# Anisotroyic critical properties of the de Gennes model for the nematic to smectic- $A$  phase transition\*

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(Received 20 June 1977)

The generalized de Gennes model for the nematic to smectic- $A$  phase transition in liquid crystals with an order parameter with  $n/2$  complex components is investigated using the  $\epsilon$  expansion in the vicinity of four dimensions. It is found that anisotropic critical behavior with correlation lengths in directions parallel and perpendicular to the direction of molecular alignment diverging at different rates described by exponents  $v_{\parallel}$ and  $v_{\perp}$  is possible. When the splay elastic constant  $K_1 = \infty$  and  $n > n_{c2} = 238.17$ , there is an accessible fixed point with  $v_{\parallel} > v_{\perp}$ . If  $K_1$  is large but not infinite and  $n = 2$ , it is expected that there will be a series of crossovers from anisotropic quasicritical behavior to isotropic heliumlike quasicritical behavior and finally to a first-order transition. Present theory and current experiments are compared briefly and found to be in incomplete agreement.

#### I. INTRODUCTION

The nematic to smectic-A phase transition in liquid crystals' has received a great deal of experimental and theoretical attention since McMillan' and Kobayashi<sup>3</sup> first suggested that it might be second order with a complex order parameter. It was an appealing transition to study because it was felt that it should fall into the same universality class as the  $\lambda$  transition in superfluid helium with the advantage that order-parameter fluctuations would be directly accessible to experimental probes. de Gennes<sup>4,5</sup> was the first to recognize the importance of fluctuations in direction of molecular orientation [described by the director  $\tilde{n}(\tilde{r})$ ] on the transition. He introduced a phenomenological Landau-Ginzburg free energy which was very similar to that of a superconductor with the director playing the role of the vector potential. It is theoretically expected that fluctuations in the vector potential will lead to a first-order transition to the superconducting state. $6$  Thus, the N-A transition is also expected to be first order.<sup>7</sup> Nevertheless, for nearly second-order transitions, it was generally assumed that effective critical exponents would be the same as the  $\lambda$  transition in helium.<sup>4-7</sup> This view was corroborated by a renormalization group calculation that indicated that anisotropies that are present in the liquid crystal, but which are not present in the superconductor, are suppressed by fluctuations.<sup>7</sup> Thus, the more nearly second order the  $N-A$  transition is, the more the critical exponents should approach those of the  $\lambda$ transition in superfluid helium.

Early experiments yielded critical exponents that Early experiments yielded critical exponents that<br>were either heliumlike<sup>8-13</sup> (i.e., had the same values as the  $\lambda$  transition in helium) or nearly meanfield-like for pure systems, but strongly purity

dependent.<sup>14</sup> More recent light-scattering experi<br>ments<sup>15–19</sup> show twist and bend elastic constants di  $\mathrm{ments}^{15-19}$  show twist and bend elastic constants diverging at different rates and apparent anisotropic critical behavior below  $T_c$ . All experiments show a transition that was more nearly second order critical behavior below  $T_c$ . All experiments sh<br>a transition that was more nearly second order<br>than theoretically predicted.<sup>6,7</sup> It was these experimental observations that prompted us to reinvestigate the critical properties of the de Gennes model. We find that anisotropy is inherent in the de Gennes model and that anisotropic quasicritical behavior is possible. In other words, we find that it is possible for correlation lengths parallel and perpendicular to  $\tilde{n}$  to diverge at different rates. This anisotropy is fundamentally different, for example, from that of an Ising model with asymmetric coupling where the ratio of the parallel to perpendicular correlation lengths is a constant as the critical point is approached. The extent to which critical behavior is anisotropic is controlled by the value of the splay elastic constant  $K_1$ : large  $K_1$  leads to large anisotropy. One can easily see how large  $K_1$  might lead to anisotropic critical behavior. If  $K<sub>1</sub>$  is infinite, splay deformations are prohibited. This means that bending of the smectic layers is prohibited in the smectic phase. Thus large  $K<sub>1</sub>$  enforces large anisotropy in the smectic phase.

Subject to some qualifications which will be discussed briefly in Sec. V, the x-ray structure gives a direct measure of the parallel and perpendicular correlation lengths in the vicinity of the nematic to smectic-A transition. As this paper was being<br>prepared, Als-Nielsen *et al*.<sup>20</sup> reported the resul prepared, Als-Nielsen  $et$   $al.^{20}$  reported the result of x-ray measurements of the structure factor that are an order of magnitude more precise than pre-<br>vious results obtained by McMillan.<sup>21</sup> These mea vious results obtained by McMillan. $^\mathrm{21}$  These measurements show parallel and perpendicular correlation lengths diverging at essentially the same

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rate (that varies with temperature) over more than two decades to within a few millikelvin of the transition. These results are in disagreement with published results obtained by light scattering. It is possible, however, that a reanalysis and reinterpretation of the light-scattering data will yield agreement.

We had originally planned to present a rather detailed analysis of experimental data in light of the new theoretical information presented in this paper. However, in view of the incompletely resolved discrepancy between x-ray and light-scattering measurements of critical exponents, we will refrain from presenting a detailed analysis. Instead, we will indicate in the final section what experimental behavior is predicted by the present theory. We do not fully understand why experiments fail to agree among themselves or why they fail to agree with the theory presented here. There are some aspects of the de Gennes model peculiar to three dimensions discussed briefly at the end of Sec. V, an understanding of which may lead to a resolution of existing discrepancies. A full study of these aspects of the model is beyond the scope of this paper. We stress, however, that the results presented in this paper stand on their own and are inescapable properties of the de Gennes model. They must be taken seriously in spite of their complexity. It has been suggested<sup>16</sup> that the de Gennes model may miss some of the physics of the nematic to smectic-A transition. We feel that all of the physics of the de Gennes model must be understood before such a drastic step is contemplated. This paper is another step towards such an understanding.

This paper is divided into five sections of which this is the first. In Sec. II, we will review the relevant properties of the de Gennes model. This section is somewhat condensed. The reader interested in further details is encouraged to consult Refs. 4, 5, 22, and 23. In Sec. III, we discuss general properties of correlation functions if anisotropic scaling holds. In Sec. IV, we develop renormalization-group (RG) recursion relations that are sufficiently general to admit the possibility of anisotropic critical behavior. We find that there is a stable fixed point with anisotropic scaling when  $K_1 = \infty$  and  $n > 238.17$ . At the end of Sec. IV, we review the various types of crossovers that are possible in the context of the present theory. In Sec. V, we review some problems that remain in reconciling theory and experiment. In particular, we reconsider the magnitude of the first-order jump, discuss what sort of crossover might be expected on the basis of the present theory and measured bare anisotropies, and indicate avenues of future research that might bring about

agreement between theory and experiment. Finally, in the Appendix, we present some calculational details.

### II. DE GENNES MODEL

Let  $\rho(\vec{x})$  be the center-of-mass molecular density at position  $\bar{x}$ . In the smectic-A phase, there is a mass density wave parallel to the director  $\overline{n}$ , and p can be decomposed into Fourier components

$$
\rho(\vec{x}) = \rho_0 \{ 1 + \left[ (1/\sqrt{2})e^{i\vec{q}_0 \cdot \vec{x}} \psi(\vec{x}) + (c.c.) \right] + \cdots \}, \tag{1}
$$

where  $\overline{\dot{q}}_0 = (2\pi/a)\overline{\dot{n}}$  and  $a$  is the interplanar spacing If the N-A transition is nearly second order, higher Fourier components can be neglected, and  $\psi(\vec{x})$ can be regarded as the order parameter for the smectic-A phase. The de Gennes free energy  $F$ in d dimensions is given by

$$
F = \int d^d x \{ A^0 | \psi |^2 + \frac{1}{2} U^0 | \psi |^4 + C_\shortparallel^0 | \nabla_\shortparallel \psi |^2
$$
  
+  $C_\perp^0 | (\vec{\nabla}_\perp - i q_0 \delta \vec{\mathbf{n}}) \psi |^2 + \frac{1}{2} K_\perp^0 (\vec{\nabla} \cdot \vec{\mathbf{n}})^2$   
+  $\frac{1}{2} K_\perp^0 (\vec{\mathbf{n}} \cdot \vec{\nabla} \times \vec{\mathbf{n}})^2 + \frac{1}{2} K_\infty^0 [\vec{\mathbf{n}} \times (\vec{\nabla} \times \vec{\mathbf{n}})]^2 \},$  (2)

where  $A^0 = a^0 t_0$ ,  $t_0 = (T - T_0^*)/T_0^*$ ,  $T_0^*$  is the meanfield transition temperature,  $\delta \overline{\mathbf{n}}$  is the deviation of the director from its uniform equilibrium value  $\overline{n}_{0}$ , || and  $\perp$  indicate, respectively, directions parallel and perpendicular to  $\overline{n}_{0}$ , and the superscript zero indicates bare values of parameters. This free energy leads to correlation functions  $G(\vec{q})$  $=\langle |\psi(\vec{q})|^2 \rangle$  and  $D_{ij}(\vec{q}) = \langle \delta n_i(\vec{q}) \delta n_j(-\vec{q}) \rangle$  with proper symmetry. If we choose  $\overline{n}_0$  to be along the 1 axis

and 
$$
\bar{q}
$$
 to be in the 1-2 plane, we have<sup>22</sup>  
\n $G(\bar{q}) = k_B T[A(t) + C_{\parallel}q_{\parallel}^2 + C_{\perp}q_{\perp}^2]^{-1}$ ,  $T > T_c$ ; (3a)  
\n $D_{33}(\bar{q}) \equiv D_t(\bar{q}) = \begin{cases} k_B T[K_3 q_{\parallel}^2 + K_2 q_{\perp}^2]^{-1}, & T > T_c, \\ k_B T[D + K_2 q_{\perp}^2 + K_3 q_{\parallel}^2]^{-1}, & T < T_c; \end{cases}$  (3b)

$$
D_{22}(\vec{q}) = D_{1}(\vec{q}) = \begin{cases} k_{B}T[K_{3}q_{0}^{2} + K_{1}q_{1}^{2}]^{-1}, & T > T_{c}, \\ k_{B}T[K_{1}q_{1}^{2} + B(q_{0}/q_{1})^{2}]^{-1}, & (3c) \end{cases}
$$

$$
T < T_{c}, q_{0} \ll q_{1},
$$

where  $t = (T - T^*)/T^*$ ,  $T^*$  is the limit of metastability of cooling, and where  $T_c$  is the actual transition temperature which will differ from  $T^*$  in a first order transition.  $D$  and  $B$  are new parameters which are respectively equal to  $2C_1\psi_0^2q_0^2$  and  $2C_{\mu}\psi_0^2q_0^2$ , where  $\psi_0$  is the equilibrium value of  $\psi$  in the ordered phase. The zero superscripts have been removed in the above to indicate that temperature-dependent normalizations of the bare parameters can, occur. For nearly-second-order transitions,  $A(t) \sim t^{\gamma}$  for  $T > T_c$ , where  $\gamma$  is the

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susceptibility exponent. For  $T < T_c$ ,  $A(t)$  has a. more complicated form unless the transition is actually second order  $(T^* = T_c)$  in which case  $A(t)$ actual $\sim$   $\mid t\mid^{\gamma}.$ 

In mean-field theory, the free energy of Eq. (2) yields correlation lengths

$$
\xi_{\rm II}^2 = C_{\rm II}^{\rm o}/A_{\rm O}^{\rm o}, \quad \xi_{\rm I}^2 = C_{\rm I}^{\rm o}/A^{\rm o}, \tag{4}
$$

describing, respectively, correlations parallel and perpendicular to  $\overline{n}_0$ . Both of these lengths diverge as  $t^{-1/2}$  in mean-field theory, and their ratio  $\xi_{\parallel}/2$  $\xi_1$  is a constant  $(C_{\rm u}^0/C_1^0)^{1/2}$ . The mean-field correlation length exponents are thus,  $v_{\mu} = v_1 = \frac{1}{2}$ . The gaugelike coupling of  $\psi$  to  $\overline{\mathbf{n}}$  leads to critical enhancements of the elastic constants  $K_2$  and  $K_3$ . We introduce exponents  $\xi_2$  and  $\xi_3$  to describe this enhancement

$$
\delta K_2 = K_2 - K_2^0 \sim |t|^{-\xi_2}, \tag{5a}
$$

$$
\delta K_3 = K_3 - K_3^0 \sim |t|^{-\epsilon_3}.
$$
 (5b)

If mean-field behavior for field  $\psi$  is assumed,  $\delta K_2$ and  $\delta K$ <sub>3</sub> can be calculated<sup>4, 23</sup>

$$
\delta K_2 = (k_B T / 24\pi) q_0^2 \xi_1^2 / \xi_{\parallel}, \qquad (6a)
$$

$$
\delta K_3 = (k_B T / 24\pi) q_0^2 \xi_{\parallel}.
$$
 (6b)

From Eq. (4),  $\xi_{\parallel}$  and  $\xi_{\perp}$  diverge in the same way in mean-field theory so that  $\delta K_2 \sim \delta K_3 \sim t^{-1/2}$  ( $\xi_2$  $= \zeta_3 = \frac{1}{2}$ . We also introduce exponents  $\varphi$  and  $\varphi'$ to describe the critical behavior of  $B$  and  $D$ ,

$$
B \sim |t|^\varphi, \quad D \sim |t|^\varphi' \,.
$$

In mean-field theory,  $\varphi = \varphi' = 1$ , and  $D/B = C_1^0/C_0^0$ . Equation (4) for  $\xi_{\parallel}$  and  $\xi_{\perp}$  is only valid in meanfield theory. When critical fluctuations become important,  $\xi_{\parallel}$  and  $\xi_{\perp}$  diverge more rapidly, and  $\nu_{\parallel}$ and  $\nu_{\perp}$  become greater than  $\frac{1}{2}$ . Since  $\psi$  is a complex number, de Gennes<sup>4,5</sup> and McMillan<sup>2</sup> argued that the  $N-A$  transition is in the same universality class as the  $\lambda$  transition in <sup>4</sup>He. They, therefore, predicted that the N-A transition would be second order and that

$$
v_{\parallel} = v_{\perp} = \zeta_2 = \zeta_3 = \varphi = \varphi' \approx 0.66.
$$

It was later predicted, using RG analysis based on an extrapolation from four dimensions that the gauge coupling of a complex order parameter to an electromagnetic field such as occurs in a superconductor would lead to <sup>a</sup> first-order transition, ' characterized by the temperature difference  $\Delta T'$  $T_c - T^*$ . A similar prediction applies to the N-A transition due to the coupling of  $\psi$  to  $\overline{\mathbf{n}}$ . Furthermore, fluctuations lead the system toward isotropy so that if  $\Delta T'$  is sufficiently small, one would indeed expect isotropic heliumlike exponents.<sup>7</sup> Thus, the generally accepted theoretical predictions based on the de Gennes free energy

[Eq. (1)] were that the  $N-A$  transition would be a nearly-second-order transition. with isotropic helium exponents.  $\Delta T'$  was estimated to be of order 10 mK (Ref. 7) or larger.

The experimental situation at the moment is somewhat ambiguous. Essentially all experiment show a  $\Delta T'$  of order 3 mK or less. X-ray measurements<sup>20</sup> seem to indicate that the correlation length exponents are isotropic. There is evident crossover for these exponents from heliumlike  $\alpha$  obsover for these exponents from heriamitike<br>values up to t of order  $10^{-3}$  to mean-field value for  $10^{-3} \le t \le 10^{-4}$ .

Published values for  $\xi_2$  and  $\xi_3$  would indicate anisotropic behavior. Chu and McMillan<sup>15</sup> find  $\zeta_2 = 0.47 \pm 0.07$  and Birecki and Litster<sup>17</sup> find  $\zeta_3$  $= 0.75 \pm 0.04$ . Both of these values were obtained by light-scattering experiments. The analysis of the raw experimental data to obtain  $\zeta$  is quite complicated, and it is possible that greater weight was given to data points far from  $t_c$  than to points close to  $t_c$ . Since x-ray experiments show  $\nu$  decreasing with t, it is possible that  $\zeta_3$  is overestimated. On the other hand, measurements of  $K_3$ using techniques other than light scattering<sup>18</sup> give approximately the same value of  $\xi_3$ . Below  $T_c$ , Birecki *et al.*<sup>16</sup> find  $\varphi = 0.333 \pm 0.05$  and  $\varphi' = 0.50$  $\pm 0.02$ . As we shall see in Sec. III, these should be equal, respectively, to  $\xi_2$  and  $\xi_3$  if anisotropic scaling is to hold. They are clearly too small to satisfy scaling. Thus, some experiments indicate the possibility of anisotropic quasicritical behavior and others do not. In Sec. III we will reinvestigate the de Gennes model to see if critical anisotropy is theoretically predicted.

#### III. ANISOTROPIC SCALING

If the  $N-A$  transition is second order, we expect scaling to hold in the vicinity of the critical point. We also wish to consider the possibility of lengths parallel and perpendicular to  $\overline{n}_0$  scaling differently. Furthermore, the elastic constant  $K<sub>1</sub>$  remains constant through the transition<sup>17, 24, 25</sup> and must, therefore, appear explicitly in any scaling relations. Thus,  $D_{ij}$  and G should obey homogeneity relations<sup>26</sup> of the form

$$
G(\vec{q}, t, K_1) = b^{2-\eta} G(b^{1+\mu_{\eta}}q_{\eta}, bq_1, b^{1/\nu_1}t, b^{-\eta}K_1),
$$
 (8a)

$$
D_{ij}(\vec{\mathbf{q}}, t, K_1) = b^{2-\eta} D_{ij} (b^{1+\mu_{ij}} q_{ij}, b q_{ij}, b^{1/\nu_{\perp}} t, b^{-\eta} K_1), \quad \text{(8b)}
$$

where  $q_{\parallel}$  and  $q_{\perp}$  are the components of the wave number  $\bar{q}$  parallel and perpendicular to  $\bar{n}_0$ . Parallel and perpendicular correlation lengths emerge naturally from Eq. (8),

$$
\xi_{\perp} \sim |t|^{-\nu_{\perp}}, \quad \xi_{\parallel} \sim |t|^{-\nu_{\parallel}},
$$
  
\n
$$
\nu_{\parallel} = (1 + \mu_{\parallel}) \nu_{\perp}. \tag{9}
$$

(10)

We can also see from the above and Eq. (3c) that  $\tau$  must satisfy

$$
\tau = \eta_n
$$

in order to keep  $K<sub>1</sub>$  constant through the transition.

Because of the gauge (rotational) invariance of this system, not all of the exponents appearing in Eq. (8) are independent. The vertex function  $\Gamma_i(k, \cdot)$  $\overline{q}$ ) defined via

$$
\langle \psi(\overline{\mathbf{k}}) \psi(-\overline{\mathbf{k}} - \overline{\dot{\mathbf{q}}}) \delta n_i(\overline{\mathbf{q}}) \rangle = G(\overline{\mathbf{k}}) D_{ij}(\overline{\dot{\mathbf{q}}}) \, \Gamma_j(\overline{\mathbf{k}},\overline{\dot{\mathbf{q}}}) G\left(-\overline{\dot{\mathbf{k}}} - \overline{\dot{\mathbf{q}}}\right) ,
$$

satisfies  $\lim_{q\to 0} \Gamma_j(\vec{k},\vec{q})$  =  $2q_0C_1k_j$  because of gauge invariance. This means that the rescaling properties of  $q_0$  can be obtained from those of  $\psi$ ,  $\delta \vec{n}$ ,  $k_{\parallel}$ , and  $k_1$  by simple power counting, and  $q_0$  $a-b^{(\epsilon - \bar{\eta}_n - \mu_{\parallel})/2} q_0$  under the rescaling transformation described in Eq. (8), where  $\epsilon = 4 - d$ . We now choose  $\eta_n$  so that  $q_0$  remains constant under rescaling. Thus we have

$$
\eta_n = \epsilon - \mu_n. \tag{11}
$$

There is a certain arbitrariness to this choice of  $\eta_{\bullet}$ . Other choices which keep other potentials constant are possible. Properties of physically observable quantities remain constant for different choices of  $\eta_r$ . Combining Eqs. (8)-(10) and (3), we obtain

$$
\delta K_3 \sim \xi_{\parallel} \xi_{\perp}^{\epsilon-1}, \quad \delta K_2 \sim \xi_{\parallel}^{-1} \xi_{\perp}^{\epsilon+1},
$$
  
\n
$$
D \sim \xi_{\parallel}^{-1} \xi_{\perp}^{\epsilon-1}, \quad B \sim \xi_{\parallel} \xi_{\perp}^{\epsilon-3},
$$
  
\n
$$
C_{\parallel} \sim \xi_{\perp}^{-2+\eta_{\perp}} \xi_{\parallel}^2, \quad C_{\perp} \sim \xi_{\perp}^{\eta_{\perp}}.
$$
 (12)

Scaling relations among exponents implied by Eq. (8) are summarized in Table L A particularly relevant prediction of this type of anisotropic scaling is that

$$
C_1/C_{\rm u}\sim \delta K_2/\delta K_3\sim t^{2\mu_{\rm H}\nu_{\rm L}}.\tag{13}
$$

IV. RENORMALIZATION-GROUP RECURSION RELATIONS

We now use Eqs. (8) as a basis for developing renormalization-group recursion relations using

TABLE I. Anisotropic scaling relations.

General dimensions	Three dimensions
$\gamma = \nu (2 - n)$	$\gamma = \nu_1(2 - n_1)$
$\alpha = 2 - (d + \mu_0) \nu_1$	$\alpha = 2 - (d + \mu_0)v_1$
$\mu_{\rm u} = (\nu_{\rm u} - \nu_{\rm u})/\nu_{\rm u}$	$\mu_0 = (\nu_0 - \nu_1)/\nu_1$
$\eta_n = \epsilon - \mu_n$	$\eta_n = 1 - \mu_0$
$\xi_3 = \nu_0 + (\epsilon - 1)\nu_1$	$\zeta_3 = \nu_{\rm H}$
$\xi_2 = (\epsilon + 1)\nu_1 - \nu_{\rm H}$	$\zeta_2 = 2\nu_1 - \nu_{\rm H}$
$\varphi = (3 - \epsilon)\nu_1 - \nu_2$	$\varphi = 2\nu_1 - \nu_2$
$\varphi' = \nu_{\rm u} + (1 - \epsilon)\nu_{\rm u}$	$\varphi' = \nu_{\rm u}$

the  $\epsilon$  expansion.<sup>27, 28</sup> We begin with an anisotropi volume-preserving rescaling of Eq. (1) so that volume-preserving rescaling of Eq. (1) so that<br> $C_0^0$ ,  $C_1^0$  +  $C_0^0$ , and  $q_0$  remains unchanged. This leads to a new Brillouin zone which is in general nonspherical and different for  $\psi$  and  $\overline{n}$ . For the purposes of this discussion, however, we will assume both Brillouin zones are spherical with radius A. We now rescale lengths so that the Brillouin zone is of radius unity and  $\psi$  so that the coefficient of  $(\nabla \psi)^2$  in  $F/T$  is unity. Furthermore, we consider the more general system where the field  $\psi$  has  $\frac{1}{2}n$ complex components. We then have

$$
H = \frac{F}{T} = \int d^d x \left( r_0 |\psi|^2 + |(\nabla - i q_0 \delta \vec{\mathbf{n}}) \psi|^2
$$
  
+  $\frac{1}{2} u_0 |\psi|^4 + \frac{1}{2} \overline{K}_1^0 (\nabla \cdot \vec{\mathbf{n}})^2$   
+  $\frac{1}{2} \overline{K}_2^0 \sum_{i > j} ' (\nabla_i n_j - \nabla_j n_i)^2$   
+  $\frac{1}{2} \overline{K}_3^0 \sum_j ' (\nabla_i n_j)^2 \right),$  (14)

where  $\overline{n}_0$  is in the 1 direction, the summations  $\Sigma'$ are over 2 to  $d$ ,

$$
\gamma_0 = (C^0)^{-1} \Lambda^{-2} A_0 ,
$$
  
\n
$$
u_0 = (C^0)^{-2} T \Lambda^{d-4} U^0 ,
$$
  
\n
$$
\overline{K}_1^0 = T^{-1} \Lambda^{4-d} (C_1^0 / C_1^0)^{2/d} K_1^0 ,
$$
  
\n
$$
\overline{K}_2^0 = T^{-1} \Lambda^{4-d} (C_1^0 / C_1^0)^{2/d} K_2^0 ,
$$
  
\n
$$
\overline{K}_3^0 = T^{-1} \Lambda^{4-d} (C_1^0 / C_1^0)^{-[(d-2)/d]} K_3^0 ,
$$

and

$$
C^0 = (C^0_0)^{1/d} (C^0_1)^{1-1/d}.
$$

 $\mathcal{L} = (\mathcal{C}_0)^{-1}$  (0,1)<br>Experimentally,  $^{20,21}$   $C_1^0 \ll C_0^0$  so that  $\overline{K}_1^0$  and  $\overline{K}_2^0$  are expected to be larger than  $\overline{K}_3^0$ . We will discuss this further below.

Recursion relations for the potentials in Eq. (14) that are valid for all values of  $\overline{K}^0$  cannot be derived without further discussions. Equation (14) is expressed in terms of what we will call the liquid-crystal gauge with  $\delta \vec{n} \perp \vec{n}_0$ . This gauge presents certain problems in three dimensions.  $D_{\perp}(\bar{q})$ diverges when  $q_{\text{u}} = 0$  and  $K_1 = 0$ . Furthermore, in three dimensions, this gauge leads to fluctuation three dimensions, this gauge leads to fluctuation<br>destruction of long-range order.<sup>29</sup> Equation (14) can be reexpressed in terms of what we call the superconducting gauge in which  $\nabla \cdot \vec{A} = 0$ , where  $\overrightarrow{A} = \delta \overrightarrow{n} - \nabla L$  and  $\Psi = e^{-i a_0 L} \psi$ ,

$$
H = \int d^d x \left( r_0 |\Psi|^2 + |(\nabla - iq_0 \overline{\mathbf{A}}) \Psi|^2 + \frac{1}{2} U_0 |\Psi|^4 \right) + \frac{1}{2} \sum_{\mathbf{\vec{q}}} \left\{ \left[ \overline{K}_3^0 q^2 + \overline{K}_1^0 \left( \frac{q_1}{q_1} \right)^2 q^2 \right] |A_1(\overline{\mathbf{q}})|^2 \right. \\ \left. + (\overline{K}_3^0 q_1^2 + \overline{K}_2^0 q_1^2) |A_t(\overline{\mathbf{q}})|^2 \right\} , \qquad (15)
$$

where  $A_{\perp}(\vec{q})$  is the component of  $\vec{A}$  in the  $\vec{q}$ -n<sub>0</sub> plane and  $\vec{A}_t(\vec{q})$  is the  $(d-2)$ -dimensional component of  $\overline{A}$  perpendicular to the  $\overline{q}$ -n<sub>0</sub> plane. The difference between the two gauges is depicted in Fig. 1. In the superconducting gauge, there are no divergences when  $\overline{K}_{1}^{0}$  + 0, and  $\Psi$  has long-range order in three dimensions. This is the gauge that was used in Ref. 7 to calculate the first-order jump for the  $N-A$  transition. Clearly, calculations of fluctuation enhancements of potentials should be done in the superconducting gauge. On the other hand, anisotropy is most naturally described in the liquidcrystal gauge. Keeping this in mind, we develop recursion relations as follows: (i) gauge transform from the liquid crystal to the superconducting gauge; (ii) integrate out degrees of freedom with wave number  $\overline{q}$  between the ellipse  $q_1^2 + b^{2\mu} q_{\parallel}^2 = b^{-2}$ and the unit sphere  $|\dot{q}| = 1$ . To obtain equation correct to order  $\epsilon$ , the ellipse may be replaced by the sphere  $|\vec{q}| = b^{-1}$  in all integrals because  $\mu_{\parallel}$ will be of order  $\epsilon$ . This process creates anisotropy in the coefficients of  $\nabla_{\bm{i}} \psi \nabla_{\bm{j}} \psi,$  i.e., it creates  $C_{\parallel} \neq C_1 \neq 1$ ; (iii) gauge transform from the superconducting to the liquid-crystal gauge; rescale lengths anisotropically  $(q_1 \rightarrow bq_1, q_1 \rightarrow b^{1+\mu} q_n)$  to regain the unit sphere Brillouin zone, rescale  $\psi$ and  $\delta \vec{n}$ ,

$$
\psi(\overline{\mathfrak{q}}/b) \to b^{(d+2+\mu_{\parallel}-\eta_{\perp})/2}\psi(\overline{q}),
$$

$$
\delta \overline{\mathfrak{n}}(\overline{q}/b) - b^{(d+2+\mu_{\parallel}-\eta_n)/2} \delta \overline{\mathfrak{n}}(\overline{q}),
$$

and choose  $\eta_{\perp}$  and  $\mu_{\parallel}$  so that  $C_{\parallel} = C_{\perp} = 1$  and  $\eta_n$  so that  $q_0$  remains unchanged under the transformation.

If we let  $b = e^t$  and remove an infinitesimal shell at each iteration, the above prescription yields the differential recursion relations



FIG. 1. Equilibrium director  $\bar{n}_0$  is along the 1 axis. Variations  $\delta\tilde{n}$  in  $\tilde{n}$  must occur in the plane perpendicular to  $\vec{n}_0$ .  $\vec{A}$  on the other hand must be purely transverse, i.e., perpendicular to the wave number  $\bar{\mathfrak{q}}$ .  $\bar{\mathfrak{A}}_{\perp}$  lies in the  $\bar{n}_0$ - $\bar{q}$  plane where as  $\bar{A}_t = \delta \bar{n}_t$  lies in the remaining  $d - 2$  dimensions.

$$
\frac{d\gamma}{dl} = (2 - \eta_{1})r + \frac{1}{2}(n+2)C_{d}\frac{u}{1+r} + C_{d}q_{0}^{2}
$$
\n
$$
\times \left[ \left( \frac{1}{\sqrt{K_{1}} + \sqrt{K_{3}}} \right)^{2} + \frac{4}{\sqrt{K_{2}}} \frac{1}{\sqrt{K_{2}} + \sqrt{K_{3}}} \right],
$$
\n
$$
\frac{du}{dl} = (\epsilon - \mu_{\text{H}} - 2\eta_{1})u - \frac{1}{2}(n+8)C_{d}\frac{u^{2}}{(1+r)^{2}}
$$
\n
$$
- 2C_{d}^{2}q_{0}^{4} \left( \frac{1}{\sqrt{K_{3}}(\sqrt{K_{1}} + \sqrt{K_{3}})^{3}} + \frac{2}{\sqrt{K_{3}}K_{2}^{3/2}} \right),
$$
\n
$$
\frac{dK_{1}}{dl} = -(\epsilon - \mu_{\text{H}})K_{1}, \qquad (16)
$$
\n
$$
\frac{dK_{2}}{dl} = -(\epsilon - \mu_{\text{H}})K_{2} + \frac{1}{6}nC_{d}q_{0}^{2},
$$
\n
$$
\frac{dK_{3}}{dl} = -(\epsilon + \mu_{\text{H}})K_{3} + \frac{1}{6}nC_{d}q_{0}^{2},
$$
\n
$$
\eta_{\perp}(l) = -4C_{d}q_{0}^{2} \left[ \frac{1}{12} \left( \frac{3\sqrt{K_{1}} + \sqrt{K_{3}}}{(\sqrt{K_{3}} + \sqrt{K_{1}})^{3}} \right) + \frac{4}{3} \frac{1}{\sqrt{K_{2}}(\sqrt{K_{2}} + \sqrt{K_{3}})} \right] \frac{1}{1+r(l)},
$$
\n
$$
\mu_{\text{H}}(l) = -2C_{d}q_{0}^{2} \left( \frac{2}{3} \frac{\sqrt{K_{3}}}{(\sqrt{K_{1}} + \sqrt{K_{3}})^{3}} - \frac{4}{3} \frac{1}{\sqrt{K_{2}}(\sqrt{K_{2}} + \sqrt{K_{3}})} \right),
$$

 $\eta_n = \epsilon - \mu_n(l)$ ,

where  $C_d^{-1} = 2^{d-1} \pi^{d/2} \Gamma(\frac{1}{2}d)$ . In this equation, we have dropped the bars over  $K_1$ ,  $K_2$ , and  $K_3$  for compactness, arid we have dropped "naught" subscripts and superscripts to indicate we are talking about renormalized quantities.

The equations for  $K_1$ ,  $K_2$ , and  $K_3$  decouple from those for  $r$  and  $u$  as does the equation for the cha'rge in a superconductor. We, therefore, investigate the fixed-point structure in this subspace. Let  $f_i = C_d q_o^2 / K_i$ ,  $i = 1, 2, 3$ , then we have

$$
\frac{df_1}{dl} = (\epsilon - \mu_{\rm H})f_1, \n\frac{df_2}{dl} = (\epsilon - \mu_{\rm H})f_2 - \frac{1}{6}nf_2^2, \n\frac{df_3}{dl} = (\epsilon + \mu_{\rm H})f_3 - \frac{1}{6}nf_3^2.
$$
\n(17)

These equations have the trivial fixed point with  $f_1^* = f_2^* = f_3^* = 0$ . In this case  $\psi$  is completely decoupled from the gauge field  $\delta \vec{n}$ , and the system reduces to the usual classical  $n$ -component gaugeless model. Below four dimensions the  $n$ -component Heisenberg fixed point is stable<sup>27</sup> with correlation-length exponent  $\nu_H(n)$ . The stability exponent<sup>30</sup>  $\lambda_{f_i} \equiv \nu_H^{-1} \varphi_{f_i}$  for turning on any of the  $f_i$ 's is  $\epsilon$ . The crossover exponent is thus  $\epsilon v_H(n)$ .

The other fixed points of these equations are most easily found by observing that the equation for  $f_1$  has a possibility of three fixed points:  $f_1$ = 0,  $f_1 = \infty$ , and  $\epsilon = \mu_{\parallel}$ . We will now consider each of these cases separately.

$$
I. \, f_1 = \infty \text{ or } K_1 = 0
$$

In this case,

 $\mu_{\text{II}} = -\frac{4}{3}f_3(1-R)(1+2R)/(1+R)$ where

 $R = (f_2/f_3)^{1/2} \equiv (K_3/K_2)^{1/2}.$ 

Thus, at the fixed point

$$
\left[\frac{1}{6}n(1+R)^2+\frac{8}{3}(1+2R)\right](1-R)=0.
$$
 (18)

 $R = 1$  is the only solution with R real and positive. Two other solutions with negative  $R$  exist, but they are of no interest to us since they are physically inaccessible. The fixed point with  $R = 1$  is that of the isotropic superconductor with

$$
f_2^* = f_3^* = 6\varepsilon/n, \quad K_1 = 0.
$$
 (19)

The stability exponents at this fixed point are

$$
\lambda_{K_1} = -\tau = -\eta_n = -\epsilon,
$$
  
\n
$$
\lambda_s = -\epsilon,
$$
  
\n
$$
\lambda_a = -\epsilon (1 + 12/n),
$$
\n(20)

where s refers to the symmetric perturbation  $(6f_2)$ +  $\delta f_3$ ) and a to the antisymmetric perturbation ( $\delta f_3$ )  $-\delta f$ <sub>2</sub>). This fixed point (if it can be reached is stable with respect to perturbations which destroy charge anisotropy as indicate'd in Ref. 7. As discussed in Ref. 1 however,  $u$  does not reach a stable fixed-point value when  $n < 365.9$  and a firstorder transition is predicted.

2.  $\epsilon = \mu_{\parallel}$ 

In this case  $f_2^* = 0$  (i.e.,  $K_2 = \infty$ ) and  $f_3^* = 12\varepsilon/n$ . These values can be inserted into the equation  $\epsilon = \mu_{\text{th}}$  to obtain an equation for  $R_1 = (f_1/f_3)^{1/2}$ . The resulting cubic equation

$$
R_1^3/(1+R_1)^3+\tfrac{1}{16}n=0
$$
 (21)

has one real root which is negative for all  $n$ . Since  $R_1$ <0 is physically inaccessible, we can ignore this fixed point.

3.  $f_1 = 0, K_1 = \infty$ 

In this case,  $\mu_{\parallel} = \frac{8}{3} f_2/(1+R)$ , where  $R = (f_2/f_3)^{1/2}$ , and the equations determining the fixed-point value for R and  $f_2$  resulting from Eqs. (16) and (17) are

 $R^3 + (1+32/n)R^2 - R - 1 = 0$ , (22a)

$$
f_2 = 6\epsilon [n + 16/(1+R)]^{-1}.
$$
 (22b)

Equation (22a) has three real roots for  $0 \le n \le \infty$ one of which is positive and two of which are negative. The negative roots are physically inaccessible and may be ignored. In terms of these variables, we have

$$
\mu_{\rm II} = \frac{8}{3} f_2 / (1 + R) \,, \tag{23a}
$$

$$
\eta_{\perp} = -\frac{16}{3} f_2 / (1+R), \qquad (23b)
$$
\n
$$
C_d u^* = \frac{\epsilon}{n+8} \left\{ \left( 1 + 8 \frac{f_2}{1+R} \right) + \left[ \left( 1 + 8 \frac{f_2}{1+R} \right)^2 - 8 f_2^2 R^{-1} (n+8) \right]^{1/2} \right\}, \qquad (23c)
$$

$$
1/\nu_{\perp} = 2 - \eta - \frac{1}{2}(n+2)C_d u^* \,. \tag{23d}
$$

 $\nu_{\shortparallel}$ ,  $\xi_{2}$ ,  $\xi_{3}$ ,..., etc., are obtained from the scaling relations in Table L As can be seen from Eq. (23),  $u^*$  may not be real. This occurs for  $n < 238.17$ , and as for the superconductor, the recursion relations drive  $u$  negative and lead to a first-order transition. For  $n > 238.17$ , a true fixed point unstable only with respect to  $K_1^{-1}$  and temperature, can be reached with critical exponents given by Eq.  $(23)$ . Even though the transition is first order for all  $n < 238.17$ , it is still instructive to note the fixed-point values of  $R$ ,  $f_2$ , and the exponents that do not depend on  $u^*$  for  $n=2$ ,

$$
R^* = 0.271308, \quad \mu_{\rm II} = 0.862877\epsilon,
$$
  
\n
$$
f_2^* = 0.411369\epsilon, \quad \eta_{\rm I} = -1.72576\epsilon,
$$
  
\n
$$
\tau = \eta_n = 0.137123\epsilon = \lambda_{f_1},
$$
  
\n
$$
\lambda_1 = -\epsilon,
$$
  
\n
$$
\lambda_2 = -1.678732\epsilon,
$$
\n(24)

where  $\lambda$ , and  $\lambda$ , are stability exponents for linear combinations of  $f_2$  and  $f_3$ . If this fixed point in the  $f<sub>2</sub> - f<sub>3</sub>$  plane is approached, the elastic-constant exponents become

$$
\xi_2 = (\epsilon - \mu_{\parallel})\nu_1 = 0.137123\epsilon\nu_1, \n\xi_3 = (\epsilon + \mu_{\parallel})\nu_1 = 1.862877\epsilon\nu_1,
$$
\n(25)

where  $\nu_{\perp}$  can be viewed as an effective exponent in a nearly-second-order transition. Note that this leads to a ratio  $\zeta_3/\zeta_2 = 13.59$  which is quite large.

It is perhaps worth reviewing in words the re- . sults of this section. Fixed points can be classified according to the number of potentials with respect to which they are unstable. Thus, fixed points for usual second-order transitions are unstable with respect to a single variable, the temperature (if anisotropies are not permitted) fixed points for tricxitical points are unstable with respect to temperature and a nonordering field, and

 $(23h)$ 

once-unstable fixed point for  $n > n_{c1} = 365.9$ . This is the isotropic superconducting fixed point discussed in Ref. 6. In addition, there are various twice unstable fixed points. Of particular interest is the fixed point at  $K_1 = \infty$  which is unstable with respect to temperature and  $K_1^{-1}$  only. It is characterized by extremely anisotropic critical behavior (i.e.,  $\nu_{\parallel} \neq \nu_{\perp}$ ). Thus, if the initial Hamiltonian is in the vicinity of this fixed point with  $K_1^{-1}$  small but not zero, there will be a crossover from mean-field to anisotropic-critical and finally to isotropic-critical behavior. Depending on initial conditions, effects of other fixed points such as the isotropic Heisenberg (chargeless) fixed point may also be felt. Even for  $n > 365.9$ , there is a domain of initial potentials that leads to a, first order rather than a second order transition. For  $238.17 \le n \le 365.9$ , there is no once unstable fixed point. 'The fixed point at  $K_1 = \infty$  and  $K_2$ ,  $K_3$ ,  $u \neq 0$  still exists, however. Thus, initial Hamiltonians starting in the vicinity of this fixed point would show crossover from mean field to anisotropic critical to isotropic critical to a first-order transition. The firstorder transition may come before the isotropiccritical behavior is seen. There is a true continuous transition only for  $K_1 = \infty$  (or for  $q_0 = 0$ ). When  $n < 238.17$ , there are no once-unstable fixed points; there are only the Gaussian and isotropic chargeless Heisenberg fixed points. Thus, the transition will be first order unless  $q_0$  is identically zero. Nevertheless, quasicritical behavior may be observed and the sequences of crossovers discussed above can also be expected to occur. 'This may make analysis of experiments somewhat difficult and even lead to apparent discrepancies between different experiments. Because the transition is never under the influence of a single fixed point, effective exponents may be nonuniversal, i.e., they may depend on starting potentials. 'This sort of behavior has been calculated for the first sort of behavior has been calculated for the first<br>order transition in superconductors.<sup>31</sup> The curve of  $\gamma_{\text{eff}}$  versus temperature, for example, depends on the initial values of  $u_0$  and  $q_0$ , and the maximum value of  $\gamma_{\text{eff}}$  is not determined by the isotropic chargeless Heisenberg fixed point as might have been expected. Similar and more complicated behavior for the nematic and smectic-A transition is to be expected. A program to calculate crossover functions from Eq. (15) is currently under way and should be relevant to the analysis of experimental data.

so on. In the de Gennes model, there is a single

#### V. DISCUSSION

In this section we will indicate what experimental behavior might be expected as a result of the

theory presented here. Since, as discussed in Sec. I, the experimental situation is not completely understood, we will not make any attempt at completeness.

We begin with some experimental information. The value of  $C_{\parallel}^0/C_{\perp}^0$  as obtained by x-ray measurements is of order 20 (somewhat smaller in McMillan's measurements<sup>21</sup> and somewhat larger McMillian's measurements " and somewhat larger<br>in those of Als–Nielsen<sup>20</sup> *et al.*).  $K_1^0$ ,  $K_2^0$ , and  $K_3^0$ <br>are equal, respectively,<sup>24,15,17</sup> to  $11.6 \times 10^{-7}$ , 5.5  $\times 10^{-7}$ , and  $5.7\times 10^{-7}$  dyn. Thus  $\overline{K}_{1}^{0}/\overline{K}_{3}^{0} = (C_{1/2}^{0})$  $(C_{\perp}^{0})K_{\perp}^{0}/K_{3}^{0}$  is of order 40,  $\overline{K}_{2}^{0}/\overline{K}_{3}^{0} = (C_{\parallel}^{0}/C_{\perp}^{0})K_{2}^{0}/K_{3}^{0}$ is of order 20, and  $\overline{K}_1^0/\overline{K}_2^0 = K_1^0/K_2^0$  is of order 2.  $\overline{K}_1^0$  is by far the largest elastic constant, and one might expect anisotropic quasicritical behavior until the renormalized value of  $\overline{K}_1^0$  is of order the renormalized values of  $\overline{K}_2^0$  and  $\overline{K}_3^0$ , at which point more isotropic behavior characteristic of the chargeless Heisenberg fixed point should set in until the transition (first order) occurs.  $\overline{K}_1^0$  becomes of order  $\overline{K}_3^0$  within a few mK of 5 mK above  $T_c$ . Thus, one might expect anisotropic-critical behavior to be almost as close to the transition as can be reached experimentally. This is not in disaccord with the behavior of  $K_2$  and  $K_3$  as obtained from light scattering<sup>15,17</sup> but is in *disaccord* with<br>the most recent x-ray measurements.<sup>20</sup> the most recent x-ray measurements.<sup>20</sup>

The analysis presented here does not change the theoretical prediction that the de Gennes model should have a first-order nematic to smectic-A theoretical prediction that the de Gennes model<br>should have a first-order nematic to smectic-A<br>transition,<sup>6,7</sup> though it probably reduces somewha the estimate of  $\Delta T'$  in the extreme type-II case. In Ref. 7,  $\Delta T'$  was calculated for type-I systems. This calculation is reproduced in the Appendix with result

$$
\Delta T' = \frac{4}{9} \mathcal{E}_c T_c \kappa^{-6}, \qquad (26)
$$

where

$$
S_c = \frac{1}{32\pi^2} \frac{(U^0)^2}{A^0} \frac{(k_B T_c)^2}{(C_{\perp}^0)^2 C_{\parallel}^0}
$$

is the Ginzburg<sup>32</sup> reduced temperature and

$$
\kappa^{-6} = \frac{2 q_0^6 C_{\parallel}^0 (C_1^0)^5}{(U^0)^3 (K_3^0)^3} \times \left( z_2 \frac{K_3^9}{K_2^0} + \frac{K_3^0 C_{\parallel}^0}{C_{\parallel}^0 K_1^0 + C_1^0 K_3^0 + 2(C_1^0 C_{\parallel}^0 K_3^0 K_1^0)^{1/2}} \right)^2, \tag{27}
$$

where  $z_2$  is unity (for type-I systems). For type-II systems, this result changes to

$$
\Delta T' = \frac{4}{9} z_1 \mathcal{E}_c T_c \kappa^{-2/\varphi} H \sim \frac{4}{9} z_1 \mathcal{E}_c T_c \kappa^{-3} , \qquad (28)
$$

where  $\varphi_H$  is the crossover exponent  $\epsilon \nu_H$  (~ $\frac{2}{3}$  for  $\epsilon$  = 1) for turning on the charge at the isotropic *n*  $=$  2 chargeless fixed point.  $z_1$  was estimated to be of order unity in Ref. 7. A recent calculation,<sup>31</sup> of order unity in Ref. 7. A recent calculation,  $31$ 

however, shows  $z_1$  to be equal to 0.3 to first order in  $\epsilon$ and very possibly much smaller to higher order in  $\epsilon$  since  $n_{c1}$  = 365.9 appears to decrease<sup>33</sup> with  $\epsilon$ . No calculation of  $z_2$  exists as yet though it appears likely that it is less than one. Note that  $K_3^0/K_2^0$ likely that it is less than one. Note that  $K_3^9/K_2^9$ <br>~1, whereas the second term in the large paren theses of Eq. (27) is of order  $\frac{1}{2}$  for large  $C_{\parallel}^0/C_{\perp}^0$ Thus  $\kappa^{-3}$  for small  $z_2$  is of order one third its value for  $z_2$  equal to one. Therefore, the estimated value of  $\Delta T'$  as calculated from Eq. (28) might be a factor of 10 or more smaller than the value calculated with  $z_1 = z_2 = 1$ . There is thus some possibility of reducing the estimate of  $\Delta T' \sim 10$  mK given in Ref. 7. A correct estimate of  $\Delta T'$  is not the whole story, however. In order for theory and experiment to agree they must produce among other things the same latent heat and size of critical region. It appears very difficult to choose a value of  $U^0$ , the only unknown in Eq. (28) other than  $z_1$  and  $z_2$  to agree with  $\Delta T' \leq 3$  mK, a critical region of order several degrees (in order that the smaller type-II prediction for  $\Delta T'$  can be used) and latent heat values obtained by scanning calorimetry<sup>34</sup> or by volume change<sup>35</sup> and pressure-temperature<sup>36</sup> data via the Gibbs-Duhem relation. Since new experimental data is constantly being obtained, we will not attempt at this point to reconcile present experiments with present theory on these issues.

It is worth noting at this point that the interpretation of x-ray experiments is not completely straightforward. X rays measure the densitydensity correlation function, i.e., they measure the Fourier transform of the order-parameter correlation function  $\langle \psi(\vec{x}) \psi^*(\vec{x'}) \rangle$  in the liquid-crystal gauge. The correlation lengths  $\xi_1$  and  $\xi_0$  appear naturally in superconducting gauge. For large separation

$$
\langle \Psi(\vec{x}) \Psi^*(\vec{x}') \rangle \sim \begin{cases} e^{-|X_{\parallel}|/|\xi_{\parallel}} & \text{if } x_{\perp} = 0, \\ e^{-|\vec{x}_{\perp}|/|\xi_{\perp}|} & \text{if } x_{\parallel} = 0, \end{cases}
$$
 (29)

where position-dependent prefactors have been omitted. The correlation function in the liquidcrystal gauge is easily related to that in the.superconducting gauge

$$
\langle \psi(\overline{\mathbf{x}})\psi^*(\overline{\mathbf{0}}') \rangle = \langle \Psi(\overline{\mathbf{x}})\Psi^{\dagger}(\overline{\mathbf{0}}') e^{i a_0 [L(\overline{\mathbf{x}}) - L(\overline{\mathbf{0}}')] } \rangle
$$
  
 
$$
\approx \langle \Psi(\overline{\mathbf{x}})\Psi^{\dagger}(\overline{\mathbf{0}}) \rangle e^{-a_0^2 \langle (L(\overline{\mathbf{x}}) - L(\overline{\mathbf{0}}))^2 \rangle/2}. \quad (30)
$$

. The second expression is only approximate. It does, however, suffice to show what problems may exist in interpreting  $\langle \psi(x) \psi^*(0) \rangle$ . From Eqs. (Al) and (A2) in the Appendix, we see that

$$
\langle (L(\bar{x}) - L(\bar{0}))^2 \rangle = k_B T \int \frac{d^3q}{(2\pi)^3} \frac{q_{\parallel}^2 (1 - e^{i\bar{q}_{\perp} \bar{x}})}{K_3 q^2 q_{\parallel}^2 + K_1 q^2 q_{\perp}^2}
$$
\n(31)

in three dimensions. This quantity is proportional to  $\vec{x}$  at large  $\vec{x}$  with angular-dependent coefficients. (For  $d>3$ , it grows more slowly than  $|\mathbf{\bar{x}}|$ at large separation.) Thus correlation lengths obtained from  $\langle \psi(x) \psi^*(0) \rangle$  contain contributions from  $\xi_{\parallel}$  and  $\xi_{\perp}$ , and from phase fluctuations, and it is not obvious that x rays measure  $\xi_{\parallel}$  and  $\xi_{\perp}$  directly This problem is current under investigation and will be discussed at some future time.

Obviously, further theoretical and experimental work is required before a full understanding of the nematic to smectic-A. transition is reached. On the theoretical side, a number of questions still within the context of the de Gennes model need to be investigated. We list some of these questions. (i) Is the experimentally observed transition much closer to the Lifshitz point<sup>37</sup> separating smectic- $A$ and smectic- $C$  phases than usually assumed? This might explain the difficulty in observing eyidence of a first-order transition. On the other hand, if this were the case, one might expect greater anisotropy than is observed. (ii) Is the system close to a tricritical point  $(u = 0)$ ? This would lead to a prediction of a smaller  $\Delta T'$  but also to a prediction of essentially mean-field exponents. (iii) Does the possible existence of different cutoffs for the order parameter and director fields play an important role in determining properties near the transition? We feel that all of these questions must be investigated before the de Gennes model is rejected as being unable to explain experiments.

## ACKNOWLEDGMENTS

We are grateful to B. I. Halperin for innumerable discussions and constant encouragement. We are also grateful to J. Als-Nielsen, R. J. Birgeneau, and J. D. Litster for communicating experimental results prior to publication and for many helpful discussions. One of us (T.C.L.) is also grateful to the Alfred P. Sloan Foundation for financial support.

#### APPENDIX

In this Appendix, we will present'various calculational details. We first present the liquidcrystal to superconducting gauge transformation. Figure 1 shows the directions of  $\overline{n}_0$ , along the 1 axis,  $\vec{q}$ ,  $\delta \vec{n}_1$  (in the  $\vec{n}_0 - \vec{q}$  plane),  $\vec{A}_1$  and  $\vec{A}_t = \delta \vec{n}_t$ . A is defined via

$$
\vec{A} = \delta \vec{n} - \nabla L \,, \tag{A1}
$$

and the constraint  $\vec{\nabla} \cdot \vec{A} = 0$ . Therefore, we have  $L(q) = -i(q_1/q^2) \delta n_1(\vec{q})$  ( $\delta n_1 \equiv \delta \vec{n}_1$ ) and  $q \equiv |\vec{q}|$ ),  $\vec{A}_1$  $A_1(-q_1/q, q_0/q, 0)$  where 0 is the  $(d-2)$ dimensional null vector with

$$
A_{\perp}(\vec{q}) = (q_{\parallel}/q)\delta n_{\perp}(\vec{q}), \qquad (A2)
$$

and finally we have

$$
\langle |A_{\perp}(\vec{q})|^2 \rangle = \left(\frac{q_{\parallel}}{q}\right)^2 \langle |\delta n_{\perp}(\vec{q})|^2 \rangle
$$

$$
= \frac{k_B T}{K_3 q^2 + K_1 (q_{\perp}/q_{\parallel})^2 q^2} \tag{A3}
$$

This result is used in Eq. (15).

The renormalization-group operation  $R$  described in Sec. IV can be written  $R = R_s G^{-1} R_s G$ , where G represents the gauge transformation from the liquid-crystal to the superconducting gauge,  $R_b$  the removal of degrees of freedom, and  $R_s$  the rescaling of length and fields. The operation  $R_b$  involves calculations of diagrams that result from a perturbation expansion in  $q_0$  and u. The propagators are

$$
D_{ij}(\overline{q}) = e_{1i}e_{1j} \frac{1}{K_3q^2 + K_1(q_1/q_1)^2q^2} + e_{ii}e_{ij} \frac{1}{K_3q_1^2 + K_2q_1^2},
$$
\n
$$
G(q) = 1/(r+q^2),
$$
\n(A4)

where  $\delta_{ij} = \hat{q}_i \hat{q}_j + e_{1i}e_{1j} + e_{ii}e_{ij}$ , with

 $\widehat{q}$  =  $\overline{\mathbf{q}}/q$  = (cosy, siny cos $\beta$ , siny sin $\beta$  cos $\alpha$ , siny sin $\beta$  sin $\alpha$ 

and

l

## $\vec{e}_1$  = (-sin $\gamma$ , cos $\gamma$  cos $\beta$ , cos $\gamma$  sin $\beta$  cos $\alpha$ , cos $\gamma$  sin $\beta$  sin $\alpha$ )

in four dimensions where  $\gamma$  and  $\beta$  run from zero to  $\pi$ , and  $\alpha$  from zero to  $2\pi$ . All diagrams can be expressed in terms of the general integral

$$
L_{mn\rho}(K_3, K_1) = \int \frac{\cos^{2m}\gamma \sin^{2n}\gamma \cos^{2\rho}\beta}{K_3 \cos^2\gamma + K_1 \sin^2\gamma} \frac{d\Omega_4}{(2\pi)^4}, \qquad (A5)
$$

where  $d\Omega_4$  is the solid angle in four dimensions.  $L_{mn\rho}$  can be evaluated using

$$
\int_0^{\pi} \frac{\cos 2n\gamma}{K_3 \cos^2 \gamma + K_1 \sin^2 \gamma} d\gamma = (-1)^n \frac{\pi}{(K_3 K_1)^{1/2}} \left(\frac{\sqrt{K_3} - \sqrt{K_1}}{\sqrt{K_3} + \sqrt{K_1}}\right)^n
$$
(A6)

and trigonometric identities relating  $\cos^n \gamma$  to  $\cos \gamma$ . We take the momentum of any external legs to be k  $=(k_{\parallel}, k_{\perp}0, 0)$ . The integrals  $I_j$  corresponding to diagram j of Fig. 2 in four dimensions are

$$
I_{1} = 4k^{2} \Biggl( \int_{b^{-1}}^{1} \frac{(\hat{k} \cdot \tilde{e}_{\perp})^{2}}{K_{3}q^{2} + K_{1}(q_{\perp}/q_{\parallel})^{2}q^{2}} - \frac{1}{q^{2} + r} \frac{d^{4}q}{(2\pi)^{4}} + \int_{b^{-1}}^{1} \frac{(\hat{k} \cdot \tilde{e}_{t})^{2}}{K_{3}q_{\parallel}^{2} + K_{2}q_{\perp}^{2}} \frac{1}{q^{2} + r} \frac{d^{4}q}{(2\pi)^{4}} \Biggr) \n= \left\{ k_{\parallel}^{2} L_{110}(K_{3}, K_{1}) + k_{\perp}^{2} [L_{200}(K_{3}, K_{1}) + L_{000}(K_{3}, K_{2}) - L_{001}(K_{3}, K_{2})] \right\} A(r) ,\n\begin{aligned}\nI_{2} &= \int_{b^{-1}}^{1} \left( \frac{1}{K_{3}q^{2} + K_{1}(q_{\perp}/q_{\parallel})^{2}q^{2}} + 2 \frac{1}{K_{3}q_{\parallel}^{2} + K_{2}q_{\perp}^{2}} \right) \frac{d^{4}q}{(2\pi)^{4}} = \left[ L_{100}(K_{3}, K_{1}) + 2L_{000}(K_{3}, K_{2}) \right] \frac{1}{2} (1 - b^{-2}) ,\n\end{aligned}
$$
\n
$$
\begin{aligned}\nI_{3} &= \int_{b^{-1}}^{1} \left[ \left( \frac{1}{K_{3}q^{2} + K_{1}(q_{\perp}/q_{\parallel})^{2}q^{2}} \right)^{2} + 2 \left( \frac{1}{K_{3}q_{\parallel}^{2} + K_{2}q_{\perp}^{2}} \right)^{2} \right] \frac{d^{4}q}{(2\pi)^{4}} = - \left( \frac{d}{dK_{3}} L_{000}(K_{3}, K_{1}) + 2 \frac{d}{dK_{1}} L_{0, -1, 0}(K_{3}, K_{2}) \right) \ln b ,\n\end{aligned}
$$
\n
$$
I_{4i}(\vec{k}) = 4 \int_{b^{-1}}^{1} D_{ij}(\vec{q}) (2k + q)_{j} G(k + q)
$$
\n
$$
= 8 \{
$$

where

$$
L_{110}(K_3, K_1) = 3 L_{201}(K_1, K_3) = \frac{1}{4} C_d (3\sqrt{K}_3 + \sqrt{K}_1) / (\sqrt{K}_1 + \sqrt{K}_3)^2,
$$
  
\n
$$
L_{000}(K_3 K_2) = 3 L_{001}(K_3 K_2) = 2 C_d [\sqrt{K}_2 (\sqrt{K}_2 + \sqrt{K}_3)]^{-1},
$$
  
\n
$$
L_{100}(K_3, K_1) = C_d \left(\frac{1}{\sqrt{K}_3 + \sqrt{K}_1}\right)^2, \quad L_{0, -1, 0} = 2 C_d \frac{1}{(K_3 K_2)^{1/2}}, \quad A(r) = \int_{b^{-1}}^{1} \frac{q^3 dq}{q^2 + r}.
$$
 (A8)

Note that  $I_{4i} = (\partial/\partial k_i)I_i$  as required by gauge invariance. Because of this,  $\eta_{\perp}$ , which appears in the rescaling factors for  $q_0$  is canceled by the contribution of  $I_{4i}$  to the recursion relations for  $q_0$ .

The momentum independent parts of diagrams  $5a$  and  $5b$  cancel as required by gauge invariance. If we set  $r = 0$ , which is consistent with the first order in  $\epsilon$  calculations presented here, we obtain

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FIG. 2. Diagrams contributing to renormalization of potentials to first order in  $\epsilon.$  Wiggly line represents  $D_{ij}$  ( $\bar{q}$ ) and solid line,  $G(\bar{q})$ . The three-point vertex is  $(2k+q)_{i}.$ 

$$
I_{5ij}(k) = (\delta_{ij} - \hat{k}_i \hat{k}_j) k^2 \frac{1}{6} n C_d.
$$
 (A9)

Equations (A7) and (A9), the well-known results for diagrams 5a and 5b, and the renormalization procedure outlines in Sec. IV yield the recursion relation Eq. (16).

Finally, we outline how Eqs. (30) and (31) are obtained. %e begin with the rescaled Hamiltonian  $3C[\Psi,\vec{A}] = \tilde{F}/T$  in Eq. (15), where  $\tilde{F}[\Psi,\vec{A}]$  is the rescaled free energy. An effective Hamiltonian which is a functional of  $\Psi$  alone can be obtained by integrating over  $\overline{A}$ ,

$$
e^{-3\mathcal{C}_{\text{eff}}\left[\Psi\right]} = \int d\left\{\vec{A}\right\} e^{-3\mathcal{C}\left[\Psi,\vec{A}\right]}.
$$
 (A10)

Following Ref. 6, we ignore spatial variations in  $\Psi$  and obtain

$$
\frac{1}{2\Omega} \frac{d \mathcal{K}_{\text{eff}}}{d|\Psi|} = r_0 |\Psi| + u_0 |\Psi|^{3}
$$
  
+  $q_0^2 |\Psi| (\langle A_{\perp}^2 \rangle + \langle A_{\ell}^2 \rangle),$  (A11)

where  $\Omega$  is the volume and

$$
\langle A_{\perp}^{2} \rangle = \int \frac{1}{K_{3}^{0} q^{2} + \overline{K}_{1}^{0} (q_{\perp}/q_{\parallel})^{2} q^{2} + 2q_{0}^{2} |\Psi|^{2}} \frac{d^{3} q}{(2\pi)^{3}},
$$
  

$$
\langle A_{t}^{2} \rangle = \int \frac{1}{\overline{K}_{3}^{0} q_{\parallel}^{2} + \overline{K}_{2}^{0} q_{\perp}^{2} + 2q_{0}^{2} |\Psi|^{2}} \frac{d^{3} q}{(2\pi)^{3}}.
$$
 (A12)

If we assume  $|\Psi|$  is small enough that we can expand the above in  $\Psi$ , we obtain

$$
\langle A_{\perp}^{2}(\Psi) \rangle = \langle A_{\perp}^{2}(0) \rangle - \frac{\sqrt{2}}{4\pi} q_{0} |\Psi| \left( \frac{1}{K_{3}^{0}} \right)^{3/2}
$$

$$
\times \left[ 1 + \left( \frac{\overline{K}_{3}^{0}}{\overline{K}_{3}^{0}} \right) \right]^{-2},
$$

$$
\langle A_{t}^{2}(\Psi) \rangle = \langle A_{t}^{2}(0) \rangle - \frac{\sqrt{2}}{4\pi} q_{0} |\Psi| \frac{1}{\overline{K_{3}^{0}} \sqrt{\overline{K_{3}^{0}}}}.
$$
(A13)

Thus,  $\mathcal{K}_{\text{eff}}$  becomes

$$
\mathcal{K} \, \mathrm{eff} \, \big/ \Omega = r_0 |\Psi|^2 - w |\Psi|^3 + \tfrac{1}{2} u_0 |\Psi|^4 \,, \tag{A14}
$$

where

$$
w = \frac{2}{3} q_0^3 \frac{\sqrt{2}}{4\pi} \left\{ \left( \frac{1}{\bar{K}_3^o} \right)^{3/2} \left[ 1 + \left( \frac{\bar{K}_1^o}{\bar{K}_3^o} \right)^{1/2} \right]^{-2} + \frac{1}{\bar{K}_2^o \sqrt{\bar{K}_3^o}} \right\}.
$$

The critical value of  $r_0$  at which the first-order transition occurs is given by

$$
r_{\rm oc} = w^2 / u_{\rm o} \,. \tag{A15}
$$

Substitution of the above expression for  $w$  and performing the transformation prescribed after Eq. (14) yields Eqs. (30) and (31).

- \*Supported in part by NSF Grant No. DMB 76-21703 and ONR Grant No. N0014-C-0106.
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