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Correlations at the nematic to smectic-A critical point when $v_{\parallel} = 2 v_{\perp}$

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Résumé. — On relie le paramètre d'ordre de la transition nématique-smectique-A (NA) à un paramètre d'ordre dans une jauge où les fluctuations de phase sont au minimum. Lorsque $v_{\parallel} = 2 v_{\perp}$ à trois dimensions, on montre que la fonction de corrélation, $G(x)$, du paramètre d'ordre physique décroît algébriquement en x pour x grand et $t \leq 0$ où t est la température réduite. Les exposants $\eta_{\parallel}(t=0)$ et $\eta_{\perp}(t=0)$ décrivant la décroissance de $G(x)$ ne sont pas égaux respectivement aux limites $\lim_{t \rightarrow 0} \eta_{\parallel}(t)$ et $\lim_{t \rightarrow 0} \eta_{\perp}(t)$. Ce résultat est en accord avec les conjectures récentes de Nelson et Toner.

Abstract. — We express the physical order parameter for the nematic to smectic-A (NA) transition in terms of an order parameter in another gauge where phase fluctuations are a minimum. We show that when $v_{\parallel} = 2 v_{\perp}$ in three dimensions, the physical order parameter correlation function $G(x)$ shows power law decay in x for reduced temperature $t \leq 0$. The exponents $\eta_{\parallel}(t=0)$ and $\eta_{\perp}(t=0)$ describing this decay are not equal to $\lim_{t \rightarrow 0} \eta_{\parallel}(t)$ and $\lim_{t \rightarrow 0} \eta_{\perp}(t)$ respectively. This result is in agreement with recent conjectures by Nelson and Toner.

The nematic to smectic-A (NA) transition in liquid crystals is one of the most intriguing, and still least understood, phase transitions that one can imagine. Properties associated with this transition include : 1) fluctuation destruction of long range order in the smectic phase [1], 2) apparent anisotropy in the correlation length exponents [2-4] ($v_{\parallel} \neq v_{\perp}$), and 3) important topological excitations in the smectic phase [5, 6]. Recently there have been several promising theoretical advances that may lead to an eventual understanding of the NA transition. These include : 1) demonstration that correlation functions depend strongly on gauge and that phase fluctuations are the strongest in the physical gauge [3, 7, 8], 2) strong arguments that the closely related normal metal to superconductor transition is second [9] rather than first order as previously thought [10], and 3) suggestions that the « unbinding » of dislocations leads to a second order transition with $v_{\parallel} = 2 v_{\perp}$ [5, 6]. In particular, the dislocation unbinding theory suggests a renormalization group flow diagram such as that shown in figure 1. Here y is the fugacity for dislocation loops and $\eta_c(t)$ (t = reduced temperature) is the Caillé exponent [1] describing the algebraic decay of order parameter correlations with distance, x ,

$$G(\mathbf{x}) \sim \begin{cases} |x_{\parallel}|^{-\eta_c(t)} & \mathbf{x}_{\perp} = 0 \\ |x_{\perp}|^{-2\eta_c(t)} & x_{\parallel} = 0 \end{cases} \quad (1)$$

Fig. 1. — Renormalization Group flows taken from reference [6]. $\eta_c(T)$ is the temperature dependent Caillé exponent ($q_0^2 k_B T / 8 \pi \sqrt{BK_1}$) and y is the fugacity for dislocation loops. The results presented in this paper are in agreement with this diagram, with proper interpretation of y , provided $v_{\parallel} = 2 v_{\perp}$. y should be interpreted as some generalized co-ordinate (e.g. u near $4-\varepsilon$) controlling flows in the superconducting gauge.

where $x_{\parallel}$ and $x_{\perp}$ are components of $\mathbf{x}$ parallel and perpendicular to the direction of molecular alignment. $\eta_c(t)$ varies continuously with temperature. Algebraic decay of correlation functions is usually described with an exponent defined via $G(x) \sim |x|^{-(d-2+\eta)}$ ($= |x|^{-(1+\eta)}$ for $d = 3$). We, therefore, introduce $\eta_{\parallel}(t)$ and $\eta_{\perp}(t)$ satisfying

$$\begin{aligned} \eta_{\parallel}(t) &= -1 + \eta_c(t) & t < 0 \\ \eta_{\perp}(t) &= -1 + 2 \eta_c(t) & t < 0. \end{aligned} \quad (2)$$

Figure 1 shows that the fixed point controlling the critical point itself does not coincide with the terminal point of the line of fixed points of the smectic phase (unlike the case for the Kosterlitz-Thouless transition [11] in the 2D XY model). Thus $\eta_{\parallel}(t = 0^-) \neq \eta_{\parallel}(t \equiv 0)$ and $\eta_{\perp}(t = 0^-) \neq \eta_{\perp}(t \equiv 0)$.

The purpose of this note is to show that the gauge transformations considered in references [3, 7, 8] lead to predictions in agreement with those of figure 1 provided the critical point is anisotropic with $v_{\parallel} = 2 v_{\perp}$. (Ref. [8] shows that this is not the case when $v_{\parallel} = v_{\perp}$). We begin with the de Gennes model [12] for the NA transition with Hamiltonian

$$H = \int d^3x \left[r |\Psi|^2 + C_{\parallel} |\nabla_{\parallel} \Psi|^2 + C_{\perp} |(\nabla_{\perp} - iq_0 \delta \mathbf{n}) \Psi|^2 + u |\Psi|^4 + \frac{1}{2} K_1 (\nabla \cdot \mathbf{n})^2 + \frac{1}{2} K_2 (\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + \frac{1}{2} K_3 (\mathbf{n} \times (\nabla \times \mathbf{n}))^2 \right] \quad (3)$$

where Ψ is the complex amplitude of the smectic mass density wave and $\mathbf{n} = \mathbf{n}_0 + \delta \mathbf{n}$ is the director ($\mathbf{n}_0$ is the equilibrium value of $\mathbf{n}$ taken along the 1-axis). To facilitate the discussion of gauge transformations, we rescale lengths as discussed in reference [3] via $x_{\parallel} \rightarrow \Lambda^{-1} l^{-2/3} x_{\parallel}$, $x_{\perp} \rightarrow \Lambda^{-1} l^{1/3} x_{\perp}$ where $\Lambda \sim q_0$ and $l = \xi_{\parallel}^0 / \xi_{\perp}^0 = \sqrt{C_{\parallel} / C_{\perp}}$ to obtain

$$H = \int d^3x \left[r |\Psi|^2 + \frac{1}{2} |(\nabla - iq_0 \delta \mathbf{n}) \Psi|^2 + u |\Psi|^4 + \right]$$

$$+ \frac{1}{2} K'_1 (\nabla \cdot \delta \mathbf{n})^2 + \frac{1}{2} K'_2 (\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + \frac{1}{2} K'_3 [\mathbf{n} \times (\nabla \times \mathbf{n})]^2 \Big] \quad (4)$$

where the primes indicate rescaled parameters $K'_{1,2} = \Lambda l^{4/3} K_{1,2}$ and $K'_3 = \Lambda l^{-2/3} K_3$.

We now introduce gauge transformations in the usual way

$$\begin{aligned} \psi &= \Psi e^{iq_0 L} \\ \mathbf{A} &= \delta \mathbf{n} + \nabla L; \end{aligned} \quad (5)$$

where we choose $\nabla \cdot \mathbf{A} = 0$ to minimize the phase fluctuations in the field ψ . In this case,

$$L = - \frac{1}{\nabla^2} \nabla \cdot \delta \mathbf{n}. \quad (6)$$

Correlations in the physical gauge can be expressed in terms of the transverse or SC gauge *via*

$$\begin{aligned} G(x) &= \langle \Psi(x) \Psi^*(0) \rangle = \langle \psi(x) \psi^*(0) e^{-iq_0(L(x) - L(0))} \rangle \\ &\cong G_{\text{SC}}(x) \langle e^{iq_0(L(x) - L(0))} \rangle \\ &= G_{\text{SC}}(x) e^{-R(x)} \end{aligned} \quad (7)$$

where

$$R(x) = \frac{1}{2} q_0^2 \langle (L(x) - L(0))^2 \rangle \quad (8)$$

in the « decoupling » approximation discussed in reference [8]. Using equation (6) we obtain

$$R(x) = q_0^2 \int \frac{d^3 p}{(2\pi)^3} \frac{p_{\perp}^2}{p^4} D_{\perp}(-p) (1 - e^{i\mathbf{p} \cdot \mathbf{x}}) \quad (9)$$

where

$$D_{\perp}(p) = K'_1 p_{\perp}^2 + K'_3 p_{\parallel}^2 + B' p_{\parallel}^2 / p_{\perp}^2 \quad (10)$$

is the director propagator [13]. B' is the rescaled compression modulus that is non-zero only in the smectic phase and is related to the unrescaled modulus *via* $B' = \Lambda^{-1} l^{-2/3} B$. The $p_{\parallel}^2 / p_{\perp}^2$ coefficient of B' is only valid for $p_{\parallel} \ll p_{\perp}$.

As discussed in references [3] and [8], $\langle \psi(x) \rangle$ is finite in the smectic phase and

$$R(x_{\parallel}, 0) \sim \eta_c \ln x_{\parallel} \quad \text{and} \quad R(0, |\mathbf{x}_{\perp}|) \sim 2 \eta_c \ln |\mathbf{x}_{\perp}|$$

for $t < 0$, so that equation (7) reproduces equation (1) exactly with a prefactor $\langle \psi \rangle^2$. For $t \rightarrow 0^+$,

$$R(x_{\parallel}, 0) \sim \left[\frac{q_0^2 k_B T}{8 \pi K_3} l^{-2} \ln (K_3 / K_1) \right] \cdot x_{\parallel}$$

and

$$R(0, |\mathbf{x}_{\perp}|) \sim [(q_0^2 k_B T) / (8 \pi \sqrt{K_1 K_3})] \cdot |\mathbf{x}_{\perp}|$$

leading to a difference between the correlation lengths $\xi_{\parallel}^{\mathbf{x}}$ and $\xi_{\perp}^{\mathbf{x}}$ measured by X-rays [8]. These results for $t < 0$ and $t > 0$ do not depend on the particular symmetry of the critical point ! Properties at the critical point $t = 0$ do, however, depend on this symmetry. For $v_{\parallel} = v_{\perp}$ [8],

$$R(x_{\parallel}, 0) \sim x_{\parallel}^{1/3} \quad \text{and} \quad R(0, |\mathbf{x}_{\perp}|) \sim |\mathbf{x}_{\perp}|^{1/2}$$

indicating that the susceptibility $\chi = \int G(x) d^3x$ is finite at $t = 0$. For $v_{\parallel} \neq v_{\perp}$, we need to know how $K'_3(p)$ behaves at $t = 0$. From scaling, we know

$$K'_3(p, t) = \xi_{\parallel} \Delta(p_{\parallel} \xi_{\parallel}, p_{\perp} \xi_{\perp}) \quad (11)$$

which implies

$$K'_3(p, t = 0) = \frac{1}{|p_{\parallel}|} \tilde{\Delta}(p_{\perp}/p_{\parallel}^{\rho}) \quad (12)$$

where $\rho = v_{\perp}/v_{\parallel}$ and

$$\tilde{\Delta}(z) \rightarrow \begin{cases} \tilde{\Delta}_0 & \text{as } z \rightarrow 0 \\ z^{-1/\rho} \tilde{\Delta}_{\infty} & \text{as } z \rightarrow \infty. \end{cases} \quad (13)$$

In this paper, we are particularly interested in the case $\rho = 1/2$ for which we have at $t = 0$

$$D_{\perp}(p) = K'_1 p_{\perp}^2 + \tilde{\Delta}_{\infty} p_{\parallel}^2/p_{\perp}^2 \quad p_{\parallel} < p_{\perp}. \quad (14)$$

Thus $D_{\perp}(p)$ has exactly the same dominant small p behaviour at $t = 0$ as it does for $t \rightarrow 0$, and we may identify $B'(t = 0)$ with $\tilde{\Delta}_{\infty}$. Furthermore, using equations (9), (10), (12) and (13), we find

$$R(\mathbf{x}, t = 0) = \begin{cases} \eta_c(0) \ln x_{\parallel} & \mathbf{x}_{\perp} = 0 \\ 2 \eta_c(0) \ln |\mathbf{x}_{\perp}| & x_{\parallel} = 0. \end{cases} \quad (15)$$

Thus for $v_{\parallel} = 2 v_{\perp}$, $R(\mathbf{x})$ is logarithmic in $\mathbf{x}$ at large $|\mathbf{x}|$ for all $t \leq 0$ with coefficients that depend continuously on t .

Recall, however, that $G(\mathbf{x})$ is also proportional to $G_{\text{sc}}(\mathbf{x})$ which dies off with a power law in $\mathbf{x}$ at large $|\mathbf{x}|$ at $t = 0$:

$$G_{\text{sc}}(\mathbf{x}) \sim \begin{cases} |x_{\parallel}|^{-(1+\eta_{\parallel}^{\text{sc}})} & \mathbf{x}_{\perp} = 0 \\ |\mathbf{x}_{\perp}|^{-(1+\eta_{\perp}^{\text{sc}})} & x_{\parallel} = 0. \end{cases} \quad (16)$$

Thus, using equations (7), (15) and (16), we obtain

$$\begin{aligned} \eta_{\parallel}(t = 0) &= \eta_{\parallel}^{\text{sc}} + \eta_c(0) \neq \eta_{\parallel}(t = 0^-) \\ \eta_{\perp}(t = 0) &= \eta_{\perp}^{\text{sc}} + 2 \eta_c(0) \neq \eta_{\perp}(t = 0^-) \end{aligned} \quad (17)$$

in contrast to equation (2) which is valid for $t < 0$.

We have shown that the picture of the NA transition proposed by Nelson and Toner [6] can be obtained, provided $v_{\parallel} = 2 v_{\perp}$, by considering phase fluctuations about a gauge transformed order parameter in which phase fluctuations are a minimum. There remains, however, the question of whether $v_{\parallel} = 2 v_{\perp}$. There are many scenarios one might imagine. The transition could be second order and in the same universality class as the « inverted XY » superconducting transition suggested by Dasgupta and Halperin [9]. In this case $v_{\parallel} = v_{\perp}$, and the picture presented in reference [8] could be correct. One would also expect K_1 to be an irrelevant variable in the vicinity of the critical point as is the case at the second order superconducting transitions in $4 - \varepsilon$ dimensions for number of components, n , of a generalized order parameter greater than 365.9 [10]. Other possibilities are that K_1 is a relevant variable at the « inverted XY » transition leading to the Nelson-Toner [6] transition with $v_{\parallel} = 2 v_{\perp}$, or there may be a critical value of K_1 separating isotropic from anisotropic behaviour (in the ε -expansion anisotropy occurs only at $K_1 = \infty$ [2]). Finally,

the transition may be weakly first order or some other altogether unexpected behaviour may result. These questions are currently under investigation.

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References

- [1] CAILLÉ, A., *C.R. Hebd. Séan. Acad. Sci.* **B 274** (1972) 891.
ALS-NIELSEN, J., LITSTER, J. D., BIRGENEAU, R. J., KAPLAN, M., SAFINYA, C. R., LINDEGAARD-ANDERSEN, A. and MATHEISEN, S., *Phys. Rev. B* **22** (1980) 312.
- [2] CHEN, J. H. and LUBENSKY, T. C., *Phys. Rev. B* **17** (1978) 366.
- [3] DUNN, S. G. and LUBENSKY, T. C., *J. Physique* **42** (1981) 1201.
- [4] DAVIDOV, D., SAFINYA, C. R., KAPLAN, M., DANA, S. S., SCHAEZING, R., BIRGENEAU, R. J. and LITSTER, J. D., *Phys. Rev. B* **19** (1979) 1657;
LITSTER, J. D., ALS-NIELSEN, J., BIRGENEAU, R. J., DANA, S. S., DAVIDOV, D., GARCIA-GOLDING, F., KAPLAN, M., SAFINYA, C. R. and SCHAEZING, R., *J. Physique Colloq.* **40** (1979) C3-339.
- [5] HELFRICH, W., *J. Physique* **39** (1978) 1199.
- [6] NELSON, D. R. and TONER, J., *Phys. Rev. B* **24** (1981) 363.
- [7] HALPERIN, B. I. and LUBENSKY, T. C., *Solid State Commun.* **14** (1973) 997.
- [8] LUBENSKY, T. C., DUNN, S. G. and ISAACSON, J., *Phys. Rev. Lett.*, to be published.
- [9] DASGUPTA, C. and HALPERIN, B. I., *Phys. Rev. Lett.* **47** (1981) 1556.
- [10] HALPERIN, B. I., LUBENSKY, T. C. and SHANG-KENG MA, *Phys. Rev. Lett.* **32** (1974) 292.
- [11] KOSTERLITZ, J. M. and THOULESS, D. J., *J. Phys. C* **6** (1973) 1181;
KOSTERLITZ, J. M. and THOULESS, D. J., *Prog. Low Temp. Phys.* **7B** (1978) 371. For reviews, see NELSON, D. R., in *Proceedings of the Enschede Summer School on Fundamental Problems in Statistical Mechanics*, 1979, edited by E. G. D. Cohen (North Holland, to be published) and HALPERIN, B. I., in *Proceedings of the Kyoto Summer School*, edited by Y. Nagaoka and S. Hikami (Publication Office, Progress in Theoretical Physics, Kyoto, 1979).
- [12] DE GENNES, P. G., *Solid State Commun.* **10** (1972) 753; *Mol. Cryst. Liq. Cryst.* **21** (1973) 49.
- [13] BROCHARD, F., *J. Physique* **34** (1973) 411.