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SOME CONSEQUENCES OF THE GINSBURG-LANDAU-DE GENNES GRADIENT TERM IN SMECTICS

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ABSTRACT. We work out some consequences of the Ginsburg-Landau-de Gennes gradient term on the properties of smectic liquid crystals. (i) Disclinations in smectic C are very much like vortex filaments in superfluids or magnetic fluxoids in superconductors. (ii) A uniform distortion of the phase factor lowers the C-A (or A-N) transition point, and at any given temperature there should occur a second order transition beyond a critical distortion. (iii) Light scattering due to phase fluctuations in smectic C should be strongly temperature dependent. (iv) In smectic A of finite size the phase change under an imposted $\nabla \times \vec{n}$ distortion can be of second order.

THE A-C TRANSITION

It is well established that the smectic C to smectic A transition is of second order. 1 Near the transition point $^{\rm C}$ the free energy density of the smectic C phase is given by 2 :

$$F = \alpha \omega^{2} + \frac{\beta}{2} \omega^{4} + \frac{1}{2} K_{11} \left(\frac{\partial n_{x}}{\partial x} + \frac{\partial n_{y}}{\partial y} \right)^{2} + \frac{1}{2} K_{22} \left(\frac{\partial n_{x}}{\partial y} - \frac{\partial n_{y}}{\partial x} \right)^{2} + \frac{1}{2} K_{33} \left(\frac{\partial n_{x}}{\partial z} + \frac{\partial n_{y}}{\partial z} \right)^{2}$$
(1)

Here $\alpha = \alpha_0$ (T - T_c) (in the mean field), $\beta = a$ small positive

quantity, $n_x = \omega \cos \phi$, $n_y = \omega \sin \phi$, $n_z = 1$, $\omega = angle$ between the director and layer normal, $\phi = azimuthal$ angle of the director, and $K_{ii} = elastic$ constants involved in in-plane distortions.

For simplicity we shall assume $K_{11} = K_{22} = K_{33} = K$, and that ω and ϕ are independent of z. Energy minimization results in the following differential equations:

$$\frac{K}{2} \left\{ \nabla^2 \omega - \omega (\nabla \phi)^2 \right\} - \alpha \omega - \beta \omega^3 = 0 \tag{2}$$

$$\omega^2 \left\{ \nabla^2 \phi \right\} + 2\omega \nabla \omega \cdot \nabla \phi = 0 \tag{3}$$

We shall work out a few implications of this model.

<u>Disclination structure</u>. Eqn.(3) admits solutions of the type

$$\phi = \pm N\theta$$
 N = integer, $\theta = \tan^{-1} \frac{y}{x}$.

These describe singularities in the in-plane director distortions. They are exactly like the integral defects found in the nematic schlieren texture. 3,4 However, in view of eqn.(2) we find that the tilt angle ω is affected by these distortions and (for N = ±1) it is described by

$$\frac{1}{\xi} \frac{\partial}{\partial \xi} \left(\xi \frac{\partial f}{\partial \xi} \right) - \frac{f}{\xi^2} + f(1 - f^2) = 0 \tag{4}$$

Here $f = \omega/\omega_0$, $\xi = r/\xi_0$, $r = (x^2 + y^2)^{\frac{1}{2}}$, ω_0 = tilt angle at $r \to \infty$, ξ_0 = coherence length = $(-K/2\alpha)^{\frac{1}{2}}$.

The above equation is exactly like the Ginsburg-Pitaevskii 5 equation for the structure of a superfluid quantum vortex or a magnetic fluxoid in a type II superconductor. 6 As we approach the centre of the singularity ω

continuously decreases to zero. Most of the decay takes place in about a coherence length. This probably explains the experimental observations of Lagerwall 3 who found near the centre of the singularity a region over which ω is significantly zero.

<u>Critical distortion</u>. We now consider an uniform inplane distortion $\nabla \phi = q$, say. Then the free energy density (if gradient terms in ω are negligible) is given by:

$$F = (\alpha + \frac{K}{2} q^2) \omega^2 + \frac{\beta}{2} \omega^4$$
 (5)

From (5) we can show that ω at any q (given by minimizing F) is

$$\omega = \{-(\alpha + \frac{K}{2} q^2)/\beta\}^{\frac{1}{2}}$$
 (6)

As q increases, ω continuously decreases. Also since α is negative (T < T_c), we find the tilt angle ω to be unfavourable beyond a critical distortion wave vector

$$q_c = (-2\alpha/K)^{\frac{1}{2}} \tag{7}$$

At this wave vector the system undergoes a second order phase transition to the smectic A phase (ω = 0).

This phenomenon is the analogue of the critical current effect found in superconductors. Equivalently it may be interpreted to mean that distortions $\nabla \phi = q$ lowers the AC transition point. This effect is quite different from the influence of a $\nabla \times \vec{n}$ distortion on the AN transition. Firstly the imposed distortion is not tolerated by an otherwise good smectic A and the distortion induced transitions is first order. Secondly the critical wave vector of a $\nabla \times \vec{n}$ distortion varies as α and not as α found in the

distortion induced AC transition (eqn.6). The only restriction for this effect is that the sample thickness should be much smaller than the coherence length.

<u>Light scattering.</u> At any temperature we have thermal fluctuations in the azimuthal angle ϕ . Equipartition theorem yields

$$\langle \phi_{\mathbf{q}}^2 \rangle = \frac{k_{\mathbf{B}}^{\mathrm{T}}}{(K_{\omega}^2)_{\mathbf{q}}^2} \tag{8}$$

These fluctuations scatter light strongly (as in nematics) resulting in turbidity. The scattering cross-section is given by

$$\sigma \sim \varepsilon_a^2 < \phi_q^2 >$$

Here ε_a is the dielectric anisotropy for light travelling along the layer normal. To a good approximation $\varepsilon_a = \varepsilon_a^0 \omega^2$. Hence

$$\sigma \sim \omega^2$$
 (9)

As ω is strongly temperature dependent, we find the scattered intensity to be strongly dependent on temperature. In this sense it behaves very differently from a nematic, wherein one finds a nearly temperature independent scattering.

THE A-N TRANSITION

Near the A-N transition which can again be of second order, the free energy density is given by $^{7}\,$

$$F = \alpha \psi^{2} + \frac{\beta}{2} \psi^{4} + \frac{B}{2} \left(\frac{\partial \mathbf{u}}{\partial z}\right)^{2} + \frac{D}{2} \left(\nabla_{\underline{\mathbf{u}}} \mathbf{u} + \delta \vec{\mathbf{n}}_{\underline{\mathbf{l}}}\right)^{2} + \frac{K}{2} \left(\nabla \times \vec{\mathbf{n}}\right)^{2} + \frac{1}{2} K_{11} \left(\nabla \cdot \vec{\mathbf{n}}\right)^{2}$$

$$(10)$$

Here α , β and K_{11} have the same meanings as in (1). Both B and D are proportional to ψ^2 and are involved in the distortions of the phase factor u. The distortions $(\partial u/\partial z)$ are $\nabla \cdot \vec{n}$ are the easiest to impose on the system. Distortions represented by the D term refer to tilting of the layers relative to the molecules. In many respects we find similarities with smectic C.

Phase changes only. Since the phase distortion factor $(\partial u/\partial z)$ is coupled to the order parameter ψ , it will influence the magnitude of ψ . This factor is particularly large near the core of a smectic A edge dislocation and hence as in smectic C we can expect a continuous decrease in ψ as we go to the centre of the defect. Also for samples smaller than the coherence length, beyond a critical uniform $(\partial u/\partial z)_{C}$ the smectic A phase should undergo a phase transformation to the N phase without any latent heat. It must be remarked that such a distortion in smectic A usually results in an undulation mode. 9 But near the AN transition it is unlikely since the critical $(\partial u/\partial z)$ for this instability (which is inversely proportion to B) becomes larger and larger as we go near the AN transition point.

Director distortions only: finite size effect. In the case of type I smectic A the penetration depth λ is smaller than the coherence length ξ_0 . In such situations, if we have a sample of thickness $\delta < \lambda$, then we find that the imposed $\nabla \times \vec{n}$ distortion completely penetrates the sample, yet the order parameter ψ is non-zero. We shall work out the critical $\nabla \times \vec{n}$ required to destroy ψ . If there are no layer deformations (10) reduces to

$$F = \alpha \psi^{2} + \frac{\beta}{2} \psi^{4} + \frac{q_{o}^{2} \psi^{2}}{2M_{\bullet}} (\delta \vec{n}_{\perp})^{2} + \frac{K}{2} (\nabla \times \vec{n})^{2}$$
 (11)

Here $\underline{M}_{\underline{I}} = (q_{\underline{O}}\psi)^2/D$ and $\delta \overrightarrow{n}_{\underline{I}}$ is the vector deviation of the local director away from the layer normal. In the present problem both ψ and $\delta \overrightarrow{n}_{\underline{I}}$ are varying from point to point and in an elementary discussion they can be replaced by their averages $\overline{\psi}$ and $\delta \overrightarrow{n}_{\underline{I}}$. Then as in the preceding discussion we must have a critical $(\delta \overrightarrow{n}_{\underline{I}})_{\underline{C}}$ at which the system undergoes a second order phase transition to the N phase. This critical value is given by

$$\frac{\rightarrow}{\delta n_c} = (-2\alpha M_1/q_0^2)^{\frac{1}{2}}$$

or

$$(\nabla \times \overrightarrow{n})_{C} \simeq \frac{\lambda}{\delta} (\nabla \times \overrightarrow{n})_{C}^{O} > (\nabla \times \overrightarrow{n})_{C}^{O}, \quad \lambda^{2} = K/D.$$
 (12)

Here $(\nabla \times \overrightarrow{\mathbf{n}})_{\mathbf{c}}^{\mathbf{O}}$ is the critical value for a first order transition in an infinite sample. Thus the finite size has a profound influence on not only the critical value of $(\nabla \times \overrightarrow{\mathbf{n}})$, which will be very large, but also on the order of the phase transition. It must be remarked that very similar effects were established long back by Ginsburg and Landau for superconductors.

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