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A new mean field $S_A - S_{A'}$ critical point in a symmetry breaking field

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We consider a $S_A - S_{A'}$ critical point in the presence of a symmetry-breaking external magnetic (electric) field with a positive magnetic (dielectric) anisotropy or a dislocation layer. Via a renormalization group analysis of the model hamiltonian, we show that the upper critical dimensions below which mean-field theory breaks down is $d_c = 2.5$. Thus the $S_A - S_{A'}$ transition in three dimensions becomes mean-field like in the presence of a symmetry-breaking field. We estimate the reduced temperature region where we can expect to see the mean field $S_A - S_{A'}$ critical point in the presence of a magnetic field or a dislocation layer.

The smectic (S_A) liquid crystal phase is a one-dimensional solid with a density modulation in the direction parallel to the equilibrium director \mathbf{n}_0 (z-axis). Recently, extensive theoretical [1] and experimental [2] studies of so-called 'frustrated smectic liquid crystal phases', which are composted of strongly polar molecules, have revealed a large number of S_A phases. In particular, there are the linear S_{A_1} , S_{A_d} , and S_{A_2} phases where the indices 1, d, and 2 indicate that the wavelength of the periodic modulation is one, d(1 < d < 2), or two times the molecular length l. The associated wavenumber of the modulation is, respectively, $q_0 = 2\pi/l$, $2\pi/dl$ and $2\pi/2l$, in the three cases.

Phase transitions between these S_A phases are of some interest and need further comment. There can be a first order transition in which there is a discontinuous change in q_0 from q_0^+ to q_0^- (e.g. an $S_{A_1}-S_{A_d}$ or $S_{A_d}-S_{A_2}$ transition) as well as second order transitions in which the amplitude ψ_{k_1} of the mass density at wavenumber $k_1 = 2\pi/2l$ grows continuously from zero. In the former case, as in the liquid-gas transition, the identical macroscopic symmetry of S_A phases allows the first order transition line to terminate in a critical point, as shown in the figure, where the difference $q_0 = q_0^+ - q_0^-$ in the wavenumber goes to zero. Such a critical point provides a continuous path between coexisting S_{A_1} (or S_{A_2}) and S_{A_d} phases.

This $S_A - S_{A'}$ critical point, C was predicted theoretically by Barois *et al.* [3] and observed in a series of experiments by Shashidhar *et al.* [4] in the binary phase diagram of (110PCBOB/90BCB). Previous experiments [5] providing evidence for its possible existence were not conclusive [5]. Alternatively, the first order $S_A - S_{A'}$ transition line can terminate on a closed re-entrant nematic domain [6]. Prost and Toner [7] predicted



Phase diagram showing the $S_A - S_{A'}$ critical point C. The two smectic phases (denoted by A and A' in the figure) coexist along a line in the concentration (or pressure)-temperature plane terminating at the critical point C.

the existence of both a 'nematic island in a smectic sea' and a $S_A - S_{A'}$ critical point using a dislocation loop theory of the $S_A - N$ transition. Park *et al.* [8] developed a nonlinear elastic model to describe the $S_A - S_{A'}$ critical point and found that this critical point belonged to a new universality class with an upper critical dimension, d_c of 6 (as opposed to $d_c = 4$ for the liquid-gas critical point).

In this paper, we consider the $S_A - S_{A'}$ transition in the presence of a symmetry breaking magnetic (electric) field with positive magnetic (dielectric) anisotropy. The Landau-Ginzburg-Wilson Hamiltonian describing this transition as a function of the displacement variable $u(\mathbf{x})$ of the smectic layers can be expressed as

$$H[u(\mathbf{x})] = H_{\rm sm}[u(\mathbf{x})] + H_1. \tag{1}$$

Here, $H_{sm}[u(\mathbf{x})]$ is the nonlinear elastic energy of elastic deformations in smectic A phases which has the following form:

$$H(u) \equiv \int d^{d}x \{ hE(u) + \frac{1}{2} BE^{2}(u) + \frac{1}{3!} wE^{3}(u) + \frac{1}{4!} vE^{4}(u) + \frac{1}{2} [K_{1}(\nabla_{\perp}^{2}u)^{2} + K_{2}(\nabla_{z}^{2}u)^{2} + 2K_{12}(\nabla_{z}\nabla_{\perp}u)^{2}] \}.$$
 (2)

with

$$E[u(\mathbf{x})] = \nabla_{z} u + \frac{1}{2} (\nabla u)^{2}$$
(3)

 $H_1[u]$ is the symmetry breaking hamiltonian arising from an external magnetic **H** or electric field **E**. It is expressed as

$$H_{1} = \int d^{d} x B_{20} (\nabla_{\perp} u)^{2}$$
 (4)

where $B_{20} = \chi_a H^2(\varepsilon_a E^2)$ with $\chi_a > 0$ ($\varepsilon_a > 0$). Since the independent variable is $u(\mathbf{x})$ not $E[u(\mathbf{x})]$, it is convenient for future analysis to re-express $H[u(\mathbf{x})]$ in terms of $\nabla_z u$ and $\nabla_\perp u$

$$H = \int d^{d}x \{h(\nabla_{z}u) + \frac{1}{2}B_{1}(\nabla_{z}u)^{2} + \frac{1}{2}B_{2}(\nabla_{\perp}u)^{2} + \frac{1}{2}[K_{1}(\nabla_{\perp}^{2}u)^{2} + K_{2}(\nabla_{z}^{2}u)^{2} + 2K_{12}(\nabla_{z}\nabla_{\perp}u)^{2}] + \frac{1}{3!}w_{1}(\nabla_{z}u)^{3} + \frac{1}{2}w_{2}(\nabla_{z}u)(\nabla_{\perp}u)^{2} + \frac{1}{4!}v_{1}(\nabla_{z}u)^{4} + v_{2}\frac{1}{4!}(\nabla_{\perp}u)^{4} + \frac{1}{12}v_{12}(\nabla_{z}u)^{2}(\nabla_{\perp}u)^{2}\},$$
(5)

where

$$B_{1} = B + h, \quad w_{1} = w + 3B, \quad v_{1} = v + 6w + 3B, \\B_{2} = h + B_{20}, \quad w_{2} = B, \quad v_{2} = 3B, \\v_{12} = 3w + 3B. \end{cases}$$
(6)

This is the hamiltonian we will use in the remainder of this paper. (Note that $B_2 \neq 0$ even in the absence of the symmetry breaking external field (h = 0).)

As discussed in [8] the order parameter for the $S_A - S_{A'}$ transition is $M_z = \langle \nabla_z u \rangle$. If $\nabla_{\perp} u = 0$ in equation (5), the resulting hamiltonian in terms of $\nabla_z u$ alone is identical in form to that describing the liquid-gas transition as a function of its scalar order parameter $\phi = n_1 - n_g$, the difference in densities of the liquid and gas phases. Thus, in mean-field theory, the $S_A - S_{A'}$ transition occurs at $h = B_1 = w_1 = 0$ and is identical to the liquid gas transition.

Mean field theory is valid above an upper critical dimension d_c below which fluctuations become important. In the LGW hamiltonian describing the liquid gas transition, there is a single third order potential which can be removed by shifting the order parameter. The upper critical dimension $d_r = 4$ is, therefore, the dimension at which the fourth order potential becomes relevant. There are two third order potentials in the hamiltonian (equation (5)) describing the $S_A - S_{A'}$ transition. In the absence of an external symmetry breaking field $(B_{20} = 0)$, the mean field propagator is proportional to ∇^{-4} at the critical point (since $h = B_1 = 0$). The S_A-S_A critical point is thus described by renormalization group transformations that leave the coefficients of $(\nabla_z^2 u)^2$, $(\nabla_\perp^2 u)^2$ and $(\nabla_z^2 u)(\nabla_\perp^2 u)$ invariant. For $d > d_c$, $u(\mathbf{q})$, the Fourier transform of $u(\mathbf{x})$, then transforms as $u(\mathbf{q}) \rightarrow b^{d-4}u(b\mathbf{q})$, and the potentials w_1 and w_2 transforms as $w'_1 = b^{-(d-6)/2} w_1$ and $w'_2 = b^{-(d-6)/2} w_2$. Thus both w_1 and w_2 become relevant for d < 6. At the liquid gas transition, there is a single third order potential that can be removed by shifting the order parameter [9]. It is impossible to remove both potentials w_1 and w_2 at the $S_A - S_{A'}$ critical point via a shift of the order parameter. The upper critical dimension for the $S_A - S_{A'}$ transition in the absence of external fields is, therefore, 6 and not 4 as the analogy with the liquid gas transition would indicate. The properties of this very complex critical point were analysed in an ε -expansion about six dimensions in [8].

In the presence of external fields, B_{20} is non-zero, and the rescaling of lengths parallel and perpendicular to the smectic layers is different even for $d > d_c$. To find d_c , we will now determine the renormalization group recursion relations to zero loop order for $B_2 \neq 0$. At the critical point, $B_1 = 0$, and we rescale to keep B_{20} and K_1 constant. Under the transformations

$$q_{\parallel} \rightarrow \exp\left(-(1 + \mu_{\parallel})l\right) q_{\parallel}, \quad q_{\perp} \rightarrow \exp\left(-l\right)q_{\perp},$$
$$u(\mathbf{q}) \rightarrow \exp\left[(d + 2 + \mu_{\parallel} - \eta_{\perp})l/2\right]u(b\mathbf{q}), \tag{7}$$

we have

$$\frac{dB_2}{dl} = -\eta_{\perp}B_2,
\frac{dK_1}{dl} = (-2 - 4\mu_{\parallel} - \eta_{\perp})K_1.$$
(8)

When $d < d_c$, B_2 and K_1 should be constant under the above transformations. This requires $\mu_{\parallel} = -\frac{1}{2} + \mu'_{\parallel}$ where μ'_{\parallel} and η_{\perp} are zero for $d > d_c$ and of order $\varepsilon = d_c - d$ for $d < d_c$. With this choice for μ'_{\parallel} we find to zero loop order

$$\frac{dB_{1}}{dl} = (1 - 2\mu_{\parallel}' - \eta_{\perp})B_{1} + \cdots,$$

$$\frac{dB_{2}}{dl} = -\eta_{\perp}B_{2} + \cdots,$$

$$\frac{dK_{1}}{dl} = (-4\mu_{\parallel}' - \eta_{\perp})K_{1},$$

$$\frac{dw_{1}}{dl} = \left[\frac{1}{2}\left(\frac{7}{2} - d\right) - \frac{7}{2}\mu_{\parallel}' - \frac{3}{2}\eta_{\perp}\right]w_{1} + \cdots,$$

$$\frac{dw_{2}}{dl} = \left[-1 + \frac{1}{2}\left(\frac{7}{2} - d\right) - \frac{3}{2}\mu_{\parallel}' - \frac{3}{2}\eta_{\perp}\right]w_{2} + \cdots,$$

$$\frac{dv_{1}}{dl} = \left[(-d + \frac{5}{2}) - 5\mu_{\parallel}' - 2\eta_{\perp}\right]v_{1} + \cdots.$$
(9)

These equations are sufficient to determine the upper critical dimension. One loop corrections are needed to determine exponents to first order in $d_c - d$. All other potentials (e.g. v_{12}) are more irrelevant than those displayed. The important result of these equations is that, because of the anisotropic rescaling imposed by the external potential, the third order potentials w_1 and w_2 are no longer of equal relevancy. w_1 becomes relevant at $d = \frac{7}{2}$ whereas w_2 and v_1 become relevant at $d = \frac{5}{2}$. The relevant potential (for $d < \frac{7}{2}$) w_1 can be removed, as in the liquid-gas case, by shifting the order parameter. The upper critical dimension is thus $d_c = 2.5$ rather than six (the $B_{20} = 0$ result) or 3.5 (the dimension at which w_1 becomes relevant). This means that physical systems in three dimensions will exhibit a mean field transition when $B_{20} \neq 0$. For $d = 2.5 - \varepsilon$ the critical point will be in a new universality class with $v_1^* \sim (w_2^*)^2 \sim \varepsilon$.

We now estimate the reduced temperature t(H) at which crossover from symmetric critical to asymmetric mean-field behaviour occurs. Mean field behaviour sets in when the $\chi_a H^2 (\nabla_\perp u)^2$ contribution to the free energy exceeds the $K_1 (\nabla_\perp^2 u)^2$ contribution to the free energy, i.e. when

$$\chi_a H^2 > K_1 \xi_{\perp}^{-2}, \tag{10}$$

where ξ_{\perp} is the perpendicular coherence length. In the vicinity of H = 0, it scales as

$$\xi_{\perp} = t^{-\nu_{\perp}} f(y(H)/t^{\phi})$$
(11)

where $y(H) = \chi_z H^2/K_1 \xi_{\perp 0}^{-2}$ is a unitless measure of the strength of the external field and $\xi_{\perp 0} \approx 10$ Å is a bare correlation length. ϕ is the crossover exponent associated with B_{20} . Rotational invariance leads [8] to $\phi = \beta$ where β is the order parameter exponent. To first order in $\varepsilon = 6 - d$, $\beta < 2v_{\perp}$. Thus equation (10) and (11) determine the reduced critical-to-mean-field crossover temperature, T(H) via

$$y(H) \sim t^{2\nu_{\perp}}(H) f^2(y(H)/t^{\phi}(H)).$$
 (12)

If ϕ remains less than $2v_{\perp}$ in three dimensions, then

$$t(H) \sim \left(\frac{\chi H^2}{K_1 \xi_{\perp 0}^{-2}}\right)^{1/(2\nu_{\perp})}$$
 (13)

If $\phi > 2v_{\perp}$ then the exponent $2v_{\perp}^{-1}$ is replaced by ϕ^{-1} . If $\chi_a = 10^{-7}$, $H = 10^4$ G, $\xi_{\perp 0} \sim 10_{-7}$ cm, $K_1 \sim 10^{-6}$ dynes, and $v_{\perp} \sim \frac{1}{2}$, this implies

$$t(H) \approx 10^{-7}.$$
 (14)

The estimate $v_{\perp} \sim \frac{1}{2}$ is crude and may be wrong. In an external electric field, $\chi_a H^2$ is replaced by $\varepsilon_a E^2$. With $\varepsilon_a \sim 10 \text{ cgs}$ and $E \sim 10^2 \text{ stat volt/cm}$, this yields

$$t(E) \sim 10^{-3}$$
 (15)

or $T_{\rm c} - T(E) \sim 10^{-3} \times 400 \sim 0.4 \,{\rm K}.$

These temperatures should be compared with the Ginzburg temperature t_G for the critical point with H = 0 (E = 0). If $t(H) > t_G$, ($t(E) > t_G$) the transition will be mean field-like. If $t(H) < t_G$ ($t(E) < t_G$), there will be a crossover from mean field to critical and then back to mean field theory. At the moment, because of our incomplete understanding of the H = 0 transition, we are unable to give a believable estimate of t_G . Thus, we cannot predict with certainty what the effects of external magnetic or electric fields will have on the $S_A - S_{A'}$ transitions. Our educated guess is that there will be critical fluctuations for experimental external magnetic fields but that reasonable electric fields could produce a crossover from critical to mean field behavior or even a purely mean field transition.

Polydomain samples experience strains which we may estimate to be of the order of one lattice spacing *a* divided by the grain size *L* independent of temperature: $\langle \nabla_z u \rangle \sim a/L$. These quenched strains create a perturbation whose effect is similar to that of an external electric field. The crossover temperature to mean-field behaviour is again given by equation (13) with $\frac{1}{2}\chi_a H^2$ replaced by $\delta H_{\rm sm}/\delta(\nabla_\perp u)^2 \sim \frac{1}{2}w_2\langle \nabla_z u \rangle$ where w_2 is the unrenormalized potential of equation (5). With $L \sim 10^{-4}$ cm and $w_2 \sim B_2 \sim 10^8 \, {\rm erg \, cm^{-3}}$, we find

$$t(\langle \nabla_z u \rangle) \sim 10^{-2}$$
 or $T_c - T(\langle \nabla_z u \rangle) \sim 400 \times 10^{-2} = 4 \text{ K.}$ (16)

Thus, quenched strains present in polycrystalline samples may explain the mean-field character of the results of [4].

In conclusion, we have studied the $S_A - S_{A'}$ critical point in the presence of an external magnetic (electric) field with positive magnetic (dielectric) anisotropy. We showed that its upper critical dimensions d_c is $\frac{5}{2}$ rather than the zero-field value of 6. Thus, this critical point in physical three-dimensional systems in a field should exhibit mean-field behaviour for temperatures sufficiently close to T_c . The reduced temperature at which mean field behaviour sets in are estimated to be 10^{-7} for magnetic fields of 10^4 G, 10^{-3} for electric fields of 10^2 stat volts/cm, and 10^{-2} for residual strains of order 3×10^{-3} .

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