Influence of magnetic field on the correlation of the displacements in smectic liquid crystals

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The influence of a magnetic field on the correlation function of the displacements in smectic liquid crystals is investigated. It is shown that the interaction of the fluctuations leads to logarithmic corrections to the correlators. These corrections are summed in the so-called parquet approximation. An analogy with the problem of the phase transition in a uniaxial ferroelectric is noted.

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1. Smectic liquid crystal are attracting much attention not only because of the possible and already existing applications of this type of liquid crystal, but also because of the very interesting and unique physics of this state. Thus, e.g., the transition from a smectic A to a nematic liquid crystal has many features that are typical of a superconductor–normal metal transition, but is much richer than the latter in the sense of the existence of stationary points of various types of renormalization-group equations.

It is known that according to a theorem of Landau and Peierls[1] long-range correlation order along one direction in a three-dimensional body is impossible. However, fluctuations of the displacements increase only logarithmically, meaning a power-law decrease of the correlations. The situation in this respect seems analogous to that in two-dimensional systems. The explicit form of the law governing the decrease of the correlations in the smectic phase is quite complicated. For the simplest particular cases it was first established by Caille[2]:

$$\exp[-g(z,r)]\sim\begin{cases}|z|^{-\eta(T)},\\ r^{-2\eta(T)},\end{cases} \tag{1}$$

where $g(z,r)$ is the correlation function of the displacements u of the smectic layers in the z direction (z is normal to the layer):

$$g(z,\ r)=\langle u(z,\ r)u(0,\ 0)\rangle, \tag{2}$$

$\eta(T)$ is an exponent that describes the falloff of the correlations. This index has a continuous (just as in two-dimensional models) temperature dependence.

There is, however, a very significant difference from two-dimensional models. The point is that the free energy of a smectic A liquid crystal (or the corresponding Hamiltonian) is of the form[3]

$$H_0=\int\left[\frac{1}{2}B\left(\frac{\partial u}{\partial z}\right)^2+\frac{1}{2}K_1\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)^2\right]d^3r, \tag{3}$$

where B is the elastic modulus connected with the compressibility of the layers, and K_1 is the Frank transverse-flexure modulus of the field of the director $\mathbf{n}$.

In terms of Fourier components we have

$$H_0=\frac{1}{2}\int d^3q[Bq_z^2+K_1q_\perp^4]|u(q)|^2. \tag{4}$$

The Hamiltonian H_0 describes the so-called Lifshitz critical point.[4] It can be stated that the entire region of existence of the smectic A phase is the Lifshitz point corresponding to $m=2$ and $n=1$ (m is the number of components of the soft mode, i.e., m shows for how many components $(\nabla_i u)^2$ the coefficient vanishes, and n is the number of components of the order parameter). At the true Lifshitz point, the Gaussian correlations at which

$$g(q_z,q_\perp)\sim\begin{cases}q_z^{-2}, & q_\perp=0,\\ q_\perp^{-4}, & q_z=0,\end{cases}$$

are unstable. An interaction proportional to u^4 leads in three-dimensional state to a change of the exponents of the correlation function, i.e., to another stable stationary point.

In contrast to the true Lifshitz point, in a smectic liquid crystal there exists no displacement-fluctuation interaction that does not vanish as $\mathbf{q}\to 0$. In this case, the most "dangerous" interaction is

$$H_1=\frac{\gamma_0}{4!}\int d^3r(\nabla_\perp u)^4. \tag{5}$$

As first noted by Grinstein and Pelcovits,[5] this interaction does not change the critical exponents, but leads to logarithmic corrections. In contrast to Ref. 5, we reduce the problem to four-dimensional and introduce a magnetic field in the Hamiltonian H_0 (4). Thus, the problem reduces to a four-dimensional problem of a phase transition with respect to the magnetic field, so that we can determine the logarithmic increments immediately and in very simple fashion. In addition, we shall discuss in a similar manner the problem of a discotic liquid crystal,[6] in which the liquid columns form a two-dimensional lattice. The simplified harmonic part of the Hamiltonian has in this case the form

$$H_0^{(d)}=\frac{1}{2}\int d^3q[Cq_\perp^2+K_3q_z^4]|\mathbf{u}(\mathbf{q})|^2, \tag{6}$$

where $\mathbf{u}$ is the two-dimensional vector of the displacement of the lattice of liquid columns. Thus, the entire region of existence of the discotic phase is the Lifshitz point $m=1, n=2$.

The most dangerous interaction is

$$H_1^{(d)}=\frac{\gamma_1}{4!}\int d^3r\left(\frac{\partial\mathbf{u}}{\partial z}\right)^4. \tag{7}$$

It is easily seen that, generally speaking, this interaction is inessential, i.e., it does not change the exponents and does not lead to logarithmic corrections. Logarithmic corrections

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FIG. 1

can be connected in this case with the interaction $(\partial u/\partial z)^3$, which is forbidden by the symmetry of the problem. However, near the transition into the nematic phase, when the elastic modulus of the two-dimensional lattice C is small, we are already near a second Lifshitz point namely $m = 3$, $n = 2$. In the vicinity of this point the interaction (7) becomes significant and leads to a change of the exponents.

2. We proceed now directly to calculate the correlations in smectic-A liquid crystals. As already noted, the interaction (5) leads in the case of the harmonic Hamiltonian (3) to logarithmic corrections. For example, the simplest diagram for the self-energy part of the Green's function $g(q_z,\mathbf{q}_\perp)$ (Fig. 1) yields

$$\Sigma(\mathbf{q}) \approx -\gamma_0^2 q_\perp^4 \ln a. \tag{8}$$

Similarly, the vertex function $\Gamma(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3,\mathbf{p}_4)$, which describes the renormalization of the interaction (Fig. 2), is equal to

$$\Gamma \approx -q_\perp^4 \gamma_0 [1-9\gamma_0 \ln a], \tag{9}$$

where a is a dimensionless cutoff parameter for the logarithmically diverging integrals.

It is obvious that logarithmic integrations accumulate also in all the three arrangements of the momentum pairs that enter in the vertex function $\Gamma(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3,\mathbf{p}_4)$. The problem of summing all the diagrams of this type at $\gamma_0 \ln a \sim 1$ is well known (the so-called parquet approximation). In principle, all the calculations can be carried out directly in the language of the Green's functions $g(q_z,\mathbf{q}_\perp)$ and of the vertices $\Gamma(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3,\mathbf{p}_4)$. However, as already mentioned above, it is more convenient to reformulate the problem first by introducing, a magnetic field, and second by taking into account some small terms in the harmonic Hamiltonian H_0(3). These terms, which are proportional to

$$\frac{\partial^2 u}{\partial z^2}\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right),$$

are usually disregarded, since they are significant only for layer displacements that depend on z and are therefore small compared with the "rigid-body" terms $(\partial u/\partial z)^2$. However, these small additions are inevitably generated, e.g., when the Hamiltonian is renormalized, and in addition, are needed to restore the symmetry of the system.

Thus, the complete Hamiltonian of the smectic A phase is

$$H = \frac{1}{2}\int d^3q \{Bq_z^2 + K' q_z^2 q_\perp^2 + \chi_a h^2 q_\perp^2 + K q_\perp^4\} |u(\mathbf{q})|^2 + \frac{\gamma_0}{4!}\int d^3q_1\, d^3q_2\, d^3q_3\, d^3q_4\, \delta(\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3+\mathbf{q}_4) \times q_{1\perp}^{\alpha} q_{2\perp}^{\alpha} q_{3\perp}^{\beta} q_{4\perp}^{\beta} u(\mathbf{q}_1) u(\mathbf{q}_2) u(\mathbf{q}_3) u(\mathbf{q}_4), \tag{10}$$

where χ_a is the anisotropic part of the magnetic susceptibility.

FIG. 2

It is convenient to introduce in place of the scalar field $u(\mathbf{q})$ a two-component vector field

$$\xi_\alpha = q_{\perp\alpha} u(\mathbf{q}). \tag{11}$$

With the aid of this vector field the Hamiltonian (10) takes the form

$$H = \frac{1}{2}\int d^3q \left\{B\frac{q_z^2}{q_\perp^2} + Kq_\perp^2 + K' q_z^2 + \chi_a h^2\right\} |\xi(\mathbf{q})|^2 + \frac{\gamma_0}{4!}\int d^3q_1\, d^3q_2\, d^3q_3\, d^3q_4\, \delta(\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3+\mathbf{q}_4) \times (\xi^\alpha(\mathbf{q}_1)\xi^\alpha(\mathbf{q}_2))(\xi^\beta(\mathbf{q}_3)\xi^\beta(\mathbf{q}_4)). \tag{12}$$

It is possible to change in obvious fashion the scale q_z and change to spherical coordinates. As a result, the unrenormalized Green's function takes the form

$$\tilde{g}_0(\mathbf{q}) \equiv T^{-1}\langle \xi^\alpha(\mathbf{q})\xi^\alpha(-\mathbf{q})\rangle = [Bx^2/(1-x^2) + \tilde{K}q^2 + \chi_a h^2]^{-1}. \tag{13}$$

In the essential region $x \ll 1$ ($x \equiv \cos\theta$, where θ is the polar angle) the problem has become equivalent to the four-dimensional phase-transition problem. The role of the "mass" (or of the proximity to the transition point) is played by the magnetic field $\chi_a h^2$.

With parquet accuracy, the equation for the vertex function Γ with all the entering momenta of the same order coincides practically literally, e.g., with the corresponding equation for the problem, solved by Larkin and Khmel'nitskii,[7] of a phase transition in a uniaxial ferroelectric. Therefore, roughly speaking, it can be stated that a smectic liquid crystal is similar not to a two-dimensional crystal, but to a "four-dimensional" one such as a uniaxial ferroelectric.

With obvious change of symbols[7] we have

$$\Gamma(y) = \gamma_0 - 10\int_y^L d\varphi \Gamma^2(\varphi), \tag{14}$$

where we have introduced the logarithmic variable y (or φ), and $L \equiv \ln(\Lambda/\chi_a h^2)$, whence

$$\Gamma(y) = \gamma_0 [1+10(L-y)]^{-1}. \tag{15}$$

To calculate the correlators we need a vertex function with entering momenta of different order. In place of calculating this function, it is more convenient to find the so-called triangular vertex function $\mathcal{T}(y)$ (Fig. 3), which in fact defines directly in terms of Ward's identities the correlation function (or the Green's function)

$$\mathcal{T}(y) = 1 - 4\int_y^L d\varphi \Gamma(\varphi)\mathcal{T}(\varphi). \tag{16}$$

From this we have with the aid of (15)

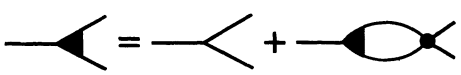

FIG. 3

$$\mathcal{T}(y)=[1+10\gamma_0(L-y)]^{-4/5}. \tag{17}$$

Now, using the Ward identity

$$\partial\tilde{g}^{-1}/\partial(\chi_a h^2)=\mathcal{T}(0), \tag{18}$$

we easily obtain the logarithmic increments to the correlators. Returning to the correlation functions of the displacements, we can deduce from (17) and (18)

$$g^{-1}(q_\perp,\ q_z=0)\sim q_\perp^4[1+\gamma_0\ln(\Lambda/\chi_a h^2)]^{4/5}. \tag{19}$$

The function $g^{-1}(q_z q_\perp=0)$ is not calculated directly in this manner, since at $q_\perp=0$ the connection between the Green's functions g and $\tilde{g}$ is not defined. In this case $x\sim 1$ and the expansion (13) is not suitable. However, simple reasoning enables us to calculate also $g^{-1}(q_z q_\perp=0)$. The point is that in all the integrals (including also at $x\sim 1$) we have $q_z^2\sim q_\perp^4$. This relation should be satisfied also for the renormalized Green's functions. From this requirement, with allowance for (9) and (19), we obtain at $\gamma_0\ln(\Lambda/\chi_a h^2)\gtrsim 1$

$$g^{-1}(q_z,\ q_\perp=0)\sim q_z^2[\ln(\Lambda/\chi_a h^2)]^{-2/5}. \tag{20}$$

We note that our Eqs. (19) and (20) agree with the expressions of Ref. 5, in which, however, $h=0$, so that cutoff is effected at the characteristic wave vectors of the problem.

It is also easy now to calculate the generalized magnetic susceptibility

$$\chi_{eff}\sim g(0)\sim h^{-2}[1+\gamma_0\ln(\Lambda/\chi_a h^2)]^{2/5}.$$

The magnetic part of the heat capacity is determined in the usual manner by the diagram shown in Fig. 4:

$$C_h\sim\int\mathcal{T}^2(q)\,\frac{q^2\,dq\,dx}{(Bx^2+Kq^2+\chi_a h^2)^2}.$$

Simple calculation with this formula yields with logarithmic accuracy

$$C_h\sim[1+10\gamma_0\ln(\Lambda/\chi_a h^2)]^{1/5}-1. \tag{21}$$

Of course, measurement of χ_{eff} and C_h is by far not a simple experimental task. It is possibly easier to measure directly the displacement correlator by means of light scattering. The scattering intensity, as is well known, is determined by the correlator of the dielectric-constant fluctuations $\delta\varepsilon_{ij}$:

$$I\sim\langle\delta\varepsilon_{ij}\delta\varepsilon_{mn}\rangle p_i p_m p_j' p_n', \tag{22}$$

where $\mathbf{p}$ and $\mathbf{p}'$ are the polarization vectors of the incident and scattered light. In smectic-A liquid crystals the fluctuating parameters that cause light scattering are the displacement u and the density change $\delta\rho$. From symmetry considerations we have

$$\begin{aligned}\delta\varepsilon_{xx}=\delta\varepsilon_{yy}&=a_\perp\delta\rho+b_\perp\partial u/\partial z,\\ \delta\varepsilon_{zz}&=a_\parallel\delta\rho+b_\parallel\partial u/\partial z,\\ \delta\varepsilon_{xz}=-\varepsilon_a\partial u/\partial x,\quad \delta\varepsilon_{yz}&=-\varepsilon_a\partial u/\partial y.\end{aligned} \tag{23}$$

Thus, at sufficiently small wave vectors (λ 5000 Å), when scattering by the density fluctuations can be neglected, the scattering cross section for polarizations in a plane perpendicular to the director is given by

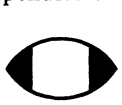

FIG. 4

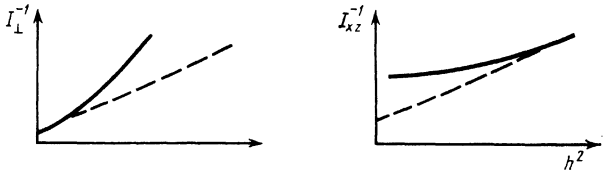

FIG. 5

$$I_\perp\sim q_z^2 g(q_\perp,\ q_z).$$

On the other hand, the scattering cross section in crossed polarizations is

$$I_{xz}\sim q_\perp^2 g(q_\perp,\ q_z).$$

At $q_\perp=0$ we therefore have

$$I_\perp\sim\frac{q_z^2}{Bq_z^2\ln^{-2/5}(\Lambda/\chi_a h^2)+\chi_a h^2},$$

and at $q_z=0$

$$I_{xz}\sim\frac{q_\perp^2}{Kq_\perp^4\ln^{2/5}(\Lambda/\chi_a h^2)+\chi_a h^2}.$$

The dependences of $I_\perp^{-1}$ and I_{xz}^{-1} on h^2 are shown schematically in Fig. 5 (the dashed straight line shows the dependences obtained without allowance for the interaction of the fluctuations).

One more measurable quantity in which, in principal, anharmonic interaction of fluctuations can manifest itself, is the structure factor

$$S(r,\ z)=\langle\rho(\mathbf{r})\rho(0)\rangle. \tag{24}$$

Separating in (24) the homogeneous part of the density from that modulated by the smectic order, we obtain in the harmonic approximation

$$S_0(r,z)=\rho_0^2+\sum_{\varkappa\neq 0}\rho_\varkappa^2\exp(i\varkappa r)\exp\left[-\frac{\varkappa^2}{2}g_0(r,z)\right],$$

where $\varkappa$ is the reciprocal-lattice vector. The explicit expressions for $g_0(r,z)$, which follow from the inverse Fourier transform of (13), depend on the ratio of the parameters, with dimension of length, which enter in the problem:

$$\lambda=(K/B)^{1/2},\quad \xi=(K/\chi_a)^{1/4}h^{-1},$$
$$l^2\equiv\max\{\lambda z,\ r^2\},\quad d\equiv\max\{a_z,\ a_\perp^2/\lambda\},$$

where a is the characteristic molecular dimension.

Thus, at $\lambda d\ll l^2\ll\xi^2$ we have

$$g_0(r,z)=\frac{T}{8\pi(BK)^{1/2}}\ln\left\{\left(\frac{z}{d}\right)^2+\left(\frac{r^2}{\lambda d}\right)^2\right\}, \tag{25}$$

and at $\lambda d\ll\xi^2\ll l^2$

$$g_0(r,z)=\frac{T}{2\pi(BK)^{1/2}}\left\{\ln\frac{4\pi\xi}{(\lambda d)^{1/2}}-\left[\left(\frac{\lambda z}{\xi^2}\right)^2+\left(\frac{r}{\xi}\right)^2\right]^{-1/2}\right\}. \tag{26}$$

Expression (25) corresponds to weak magnetic fields. The structure factor behaves in this case in power-law fashion, just as in the absence of the field. However, the interaction of the fluctuations is "cutoff" at the magnetic coherence

length. A simple calculation with the aid of (25) and (19) yields a formula of type (1) with the substitution

$$\eta(T) \to \eta(T)\,[\ln(\Lambda/\chi_a h^2)]^{1/5}.$$

The second region (26) corresponds to an ordered phase, and the logarithmic corrections in it are small.

3. We discuss briefly, in conclusion, the already noted case of discotic liquid crystals near the transition into the nematic phase. We introduce in (6) and (7) a new field ψ in analogy with the procedure used for smectic liquid crystals: $\psi = \partial u/\partial z$;

$$H^{(d)} = \frac{1}{2}\int d^3q \left\{ C\frac{q_\perp^2}{q_z^2} + K_3 q_z^2 \right\} |\psi(\mathbf{q})|^2 + \frac{\gamma_1}{4!}\int d^3q_1\, d^3q_2\, d^3q_3\, d^3q_4\, \delta(\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3+\mathbf{q}_4) \times (\psi(\mathbf{q}_1)\psi(\mathbf{q}_2))\,(\psi(\mathbf{q}_3)\psi(\mathbf{q}_4)),$$

or in spherical coordinates

$$\tilde{g}_0^{(d)} \equiv T^{-1}\langle \psi(\mathbf{q})\psi(-\mathbf{q})\rangle = [C(1-x^2)/x^2 + K_3 q^2 x^2]^{-1}.$$

The form of the interaction (7) shows that the significant values are $x \sim 1$. In this region we have a phase-transition problem in which the role of the temperature is played by the quantity C (the critical temperature corresponds to $C = 0$). All the exponents are determined in the usual manner by expansion in $\varepsilon = 4 - d$ (d is the dimensionality of space). It must only be borne in mind that our vector field has two components ($n = 2$).

In particular, the susceptibility exponent, which shows in our case the dependence of the correlation function on C (and consequently on the proximity to the point of transition into the nematic phase),[8] is equal to

$$\gamma = 1 + [(n+2)/2(n+8)]\,\varepsilon = 1.2.$$

In contrast to the case of smectics, the interaction of the fluctuations does not yield simply logarithmic corrections, but makes the exponents different from their classical values (obtained in the self-consistent-field approximation).

As usual, the exponent η differs from zero only in second order ε:

$$\eta = [(n+2)/2(n+8)^2]\,\varepsilon^2 = 0.02.$$

This means, e.g., that at $q_\perp = 0$ the correlator is

$$\langle \mathbf{u}(\mathbf{q})\mathbf{u}(-\mathbf{q})\rangle \sim q_z^{-4+0.02}.$$

We note that such a correction is within the limits of the accuracy of modern precision x-ray and neutron methods of measure of scattering line shapes. In addition, the deviation from the classical law should increase as the point of transition to the nematic phase is approached.

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