cdot 4!} \phi^4 \psi_x^2 + \frac{w_{4y}}{2\cdot 4!} \phi^4 \psi_y^2 \Big] . \end{aligned} \tag{2.10}$$

To make Eq. (2.10) equivalent to Eq. (2.7), we must have $r_x = r - w$, $r_y = r + w$, $w_1 = w_3 = w_{2x} = w_{2y} = w$, $c_x = c_y = 1$, and $u_x = u_y = u_{xy} = u$. In this case the Ward identities of Eq. (2.9) are easily seen to be valid to lowest order in a loop expansion where $\Gamma^{(2)}_{xx}(0) = r_x$, $\Gamma^{(2)}_{yy}(0) = r_y$, $\Gamma^{(3)}_{\phi xy}(0,0,0) = w_1$, $\Gamma^{(4)}_{\phi\phi xx} = -w_{2x}$. We will use the Hamiltonian of Eq. (2.10) in subsequent sections, always remembering the relations among the bare potentials imposed by Eq. (2.9).

III. ϵ EXPANSION

The momentum-shell recursion relations of the ϵ expansion map the original Hamiltonian H with a spherical Brillouin zone of unit radius onto a Hamiltonian $H' \equiv RH$ by first removing degrees of freedom with wave number $\vec{q}$ between b^{-1} and 1 and rescaling the fields: $\psi_x \to \zeta_x \psi_x$, $\psi_y \to \zeta_y \psi_y$, and $\phi \to \zeta_\phi \phi$. Vertex and correlation functions can be expressed in terms of H or H'. For example,

$$\begin{aligned} \Gamma^{(2)}_{\phi\phi}(q,H) &= b^{-d} \zeta_\phi^2\, \Gamma^{(2)}_{\phi\phi}(q/b,H')\,, \\ \Gamma^{(2)}_{xx}(q,H) &= b^{-d} \zeta_x^2\, \Gamma^{(2)}_{xx}(q/b,H')\,. \end{aligned} \tag{3.1}$$

The Ward identities discussed in the previous section are satisfied by vertex functions of the original Hamiltonian; they are not, however, satisfied by those of the rescaled Hamiltonian H'. This is because H' is not invariant with respect to the simple transformations of Eq. (2.8) but rather to more general transformations involving rescaling of the fields. The Ward identity Eq. (2.9a) is, however, valid in all rescaled Hamiltonians $R^n H$ along the renormalization-group trajectory including any fixed-point Hamiltonian H^*. This provides a valuable check of the validity of our recursion relations.

The important vertex functions for this problem are evaluated in Appendix B to one-loop order for arbitrary potentials of Eq. (2.10) using the diagrams of Fig. 3. They satisfy the Ward identities as required. In this section, we will need to consider the vertex function $\Gamma^{(2)}_{\phi\phi}$ carefully. To one-loop order, it satisfies

$$\begin{aligned} \Gamma^{(2)}_{\phi\phi}(k) = K k^2 - w_1^2 \int_q & \frac{1}{r_x + c_x q^2} \frac{1}{r_y + c_y (\vec{k} + \vec{q})^2} \\ & + \tfrac{1}{2} w_{2x} \int_q \frac{1}{r_x + c_x q^2} \\ & - \tfrac{1}{2} w_{2y} \int_q \frac{1}{r_y + c_y q^2}\,, \end{aligned} \tag{3.2}$$

where

$$\int_q = \int \frac{d^d q}{(2\pi)^d}\,.$$

As just discussed, $\lim_{k\to 0} \Gamma^{(2)}_{\phi\phi}(k) = 0$ for all Hamiltonians along the RG trajectory.

To derive the momentum-shell recursion relations, we note that ψ_x is critical whereas ψ_y is non-critical. Usually in situations like this, the non-critical field is simply removed to produce a new effective Hamiltonian that is a function of the critical fields only. We will discuss this approach at the end of the section. Since ψ_y plays an

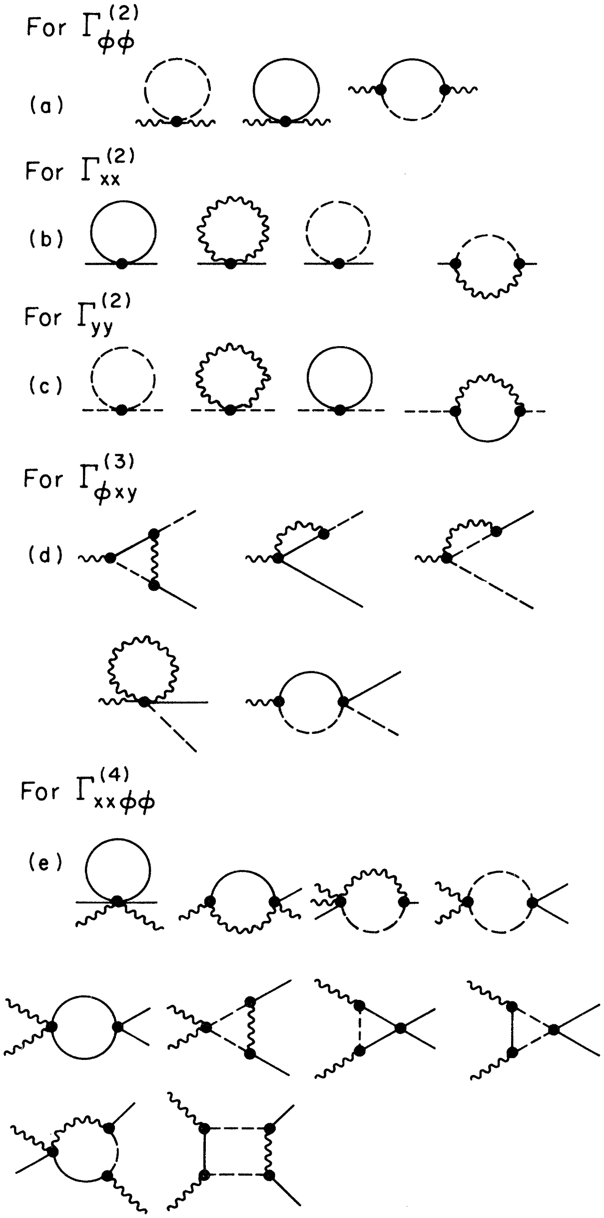

FIG. 3. Diagrams for some vertex functions. The unbroken lines represent G_{xx}, the broken lines G_{yy}, and the wavy lines $G_{\phi\phi}$. (a), (b), (c), (d), and (e), respectively, show diagrams for $\Gamma^{(2)}_{\phi\phi}$, $\Gamma^{(2)}_{xx}$, $\Gamma^{(2)}_{yy}$, $\Gamma^{(3)}_{\phi xy}$, and $\Gamma^{(4)}_{\phi\phi xx}$.

essential role in maintaining Ward identities, we find it convenient, for the moment, not to remove it. We will, however, rescale ψ_x and ψ_y differently. We set

$$\begin{aligned} \zeta_x^2 &= b^{d+2-\eta} , \\ \zeta_y^2 &= b^d , \\ \zeta_\phi^2 &= b^{d+2-\eta_\phi} , \end{aligned} \tag{3.3}$$

where η and η_ϕ are chosen to keep the coefficients c_x and K constant and equal to unity. With this choice of rescaling, all potentials involving ψ_y except w_1 and r_y are irrelevant. Furthermore, the potentials r_y and w_1 always occur in the combination $g = w_1^2/r_y$ since c_y is irrelevant. The differential recursion relations for $b = e^{\delta l}$ to first order in ϵ for the potentials of interest are therefore

$$\begin{aligned} \frac{du_x}{dl} &= \epsilon u_x - \tfrac{3}{2}K_d u_x^2 - \tfrac{3}{2}K_d w_{2x}^2 \\ &\quad + 6K_d g w_{2x} - 6K_d g^2 , \\ \frac{dw_{2x}}{dl} &= \epsilon w_{2x} - 2K_d g u_x + 4K_d g w_{2x} \\ &\quad - \tfrac{1}{2}K_d u_x w_{2x} - 2K_d w_{2x}^2 , \\ \frac{dg}{dl} &= \epsilon g + 3K_d g^2 - 2K_d w_{2x} g , \\ \frac{dr_x}{dl} &= 2r_x + \tfrac{1}{2}K_d w_{2x} + \tfrac{1}{2}K_d \frac{u_x}{1+r_x} - K_d g , \end{aligned} \tag{3.4}$$

where $K_d = \Omega_d/(2\pi)^d$ where Ω_d is the solid angle subtended by the unit sphere in d-dimension. η_ϕ and η are zero to first order in ϵ. The general fixed point structure of these equations is quite complex. We know, however, from Eq. (3.2) that at the fixed point $g = g^* = w_1^{*2}/r_y^* = w_{2x}^*/2$ in order to ensure that $\Gamma^{(2)}_{\phi\phi}(q) \sim q^2$ at small q because the potentials w_y and c_y are zero. Equations (3.4) have a stable fixed point satisfying these conditions with

$$K_d u_x^* = \tfrac{3}{2}\epsilon , \quad K_d g^* = \tfrac{1}{2}\epsilon , \quad K_d w_{2x}^* = \epsilon \tag{3.5}$$

and

$$\nu = \tfrac{1}{2} + \tfrac{1}{12}\epsilon , \quad \eta = 0 . \tag{3.6}$$

It is clear that this is a fixed point with Ising symmetry since the equations for u_x and r_x decouple completely from those for g and w_{2x} if $g = w_{2x}/2$. In other words, the fixed-point Hamiltonian consists of two disjoint parts for the critical fields ψ_x and ϕ: the Ising Hamiltonian for the field ψ_x and a non-interacting Gaussian spin-wave Hamiltonian for the field ϕ.

Another way of seeing this result is to consider the effective Hamiltonian for ψ_x and ϕ with the non-critical field ψ_y removed. We find

$$\begin{aligned} H_{\text{eff}} = &\int d^dx \left[\tfrac{1}{2}r_x\psi_x^2 + \tfrac{1}{2}(\nabla\psi_x)^2 + u_x\psi_x^4\right] + \int d^dx \left[\frac{r_\phi}{2}\phi^2 + \tfrac{1}{2}K(\nabla\phi)^2\right] \\ &- \int d^dx \int d^dx'\, u_{\phi x}(x,x')\phi(x)\psi_x(x)\phi(x')\psi_x(x') , \end{aligned} \tag{3.7}$$

where

$$u_{\phi x}(x,x') = 1/4[w_{2x}\delta(\vec{x}-\vec{x}') - 2w_1^2 G_{yy}(\vec{x},\vec{x}')]$$

and $r_\phi = -\frac{1}{2} w_{2y} G_{yy}(\vec{x},\vec{x})$ where $G_{yy}(\vec{x},\vec{x}') = \langle \psi_y(\vec{x}) \psi_y^*(\vec{x}') \rangle$. To one-loop order, the contribution from $u_{\phi x}$ cancels the r_ϕ term keeping $\Gamma^{(2)}_{\phi\phi}(q=0)=0$ as required. At the fixed point, $u_{\phi x} = 0$ and $r^*_\phi = 0$. It seems likely to us that the decoupling of ψ_x and ϕ remains true to higher order in ϵ. We have, however, not found a general symmetry argument leading to this result nor have we carried out the rather tedious calculations needed to verify this to second order in ϵ.

IV. GENERAL MODEL

The model presented in Sec. II is incomplete in two respects: it does not include anisotropy and coupling of the order parameters ψ_1 and ψ_2 to the Frank director $\vec{n}$. The invariance of the Hamiltonian with respect to simultaneous rotations of the director and the smectic planes leads to a gaugelike coupling between $\delta\vec{n} = \vec{n} - \vec{n}_0$ (where $\vec{n}_0$ is the uniform equilibrium director) and both ψ_1 and ψ_2 to quadratic order in $\delta\vec{n}$. The non-interacting Hamiltonian of Eq. (2.2) is thus replaced by

$$\bar{H}_0 = \int d^dx \tfrac{1}{2}[r_1|\psi_1|^2 + r_2|\psi_2|^2 + |\nabla_{||}\psi_1|^2 + c_{||}|\nabla_{||}\psi_2|^2 + |(\nabla_\perp - iq_0\delta\vec{n})\psi_1|^2 + c_\perp|(\nabla_\perp - 2iq_0\delta\vec{n})\psi_2|^2] , \tag{4.1}$$

where we have chosen length scales so that the coefficients of $|\nabla_{||}\psi_1|^2$ and $|\nabla_\perp\psi_1|^2$ are unity. The full Hamiltonian is

$$H = \bar{H}_0 + \bar{H}_{\text{int}} + H_F , \tag{4.2}$$

where $\bar{H}_{\text{int}}$ is given in Eq. (2.3) and H_F is the usual Frank Hamiltonian

$$H_F = \int d^dx \tfrac{1}{2}\{K_1(\nabla\cdot\vec{n})^2 + K_2(\vec{n}\cdot\nabla\times\vec{n})^2 + K_3[\vec{n}\times(\nabla\times\vec{n})]^2\} . \tag{4.3}$$

This Hamiltonian leaves out non-linear terms needed to ensure global rotational invariance.[7] Though these terms do affect the elastic properties of the smectic phases, we do not believe they have an important effect on the S_{A_1}-S_{A_2} transition, and we will ignore them.

Equation (4.2) is the analog of Eq. (2.1). To obtain the analog of Eq. (2.4), we set $\psi_2 = e^{i\phi'}$ as before to obtain

$$H_0 = \int d^dx \tfrac{1}{2}[r|\psi_1|^2 + |\nabla_{||}\psi_1|^2 + |(\nabla_\perp - iq_0\delta\vec{n})\psi_1|^2 + K_{||}(\nabla_{||}\phi')^2 + K_\perp(\nabla_\perp\phi' - 2q_0\delta\vec{n})^2] \tag{4.4}$$

and

$$H = H_0 + H_{\text{int}} + H_F , \tag{4.5}$$

where H_{int} is expressed in Eq. (2.6). The simplest way to study the effects of couplings to the director is to perform a change of variables to decouple ϕ' from $\delta\vec{n}$. This change of variables has the appearance of gauge transformation [8,9]

$$\begin{aligned} \delta\vec{n} &= \vec{A} + \nabla L , \\ \phi' &= \phi + 2q_0 L , \\ \psi_1 &= \psi e^{iq_0 L} . \end{aligned} \tag{4.6}$$

After this transformation, H_{int} is unchanged,

$$H_0 = \int d^dx \tfrac{1}{2}[r|\psi|^2 + |(\nabla_{||} - iq_0A_{||})\psi|^2 + |(\nabla_\perp - iq_0\vec{A}_\perp)\psi|^2 + K_{||}(\nabla_{||}\phi - 2q_0A_{||})^2 + K_\perp(\nabla_\perp\phi - 2q_0\vec{A}_\perp)^2] , \tag{4.7}$$

and H_F becomes a function of both L and $\vec{A}$. To decouple $\vec{A}$ and ϕ, we choose

$$K_{||}\nabla_{||}A_{||} + K_\perp\nabla_\perp\cdot\vec{A}_\perp = 0 . \tag{4.8}$$

When $K_{||} = K_\perp$, this is the usual transverse constraint of the "SC" gauge.[8,9] Equation (4.8) determines L in terms of $\delta\vec{n}$ via Eq. (4.6a) and allows $\delta\vec{n}$ and thus H_F to be expressed in terms of $\vec{A}$ only. Defining $\vec{A}_s$ to be the component of $\vec{A}$ in the $\vec{n}_0$-$\vec{q}$ plane and A_t the component of $\vec{A}$ in the space perpendicular to the $\vec{n}_0$-$\vec{q}$ plane, we obtain

$$H = H_0' + H_{\text{int}} + H_A , \tag{4.9}$$

where

$$H_0' = \int d^dx \, \tfrac{1}{2}[r|\psi|^2 + |(\nabla - iq_0\vec{A})\psi|^2] + \int d^dx \, \tfrac{1}{2}[K_{||}(\nabla_{||}\phi)^2 + K_\perp(\nabla_\perp\phi)^2] \tag{4.10}$$

and

$$H_A = \int_q \frac{1}{2}\left\{\left[4q_0^2K_{||}K_\perp + \left[K_3 + K_1\frac{q_\perp^2}{q_{||}^2}\right]K(q)\right]\left[\frac{K(q)}{K_{||}^2q_{||}^2 + K_\perp^2q_\perp^2}\right]\vec{A}_s^2 + (4q_0^2K_\perp + K_2q_\perp^2 + K_3q_{||}^2)A_t^2\right\} , \tag{4.11}$$

where

$$K(q)=K_{\|}q_{\|}^2+K_{\perp}q_{\perp}^2 \;.$$

We are now in a position to analyze the effect of anisotropy and couplings to $\delta\vec{n}$ on the S_{A_1}-S_{A_2} transition. The first thing to note is that $\vec{A}$ is not a hydrodynamic variable: its independent components have "masses" determined by $K_{\|}$ and $K_{\perp}$ and the constraint, Eq. (4.8). Thus $\vec{A}$ can be removed to produce an effective Hamiltonian that is identical in form to that of Eq. (2.2) except for the anisotropy imposed by $K_{\|}\neq K_{\perp}$. At the Ising fixed point discussed in the previous sections, the critical fields ψ_x and ϕ decouple completely. Since anisotropy has no effect on the critical exponents of the Ising fixed point associated with an independent ψ_x or the Gaussian fixed point associated with an independent ϕ, it is clear that introduction of anisotropy in the original Hamiltonian will have no effect on critical exponents. This has been explicitly verified to first order in ϵ using recursion relations appropriate to the anisotropic system.

Though the S_{A_1}-S_{A_2} transition is in the same universality class as the Ising model, the coupling of ψ to $\delta\vec{n}$ leads to anomalous behavior for the physical correlation function $G(\vec{x},\vec{x}\,')=\langle\psi_1(\vec{x})\psi_1^*(\vec{x}\,')\rangle$. The correlation function in the "SC" gauge is, apart from dependence on irrelevant variables, identical to the spin-correlation functions of the Ising model. Correlations in the physical field ψ_1 can be related to correlations in ψ_{SC} via

$$\begin{aligned}G_{\mathrm{SC}}(\vec{x},0)&=\langle\psi_{\mathrm{SC}}(\vec{x})\psi_{\mathrm{SC}}^*(0)e^{-iq_0[L(\vec{x})-L(0)]}\rangle\\&\equiv\widetilde{G}_{\mathrm{SC}}(\vec{x},0)\,C(\vec{x})\;,\end{aligned}\tag{4.12}$$

where

$$\widetilde{G}_{\mathrm{SC}}(\vec{x},0)=\frac{\langle\psi_{\mathrm{SC}}(\vec{x})\psi_{\mathrm{SC}}^*(0)e^{-iq_0[L(\vec{x})-L(0)]}\rangle}{\langle e^{-iq_0[L(\vec{x})-L(0)]}\rangle}\tag{4.13}$$

and

$$C(\vec{x})=\langle e^{-iq_0[L(\vec{x})-L(0)]}\rangle\;.\tag{4.14}$$

The large-$|\vec{x}|$ behavior[8,10] of $C(\vec{x})$ is dominated by the cumulant $\langle[L(\vec{x})-L(0)]^2\rangle$ which can be calculated using

$$\langle|L(\vec{q})|^2\rangle=\frac{K_{\perp}q_{\perp}^2}{K^2(q)}D_{\perp}(\vec{q})\;,\tag{4.15}$$

where

$$D_{\perp}(\vec{q})\;=\;(K_1q_{\perp}^2\;+\;Bq_{\|}^2/q_{\perp}^2)^{-1}\;,\tag{4.16}$$

where B is the usual compression modulus for smectics. In the present model, $B=4q_0^2K_{\perp}$ to lowest order in perturbation theory. Using Eqs. (4.14) and (4.15), it is easy to verify that at large $|\vec{x}|$ $C(\vec{x})$ is identical to the function calculated by Caillé:[5]

$$C(\vec{x})\;=\;\begin{cases}x_{\|}^{-\eta_c} & x_{\perp}=0\\ x_{\perp}^{-2\eta_c} & x_{\|}=0\end{cases}\tag{4.17}$$

where

$$\eta_c\;=\;\frac{q_0^2k_BT}{8\pi\sqrt{K_1B}}\;.\tag{4.18}$$

Note that $C(\vec{x})$ dies off algebraically rather than exponentially as it does in the nematic phase and at the nematic to smectic-A critical point.[8–10] To complete the calculation of $G(\vec{x},0)$, we need to consider $\widetilde{G}_{\mathrm{SC}}(\vec{x},0)$ which can be expanded in a power series[10] in q_0. Low-order diagrams in this expansion are shown in Fig. 4. The first term is precisely $G_{\mathrm{SC}}(\vec{x},0)$ which has Ising critical behavior. Higher-order diagrams [Figs. 4(b) and 4(c)] involve both $G_{\mathrm{SC}}(\vec{x},0)$ and $D_{LA_i}(\vec{x},\vec{x}\,')=\langle L(\vec{x})A_i(\vec{x}\,')\rangle$ which die off, respectively, with characteristic lengths $\xi\sim t^{-\nu}$ and $\lambda=(K_1/B)^{1/2}$ where t is the reduced temperature. It is tedious but straightforward to verify that there are no infrared singularities in these diagrams[10] so that they die off with a length $l\sim\min(\lambda,\xi)$. λ is not a critical function of temperature in the S_{A_1} phase as the S_{A_2} line is approached so that $l\sim\lambda$ as $t\to0$. Thus $\widetilde{G}_{\mathrm{SC}}(\vec{x},0)\sim G_{\mathrm{SC}}(\vec{x},0)$ as $t\to0$ and

$$G(\vec{x},0)=C(\vec{x})\,|\vec{x}|^{-(d-2+\eta)}f\left[\frac{|\vec{x}|}{\xi}\right],\tag{4.19}$$

where we have inserted the isotropic scaling form for $G_{\mathrm{SC}}(\vec{x},0)$ near the critical point. This form implies that $G(\vec{x},0)$ has anisotropic power-law behavior with critical exponents varying continuously along the S_{A_1}-S_{A_2} critical line:

$$G(\vec{x},0)\;\sim\;\begin{cases}x_{\|}^{-(d-2+\eta+\eta_c)} & x_{\perp}=0\\ |x_{\perp}|^{-(d-2+\eta+2\eta_c)} & x_{\|}=0\end{cases}\;.\tag{4.20}$$

Equations (4.18) and (4.19) imply that the susceptibility χ satisfies

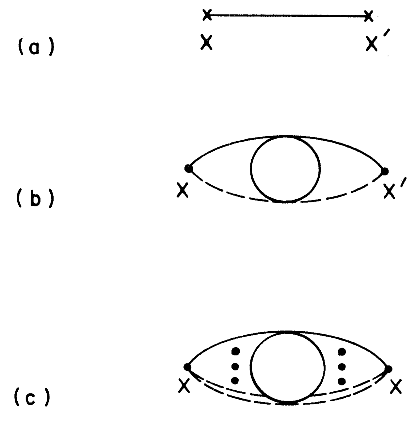

FIG. 4. Diagrams contributing to $\widetilde{G}_{\mathrm{SC}}(\vec{x},\vec{x}\,')$. The unbroken line represents $G_{\mathrm{SC}}(\vec{x},\vec{x}\,')$ and the broken line D_{LA_i}. The circles in (b) and (c) represent vertex functions. (a) is simply G_{SC} and is the dominant contribution to $\widetilde{G}_{\mathrm{SC}}$ near $t=0$. The D_{LA_i} propagators in (b) and (c) cause these diagrams to decay to zero for $|\vec{x}-\vec{x}\,'|>\lambda$.

$$\chi = \int d^d x\, G(\vec{x},0) \sim \xi^{2-\eta-2\eta_c} \tag{4.21}$$

so that

$$\gamma = (2-\eta-2\eta_c)\nu \tag{4.22}$$

is not universal but depends on the values of B and K_1 at the critical point. η_c can be calculated using Eq. (4.18). Using $q_0 = 0.222 \times 10^8 \text{cm}^{-1}$, $K_1 = 10^{-6}$ dynes, $B = 10^8$ dynes/cm^2, and $T = 360$ K, we obtain $\eta_c \sim 0.1$. Thus we predict that γ is of order 0.1 to 0.2 less than the Ising value of 1.242 (Ref. 11) that is presumed to be appropriate for the SC gauge in three dimensions.

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APPENDIX A

To derive the Ward identities discussed in the text, we consider the partition function

$$Z(h_x,h_y,h_\phi) = \int D\psi_x D\psi_y D\phi\, e^{-H-H_{\text{ext}}}\ , \tag{A1}$$

where H is given by Eqs. (2.4) to (2.6) and

$$H_{\text{ext}} = -\int d^d x [h_x(x)\psi_x(x) + h_y(x)\psi_y(x) + h_\phi \phi(x)]\ . \tag{A2}$$

The invariance of H under the transformations of Eq. (2.8) implies that

$$Z(h_x,h_y,h_\phi) = \exp\left[\int d^d x 2h_\phi(x)\theta\right] Z(h_x\cos\theta + h_y\sin\theta,\ -h_x\sin\theta + h_y\cos\theta,\ h_\phi) \tag{A3}$$

or that

$$\frac{\partial \ln Z}{\partial \theta} = \int d^d x\, [2h_\phi(x) + \langle\psi_x(x)\rangle h_y(x) - \langle\psi_y(x)\rangle h_x(x)]\ , \tag{A4}$$

where $\langle\psi_x(x)\rangle$ and $\langle\psi_y(x)\rangle$ are the averages of $\psi_x(x)$ and $\psi_y(x)$ with respect at $H + H_{\text{ext}}$. Introducing the Legendre-transformed free energy

$$\Gamma(\langle\psi_x\rangle,\langle\psi_y\rangle) = -\ln Z + \int d^d x\, [h_x(x)\langle\psi_x(x)\rangle + h_y(x)\langle\psi_y(x)\rangle + h_\phi(x)\langle\phi(x)\rangle]\ , \tag{A5}$$

Eq. (A3) can be reexpressed as

$$\int d^d x\, [2\Gamma_\phi^{(1)}(x) + \langle\psi_x(x)\rangle\Gamma_y^{(1)}(x) - \langle\psi_y(x)\rangle\Gamma_x^{(1)}(x)] = 0\ , \tag{A6}$$

where these vertex functions are defined as

$$\Gamma^{(n)}_{a_1 \cdots a_n}(x_1,\ldots,x_n) = \frac{\delta^n \Gamma}{\delta a_1(x_1)\cdots\delta a_n(x_n)}\ , \tag{A7}$$

where a_i can be ψ_x, ψ_y, or ϕ with the convention that x and y rather than ψ_x and ψ_y be used as subscripts on the left-hand side of the equation. Successive differentiation of Eq. (A5) yields the Ward identities of Eqs. (2.9) where

$$\Gamma^{(2)}_{ab}(q) = \int d^d x\, e^{-i\vec{q}\cdot\vec{x}}\, \Gamma^{(2)}_{ab}(\vec{x},0) \tag{A8}$$

and

$$\Gamma^{(n)}_{a_1 \cdots a_n}(k_1,\ldots,k_n)\delta^{(d)}(\vec{k}_1 + \cdots + \vec{k}_n) = \int d^d x_1 \cdots d^d x_n e^{-i\vec{k}_1\cdot\vec{x}_1} \cdots e^{-i\vec{k}_n\cdot\vec{x}_n} \Gamma^{(n)}{}_{a_1 \cdots a_n}(\vec{x}_1,\ldots,\vec{x}_n)\ . \tag{A9}$$

APPENDIX B

Perturbation expressions for the vertex functions are easily derived from the general Hamiltonian of Eq. (2.10). One-loop diagrams for some vertex functions are shown in Fig. 3. From these, we obtain the following one-loop expressions for $\Gamma^{(2)}_{xx}$, $\Gamma^{(2)}_{yy}$, $\Gamma^{(3)}_{\phi xy}$, and $\Gamma^{(4)}_{\phi\phi xx}$:

$$\Gamma^{(2)}_{xx}(\vec{q}=0) = r_x + \tfrac{1}{4}w_{2x}\int_q G_{\phi\phi}(\vec{q}) + \tfrac{1}{2}u_x\int_q G_{xx}(\vec{q}) + \tfrac{1}{6}u_{xy}\int_q G_{yy}(\vec{q}) - w_1^2\int_q G_{\phi\phi}(\vec{q})G_{yy}(\vec{q})\ , \tag{B1}$$

$$\Gamma^{(2)}_{yy} = r_y - \tfrac{1}{2}w_{2y}\int_q G_{\phi\phi}(\vec{q}) + \tfrac{1}{2}u_y\int_q G_{yy}(\vec{q}) + \tfrac{1}{6}u_{xy}\int_q G_{xx}(\vec{q}) - w_1^2\int_q G_{\phi\phi}(\vec{q})G_{xx}(\vec{q})\ , \tag{B2}$$

$$\begin{aligned}\Gamma^{(3)}_{\phi xy} = {} & w_1 - \tfrac{1}{2}w_3\int_q G_{\phi\phi}(\vec{q}) + w_1 w_{2y}\int_q G_{\phi\phi}(\vec{q})G_{yy}(\vec{q}) - w_1 w_{2x}\int_q G_{\phi\phi}(\vec{q})G_{xx}(\vec{q}) \\ & + w_1^3\int_q G_{\phi\phi}(\vec{q})G_{xx}(\vec{q})G_{yy}(\vec{q}) - \tfrac{1}{3}u_{xy}w_1\int_q G_{xx}(\vec{q})G_{yy}(\vec{q})\ ,\end{aligned} \tag{B3}$$

$$\begin{aligned}\Gamma^{(4)}_{\phi\phi xx} = {} & w_{2x} - \tfrac{1}{2} w_{4x} \int_q G_{\phi\phi}(\vec{q}) - 2w_{2x}^2 \int_q G_{\phi\phi}(\vec{q}) G_{xx}(\vec{q}) + w_1 w_3 \int_q G_{\phi\phi}(\vec{q}) G_{yy}(\vec{q}) + \tfrac{1}{6} u_{xy} w_{2y} \int_q G_{yy}^2(\vec{q}) \\ & - \tfrac{1}{2} w_{2x} u_x \int_q G_{xx}^2(\vec{q}) - w_1 w_{2y} \int_q G_{\phi\phi}(\vec{q}) G_{yy}^2(\vec{q}) + \tfrac{1}{3} w_1^2 u_{xy} \int_q G_{xx}(\vec{q}) G_{yy}^2(\vec{q}) \\ & + 4 w_{2x} w_1 \int_q G_{\phi\phi}(\vec{q}) G_{xx}(\vec{q}) G_{yy}(\vec{q}) + w_1^2 u_x \int_q G_{xx}^2(\vec{q}) G_{yy}(\vec{q}) - 2 w_1^2 \int_q G_{\phi\phi}(\vec{q}) G_{xx}(\vec{q}) G_{yy}^2(\vec{q}) \, . \end{aligned} \tag{B4}$$

One can easily see that the Ward identities of Eqs (2.9) are satisfied when $w_1 = w_{2x} = w_{2y} = w_3 = w_{4x} = w_{4y}$ and $u_x = u_y = u_{xy}$.

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