Theory of the smectic-*A*–smectic-*C* phase transition

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(Submitted 2 December 1985)
Zh. Eksp. Teor. Fiz. **90**, 111–123 (January 1986)

The smectic-*A*–smectic-*C* phase transition is investigated by the renormalization-group method. In the region $7 < \ln(10^3/\tau) < 10^2$ (τ is the dimensionless distance from the transition point) the corrections to the Frank constants are small. Therefore, the critical indices describing the temperature dependences of the compressibility of the smectic layers, susceptibility, and specific heat in this region are functions of K_1/K_2. These indices are calculated in the one-loop approximation. The renormalization-group equations for the Frank constants are found in the two-loop approximation.

1. INTRODUCTION

Liquid crystals are substances which have undergone spontaneous breaking of rotational invariance but which are not true three-dimensional crystals (see, e.g., Ref. 1). Such a state is possible by virtue of the fact that liquid crystals consist of molecules with a strongly anisotropic shape (in most cases, rod-like). The average direction of the liquid-crystal molecules is characterized by a unit vector **n**, called the director. A nonuniform deformation of the director in the liquid crystal requires the expenditure of energy; the corresponding term in the expansion of the free energy is called the Frank energy:

$$F_F={}^1\!/_2K_1(\nabla\mathbf{n})^2+{}^1\!/_2K_2(\mathbf{n}[\nabla\mathbf{n}])^2+{}^1\!/_2K_3((\mathbf{n}\nabla)\mathbf{n})^2. \qquad (1)$$

Here square brackets are used for cross products, so $[\nabla n]$ denotes the curl of **n**, and K_1, K_2, and K_3 are the Frank constants.

The liquid-crystalline phase of a substance exists in a temperature range $\Delta T\sim 10$ K between the liquid and solid phases. However, even in this narrow temperature range liquid crystals undergo numerous phase transformations, one of which (the smectic-*A*–smectic-*C* transition) will be investigated in this paper. As is well known, smectics are liquid crystals in which besides the spontaneous breaking of rotational invariance there is also spontaneous breaking of translational invariance in one of the directions. As a result of this there appears a layer structure with period l of the order of the length of a liquid-crystal molecule. We shall describe this layer structure by means of a function $W(t,\mathbf{r})$, which has the property that the equation $W=$ const specifies the position of a smectic layer in space (and the evolution of the layer in time). We note that, by the definition of the function W, the vector ∇W specifies the direction of the normal to the layer.

2. FREE ENERGY FOR THE SMECTIC-*A*-SMECTIC-*C* PHASE TRANSITION

In equilibrium the smectic layers are parallel and equidistant. If the z axis is perpendicular to these layers, this structure will correspond to the function $W=z/l$, where l is the interlayer distance. Away from equilibrium we must put

$$W=(z-u)/l. \qquad (2)$$

Here u has the meaning of the displacement vector of the layers along the z axis. In the expansion of the free energy the corresponding term that reaches a minimum at $u=0$ has the form

$$F_S={}^1\!/_8B[l^2(\nabla W)^2-1]^2. \qquad (3)$$

In order that the energy (3) have a minimum we must set $B>0$. Besides the terms (1) and (3) we must include in the expansion of the free energy a term specifying the relationship between the orientation of a layer and the direction of the molecules in it. We write this term in the form

$$\begin{aligned}F_A=&-{}^1\!/_2A[(\nabla W)^{-2}(\mathbf{n}\nabla W)^2-1]\\&+{}^1\!/_4(U_1+2U^2/B)[(\nabla W)^{-2}(\mathbf{n}\nabla W)^2-1]^2\\&+{}^1\!/_2U[l^2(\nabla W)^2-1][(\mathbf{n}\nabla W)^2(\nabla W)^{-2}-1]. \qquad (4)\end{aligned}$$

Henceforth we shall take $U_1>0$, which corresponds to the real situation in the *A–C* transition.

At equilibrium **n** and ∇W are uniform, and the angle between them is determined by the parameters of (4) and can be found by minimizing the energy (4) with respect to $\mathbf{n}\cdot\nabla W$. If $A>0$ the energy (4) is a minimum when **n** is parallel to ∇W (i.e., the orientation of the molecules is perpendicular to the layer), corresponding to a smectic-*A*. For $A<0$ the interlayer distance turns out to be different from l and equal to

$$l'=l(1+2U|A|/BU_1)^{-1/2}. \qquad (5)$$

If $A<0$ the energy (4) is a minimum when **n** and ∇W are at an angle θ determined by the condition

$$\cos^2\theta=1+A/U_1. \qquad (6)$$

This case corresponds to a smectic *C*, in which the molecules are oriented obliquely to the layer. We note that for $A>0$ the presence of the energy (4) does not affect the interlayer distance, which is simply equal to l. In smectics *A* the direction of **n** if fixed uniquely by the vector ∇W, while in smectics *C* only the projection of **n** on ∇W is fixed; the azimuthal angle describing the director remains free, and is in this case an additional Goldstone variable. Thus, when the sign of A in (4) changes, the symmetry of the system changes, and, correspondingly, a phase transition (from the *A* phase to the *C* phase) should occur.

We shall give estimates of the quantities appearing in the expressions written out above. The characteristic scale of

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the energies is the atomic energy density, which can be estimated in terms of ρc^2, where $\rho \sim 1$ g/cm^3 is the mass density and $c \sim 10^5$ cm/sec is the speed of sound in the liquid crystals. For the Frank constants that specify the energy of deformation of the director field we have the following natural estimate: $K \sim \rho c^2 a^2 \sim 10^{-6}$–$10^{-7}$ erg/cm.

Here $a \sim 10^{-8}$ cm is the atomic size. As regards to constant B that appears in the smectic energy (3), we have the estimate

$$B \sim 10^{-3} \rho c^2 \sim 10^7 \text{ erg/cm}^3.$$

The small magnitude of this expression is due to the weakness of the modulation of the density in smectics. The latter circumstances, in turn, is associated with the fact that the transition from the nematic to a smectic phase of liquid crystals is second-order, and, therefore, because of the narrowness of the region of existence of the smectic phase, the smectic is always close to this transition point. An estimate analogous to that for B holds for the constant U appearing in the energy (5), and so we shall assume that $U \sim B \sim U_1$.

This distance of the smectic from the A–C-phase-transition point is characterized by the dimensionless parameter

$$\tau = A/U_1. \tag{7}$$

In the A phase $\tau > 0$, and in the C phase $\tau < 0$; for this parameter we have the estimate

$$\tau \sim (T - T_c)/T_c.$$

Here T_c is the temperature of the A–C transition. From this, by virtue of the narrowness of the temperatue range of existence of the liquid-crystalline phase ($\Delta T \sim 10$ K), it follows that $|\tau|$ is small in the entire region of existence of the smectic phase. In particular, this explains the observed smallness of the angles θ of tilt of the director with respect to the normal to the layer in smectics C; from formula (6) it follows that $\theta \cong |\tau|^{1/2}$, and $\theta < 0.1$ in real smectics C. We note two further facts. First, liquid crystals exist at temperature $T \sim 100$ K $\sim \rho c^2 a^3$, and, consequently, the temperature does not specify any additional energy scale. Secondly, the region of applicability of the treatment given above is bounded by the scale $\gtrsim 10^3 a$; the large factor in this estimate is associated with the above-mentioned closeness of the transition to the nematic phase.

To describe the phase transition from the A phase to the C phase we shall use the following parameter:

$$\varphi_i = \varepsilon_{ikn} n_k \nu_n, \qquad \boldsymbol{\nu} = \nabla W / |\nabla W|. \tag{8}$$

This quantity is equal to zero in the A phase and becomes nonzero in the C phase. The director is expressed as follows in terms of ψ:

$$n = |\nabla W|^{-1} (\nabla W (1 - \psi^2)^{1/2} + [\nabla W, \psi]). \tag{9}$$

Substituting (9) into (1), (3), and (4) and retaining the leading terms in the resulting expressions, we find the following free energy:

$$\begin{aligned} F_{C\text{-}A} = {}& {}^1/_8 B [l^2 (\nabla W)^2 - 1]^2 + {}^1/_2 K l^2 (\nabla^2 W)^2 + {}^1/_2 A \psi^2 \\ & - {}^1/_2 U \psi^2 [l^2 (\nabla W)^2 - 1] + {}^1/_4 (U_1 + 2U^2/B) \psi^4 + {}^1/_2 K_1 (\boldsymbol{\nu} [\nabla \psi])^2 \\ & + {}^1/_2 K_2 [(\nabla \psi)^2 - ((\boldsymbol{\nu} \nabla) \psi)^2] + {}^1/_2 K_3 (\boldsymbol{\nu} \nabla \psi)^2. \end{aligned} \tag{10}$$

Here the constant $K = K_1$. We note also the conditions $U > 0$, $B > 0$, and $U_1 > 0$. The first two terms in the expansion (10) are the standard smectic energy, the last terms in (10) give the energy of the critical mode, and the term with U describes the interaction of the critical mode and the smectic mode.

3. RENORMALIZATION GROUP

If the distribution function $\exp(-F_{C\text{-}A}/T)$ is integrated over the fluctuations of W, leading to the effective elimination of the smectic degree of freedom from the analysis, we arrive at a model with a ψ^4 interaction. Such models are conventionally used for the description of phase transitions.[2,3] However, in the case of the smectic-A–smectic-C transition the order parameter ψ realizes a representation of the rotation energy group in real space; it therefore couples with the spatial derivatives, and the situation becomes substantially anisotropic. Because of this, the problem under consideration does not reduce to familiar models, even with a many-component order parameter. However, the phase transition in the system described by the free energy (10) can be investigated with the aid of the standard renormalization-group methods of the theory of phase transitions. In particular, the expression (10) is renormalizable; in calculating the renormalizations of the parameters in (10) we shall use the well-developed perturbation-theory procedure that reduces to the so-called loop expansion. In contrast to the ε-expansion method,[2,3] we shall find it more convenient to perform the acted calculations directly in three-dimensional space, because of the above-mentioned specific features of the problem.

Before proceeding to the calculations, we shall give some estimates. For the fluctuation effects of interest to play an important role, it is necessary that there be a wide range of wave vectors q in which the fluctuations of the order parameter can be regarded as gapless. It is precisely in this region that the main fluctuation contributions to all the observable quantities are formed. It is not difficult to estimate that (in the gapless region) fluctuation corrections become appreciable at the scale

$$10 K^2 / T U \sim 10^4 a. \tag{11}$$

For it to be possible to regard the fluctuations of the order parameter on this scale as gapless it is necessary that the inequalities[1)]

$$|\tau| < T^2 U / K^3 \sim 10^{-3} \tag{12}$$

be fulfilled. To describe the fluctuation effects it is convenient to introduce the following quantity:

$$L = \min\{\ln(2\pi/ql); \quad {}^1/_2 \ln(10^3/|\tau|)\}. \tag{13}$$

This logarithm is characterized by the scale (or temperature factor) at which the integrals appearing in the calculation of the fluctuation corrections are cut off. In accordance with the estimates (11) and (12) these corrections become important for $L > 7$.

We note that for $L > 7$ the effective parameters A, B, U, and U_1 in (10) begin to be substantially renormalized,[2)] while the quantities K_{1-3} in this expression are renormalized much more weakly, this being a reflection of a well known fact in the theory of phase transitions, namely, that the anomalous critical index η is small. Estimates show that there exists a wide range of scales (or temperatures) in which the corrections to K_{1-3} can be assumed to be small. This region is determined by the inequality $L < 10^2$. Evidently, the region $L > 10^2$ is experimentally inaccessible, and, therefore, we shall concentrate our main attention on the region $7 < L < 10^2$ in which fluctuation effects are important but the moduli K in (10) can be regarded as constants. However, it is of undoubted methodological interest to analyse the behavior of the parameters of the free energy (10) for $L > 10^2$; this analysis will also be given in the present paper.

In the calculation of the fluctuation corrections we can neglect completely the fluctuations of W in the last terms in (10), i.e., we can assume that $\mathbf{v}$ in this expression is the unit vector along the z axis. The same can be said of the vector $\mathbf{v}$ in the definition (8). Thus, the order parameter ψ, in accordance with this definition, will have only components along the x and y axes, and we shall denote these components by Greek indices: $\psi_\alpha = (\psi_x, \psi_y)$.

Using analogous notation for the spatial derivatives, we find from (10) the following expression for the gradient part of the energy:

$$F_\psi^{(2)} = {}^1/_2 K_1 (\varepsilon_{\alpha\beta} \nabla_\alpha \psi_\beta)^2 + {}^1/_2 K_2 (\nabla_\alpha \psi_\alpha)^2 + {}^1/_2 K_3 (\nabla_z \psi_\alpha)^2. \qquad (14)$$

Here $\varepsilon_{\alpha\beta}$ is the two-dimensional antisymmetric unit tensor ($\varepsilon_{xy} = -\varepsilon_{yx} = 1$). Hence, in the fluctuation region we obtain the following correlator of the Fourier components:

$$\Delta_{\alpha\beta}(\mathbf{q}) = \langle \psi_\alpha(\mathbf{q}) \psi_\beta(-\mathbf{q}) \rangle = \frac{q_\alpha q_\beta}{q_\perp{}^2} T (K_2 q_\perp{}^2 + K_3 q_z{}^2)^{-1}$$
$$+ \left(\delta_{\alpha\beta} - \frac{q_\alpha q_\beta}{q_\perp{}^2} \right) T (K_1 q_\perp{}^2 + K_3 q_z{}^2)^{-1}, \qquad (15)$$
$$q_\perp{}^2 = q_\alpha{}^2 = q_x{}^2 + q_y{}^2.$$

Expanding now the smectic part of the free energy (10) to second order in the displacement vector u defined as in (2), we find

$$F_u^{(2)} = {}^1/_2 B (\nabla_z u)^2 + {}^1/_2 K (\nabla^2 u)^2. \qquad (16)$$

Hence we obtain the following correlator of the Fourier components:

$$\Delta(\mathbf{q}) = \langle u(\mathbf{q}) u(-\mathbf{q}) \rangle = T (B q_z{}^2 + K q^4)^{-1}. \qquad (17)$$

Expanding the term with U in the free energy (10) to first order in the displacement vector u and combining the result with the term proportional to ψ^4 in (10), we finally obtain the following expression:

$$F_{int} = -U \psi^2 \nabla_z u + {}^1/_4 (U_1 + 2U^2/B) \psi^4. \qquad (18)$$

The free energy (18) describes the interaction of the modes. The first term in (18) gives the three-point vertex of the interaction of the smectic mode and the critical mode, and the second term in (18) gives the four-point vertex of the self-interaction of the critical mode. In the one-loop approximation the interaction term (18) generates corrections to the parameters of (16) and (18), these corrections being depicted by the Feynman diagrams given in Figs. 1–3. In these diagrams a solid line corresponds to the correlator (15), a wavy line to the correlator (17), and the points to the vertices generated by (18). The corrections to B are depicted by the diagram in which two three-point vertices appear (Fig. 1). The corrections to U are depicted by the diagram with one three-point and one four-point vertex (Fig. 1), and also by the diagram with three three-point vertices (Fig. 2). The corrections to the four-point vertex are depicted by the diagrams with two four-point vertices (Fig. 1), by the diagrams with one four-point and two three-point vertices (Fig. 2), and also by the diagram with four three-point vertices (Fig. 3). Finally, the corrections to the two-point vertex A are determined by the diagrams containing one two-point vertex A and either one four-point vertex (Fig. 1) or two three-point vertices (Fig. 2).

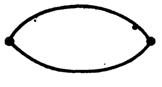

FIG. 1

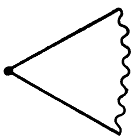

FIG. 2

In the calculation of these diagrams we introduce an intermediate cutoff μ, replacing q_z^2 by $q_z^2 + \mu^2$ in the expression (15). We now investigate how the answers obtained for the fluctuation contributions depend on the factor μ, which has the meaning of the characteristic wave vector on which all the vertices introduced above become dependent when the fluctuation corrections are taken into account. The specific details of the calculations are presented in the Appendix, and as a result we obtain (in the one-loop approximation) the following renormalization-group equations:

$$\frac{\partial U_1}{\partial \ln \mu^{-1}} = -\frac{5TU_1{}^2}{4\pi\mu K_3 K_4}, \qquad \frac{\partial \ln (U/B)}{\partial \ln \mu^{-1}} = -\frac{TU_1}{2\pi\mu K_3 K_5},$$
$$\frac{\partial B}{\partial \ln \mu^{-1}} = -\frac{TU^2}{2\pi\mu K_3 K_5}, \qquad \frac{\partial \ln A}{\partial \ln \mu^{-1}} = -\frac{TU_1}{2\pi\mu K_3 K_5}. \qquad (19)$$

Here we have introduced the notation

$$\frac{10}{K_4} = \frac{9}{2} \left(\frac{1}{K_1} + \frac{1}{K_2} \right) + \frac{\ln (K_1/K_2)}{K_1 - K_2}, \qquad \frac{2}{K_5} = \frac{1}{K_1} + \frac{1}{K_2}. \qquad (20)$$

If $K_1 = K_2$, then $K_4 = K_5 = K_1$. The system of equations (19) is valid in the region of applicability of our analysis, i.e.,

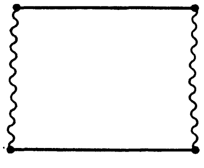

FIG. 3

in the region determined by the inequality $\mu < \mu_0 \sim 10^2 a^{-1}$. On the other hand, the region of applicability of the system (19) is bounded by the inequality $\mu > \mu_1$, where

$$K\mu_1^2 = A \tag{21}$$

(this inequality ensures that the critical mode is gapless). At larger scales μ^{-1} the constants of the theory cease to change.

In the one-loop approximation there are no corrections to the constants K, and, therefore, in solving the system of renormalization-group equations (19) we can regard K_1, K_2, and K_3 as constants. Under this condition the system (19) is trivially integrated, and as a result we find the solution

$$U_1^{-1} = U_{1,0}^{-1} + 5T(\mu^{-1} - \mu_0^{-1})/4\pi K_3 K_4, \tag{22}$$

$$\frac{U}{B} = \frac{U_0}{B_0}\left(\frac{U_1}{B_1}\right)^{\sigma}, \tag{23}$$

$$B^{-1} = B_0^{-1} + \frac{U_0^2}{U_{1,0} B_0^2} \frac{2K_4}{5K_5 - 4K_4}\left[\left(\frac{U_{1,0}}{U_1}\right)^{1-2\sigma} - 1\right], \tag{24}$$

$$A = \tau U_0 (U_1/U_{1,0})^{\sigma}, \qquad \sigma = 2K_4/5K_5. \tag{25}$$

Here we have used the subscript 0 to denote the bare values that the corresponding quantities take at $\mu = \mu_0$, and in (25) we have taken definition (7) into account. If we use now the estimates given above it is straightforward to show that (in accordance with the estimate (11)) for $\mu \ll 10^3 a^{-1}$ the behavior of the solutions (22)–(25) acquires a universal character that does not depend on the initial conditions:

$$U_1 \propto \mu, \quad B \propto \mu^{1-2\sigma}, \quad U \propto \mu^{1-\sigma}, \quad A \propto \tau\mu^{\sigma}. \tag{26}$$

The behavior of the constants of the theory at large scales can be obtained from the solutions (22)–(25) by substituting $\mu = \mu_1$, where μ_1 is defined in (21). Taking into account the proportionalities (26), we find

$$\begin{aligned}
\ln U_1 &\approx \text{const} - \frac{5K_5}{2(5K_5 - K_4)} \ln|\tau|^{-1},\\
\ln B &\approx \text{const} - \frac{5K_5 - 4K_4}{2(5K_5 - K_4)} \ln|\tau|^{-1},\\
\ln U &\approx \text{const} - \frac{5K_5 - 2K_4}{5(5K_5 - K_4)} \ln|\tau|^{-1},\\
\ln A &\approx \text{const} - \frac{5K_5}{5K_5 - K_4} \ln|\tau|^{-1}.
\end{aligned} \tag{27}$$

The expressions (27) are valid when the condition (12) is fulfilled.

Above we have neglected effects associated with the intrinsic fluctuations of W—effects that lead, outside the critical region, to a logarithmic renormalization of the constants B and K in (10).[4,5] Thus, in the one-loop approximation the renormalization of the constant B is determined by the diagram given in Fig. 4, which contains two vertices obtained by expansion of the coefficient of B in (10) to third order in u. The explicit expression for the corresponding correction to B is given in the Appendix; as a result of the integration over q_z we find

$$\Delta B = -\frac{T}{16\pi K^{3/2}} \int \frac{dq_\perp}{q_\perp} B^{3/2}. \tag{28}$$

By virtue of the proportionality (26) for B this integral converges in the fluctuation region, and, consequently, is a constant,[3] to which the main contribution is made by the integration over $q_\perp \sim \mu_1$. This constant is of absolutely no importance, since it simply renormalizes the bare value B_0, and, moreover, the magnitude of this renormalization is small: $\Delta B / B_0 \sim 10^{-3}$. The same applies to the corrections contributed to U and U_1 by diagrams of the type given in Fig. 4, and it is this which justifies the neglect of the intrinsic fluctuations of W.

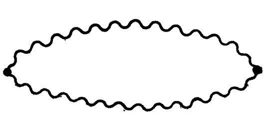
FIG. 4

Corrections of the constants K in (10) and (14) appear only in the two-loop approximation. An example of such a correction generated by (18) is given by the diagram of Fig. 5. It is not difficult to show that all two-loop corrections to the constants K are reduced to this diagram if we take U_1 as the four-point vertex. This diagram is calculated more easily in the **r**-representation (see the Appendix.) We represent the result of the calculation in the following form:

$$\frac{dK_{1,2}}{d\ln\mu^{-1}} = \frac{T^2 U_1^2 (K_1 + K_2)}{2^2 \cdot 3^3 \pi^2 \mu^2 K_1 K_2 K_3^2} j_{1,2},$$

$$\frac{dK_3}{d\ln\mu^{-1}} = \frac{T^2 U_1^2 (K_1 + K_2)^2}{2^3 \cdot 3^3 \cdot \pi^2 \mu^2 K_3 K_1^2 K_2^2} j_3.$$

Here j_1, j_2, and j_3 are numbers of order unity that are functions of K_1/K_2. Expressions for these functions in the form of (single) integrals are given in the Appendix. We note that the following relations hold:

$$j_1\left(\frac{K_1}{K_2}\right) = j_2\left(\frac{K_2}{K_1}\right), \quad j_3\left(\frac{K_1}{K_2}\right) = j_3\left(\frac{K_2}{K_1}\right). \tag{30}$$

These relations are a consequence of a symmetry of the system under considerations; namely, under the replacement $\psi_\alpha \to \varepsilon_{\alpha\beta}\psi_\beta$ the expression (18) does not change, while the expression (14) for the gradient energy is reproduced but with K_1 and K_2 interchanged. The general form of the functions j obtained as a result of a numerical calculation is presented in Fig. 6.

As already noted, the constants K change much more slowly than U_1, and, therefore, for U_1, as before, the expression (22), in which we can also neglect the bare terms, is valid. Substituting this expression into (30), we find

$$\frac{d\ln K_1}{d\ln\mu^{-1}} = \frac{2^2 (K_1 + K_2) K_4^2}{3^3 \cdot 5^2 K_1^2 K_2} j_1, \tag{31a}$$

$$\frac{d\ln K_3}{d\ln\mu^{-1}} = \frac{2(K_1 + K_2)^2 K_4^2}{3^3 \cdot 5^2 K_1^2 K_2^2} j_3. \tag{31b}$$

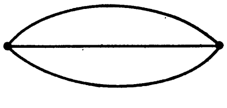
FIG. 5

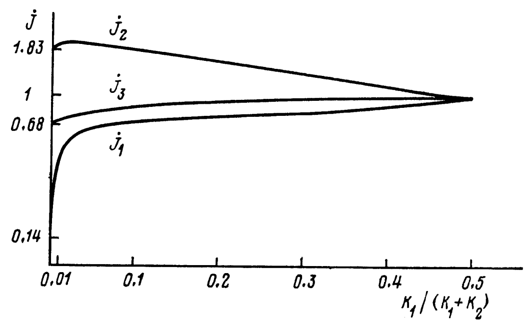

FIG. 6

The equation for K_2 is obtained from (31a) by interchanging the indices 1 and 2. Since the j are numbers of order unity, we obtain from this the estimate

$$d\ln K/d\ln\mu^{-1}\sim 10^{-2},$$

which determines the region $L > 10^2$ in which the constants K begin to change appreciably. In the limit $K_1 \ll K_2$ we have

$$\frac{d\ln K_1}{d\ln\mu^{-1}}=\frac{2^6}{3^7}j_1,\qquad \frac{d\ln K_2}{d\ln\mu^{-1}}=\frac{2^6}{3^7}\frac{K_1}{K_2}j_2;\qquad \frac{d\ln K_3}{d\ln\mu^{-1}}=\frac{2^5}{3^7}j_3. \tag{32}$$

Thus, in this case the constants K_1 and K_3 have indices of the same order 10^{-2}, while the constant K_2 remains constant. An analogous situation obtains in the limit $K_1 \gg K_2$ with K_1 and K_2 interchanged.

If follows from the symmetry of the problem under interchange of K_1 and K_2 that the system (31) admits the solution $K_1 = K_2$. This solution corresponds to the isotropic case, since here, by a change of scale along the z axis, we can also arrange that $K_3 = K_1$, after which (14) is transformed into the standard isotropic gradient energy for a two-component order parameter. The quantities j in this case are calculated analytically (see the Appendix) and turn out to be equal to unity.

It is not difficult to calculate the index of the difference $K_1 - K_2$ near this fixed point (see the Appendix):

$$\frac{d\ln(K_1-K_2)}{d\ln\mu^{-1}}=\frac{T^2U_1^2}{3^4\pi^2K_1^2K_3^2\mu^2}=\frac{2^4}{3^4\cdot 5^2}. \tag{33}$$

This index is smaller than the index of K_1, which, in accordance with (31), is equal to $2^3/3^35^2$. Therefore, the relative magnitude of $(K_1 - K_2)/K_1$ decreases with increase of L, so that the isotropic fixed point is found to be stable.

4. CONCLUSION

We shall summarize our work. We have calculated the change with temperature of the parameters of a smectic A (the compressibility of the layers, the Frank elastic constants, and certain other parameters) in the region of the phase transition from smectic A to smectic C. We have shown that when the dimensionless distance from the transition point has a value $\tau \ll 10^{-3}$ the compressibility B varies as

$$B\propto\tau^{\lambda},\qquad \lambda=\frac{5K_5-4K_4}{2(5K_5-K_4)},$$

where

$$\frac{10}{K_4}=\frac{9}{2}\left(\frac{1}{K_1}+\frac{1}{K_2}\right)+\frac{\ln(K_1/K_2)}{K_1-K_2},\qquad \frac{2}{K_5}=\frac{1}{K_1}+\frac{1}{K_2}.$$

The Frank constants themselves do not change in this approximation (the one-loop approximation of the renormalization group, for the applicability of which it is required that the logarithms L specified by formula (13) that appear in the theory satisfy the inequality $7 < L < 10^2$). Therefore, the index of B depends on the bare Frank-constant ratio K_1/K_2. If $K_1 = K_2$, then $B \propto \tau^{1/8}$, while if $K_1 \gg K_2$ (or $K_2 \gg K_1$), then $B \propto \tau^{1/14}$. The indices, unfortunately, are small, but the change of B, in principle, lies within reach of the present-day experimental accuracy of x-ray or ultrasound methods.

In this same region it is easy to find the change of the specific heat of the system:

$$C\propto -T_c\left(\frac{\partial T_c}{\partial A}\right)^{-2}\frac{\partial^2F_{A-C}}{\partial A^2}=-T_c\left(\frac{\partial T_c}{\partial A}\right)^{-2}\Pi,$$

where the polarization operator Π is determined by a diagram of the type depicted in Fig. 1, in which in the correlators (15) we must take into account the gap $\propto A$ and vertices $\propto 1$. A simple calculation of this diagram gives the following expression for the specific-heat index:

$$\alpha=-(4K_4-5K_5)/2(5K_5-K_4),$$

i.e., the specific-heat index is equal to minus the index of the elastic constant B ($\alpha = 1/8$ for $K_1 = K_2$, and $\alpha = 1/14$ for $K_1 \gg K_2$ or $K_1 \ll K_2$).

According to (27), the susceptibility index is equal to

$$\gamma=5K_5/(5K_5-K_4).$$

At the point $K_1 = K_2$ we have $\gamma = 5/4$, which agrees with the known experimental data.[6,7] In an analogous way, from the definition of the order parameter in the C phase and estimates of the type (27) we can find the order-parameter index

$$\beta={}^1/_4(5K_5+2K_4)/(5K_5-K_4).$$

For $K_1 = K_2$ we have $\beta = 7/16 \cong 0.43$, which also does not contradict the experimental data.[7]

We draw attention to a difference between our work and all previous papers on this subject (see, e.g., the review Ref. 8 and the literature cited therein). The theoretical description of the smectic-A–smectic-C phase transition goes back to the work of de Gennes,[9] who drew attention to the analogy between the transition and the transition in helium-4. However, this analogy takes no account of substantial differences in the order parameters of the two types of transition. The order parameter in liquid crystals is coupled to the spatial coordinates, and it is this which leads to the entirely distinctive character of the phase transitions, one of which (the A–C transition) is considered in our paper. Finally, the region $L > 10^2$ in which the Frank constants change substantially with temperature is hardly accessible to experiment. We note only that in this region isotropization of the system in the plane of the layers should occur.

In conclusion the authors express their gratitude to V. A. Avilov for assistance in the computer calculations.

APPENDIX

We shall consider first the expression for the correction to the constant B. This correction is determined by the diagram of Fig. 1:

$$\Delta B=-\frac{2}{T}\int\frac{d^3q}{(2\pi)^3}U^2\Delta_{\alpha\beta}\Delta_{\alpha\beta}. \tag{A.1}$$

Substituting the expression (15) into this and introducing the intermediate cutoff, we find

$$\Delta B=-\frac{T}{2\pi^2}\int_{-\infty}^{\infty}dq_z\int_0^{\infty}q_\perp dq_\perp\frac{U^2}{K_3^2}\left[\left(q_z^2+\frac{K_1}{K_3}q_\perp^2+\mu^2\right)^{-2}+\left(q_z^2+\frac{K_2}{K_3}q_\perp^2+\mu^2\right)^{-2}\right]. \tag{A.2}$$

Performing the integration in the order indicated in (A.2), we finally obtain

$$\Delta B=-\frac{TU^2}{4\pi\mu K_3}\left(\frac{1}{K_1}+\frac{1}{K_2}\right). \tag{A.3}$$

Differentiating now with respect to μ, we obtain the expression for $\partial B/\partial\ln\mu^{-1}$ in (19). The correction contributed to the vertex U by the diagrams in Figs. 1 and 2 has, after averaging over the angles, the following form:

$$\Delta U=-\frac{2}{T}\int\frac{d^3q}{(2\pi)^3}U\tilde{U}_1\Delta_{\alpha\beta}\Delta_{\alpha\beta}+\frac{2}{T^2}\int\frac{d^3q}{(2\pi)^3}U^3\Delta_{\alpha\beta}\Delta_{\alpha\beta}\,\Delta q_z^2. \tag{A.4}$$

Here $\tilde{U}_1=U+2U^2/B$, and Δ is determined by the expression (17). In the region $\mu<10^{-3}a^{-1}$ in which, in accordance with the estimate (11), fluctuation corrections become important, the ratio of the second term in the denominator of (17) to the first is of the order of

$$(K/B)\mu^2<10^{-3}. \tag{A.5}$$

Therefore, we can neglect this second term, as a result of which we obtain

$$q_z^2\Delta\approx T/B. \tag{A.6}$$

Thus, the integrals in (A.4) are completely identical to the integral in (A.1), and are taken in exactly the same way. Differentiating the result with respect to μ, we find the derivative of U/B in (19). The correction to A is determined by the analogous diagrams. Averaging over the angles and substituting (A.6), we find

$$\Delta A=-\frac{2}{T}\int\frac{d^3q}{(2\pi)^3}AU_1\,\Delta_{\alpha\beta}\Delta_{\alpha\beta}. \tag{A.7}$$

From this follows the expression given in (19) for the derivative of A. Finally, the corrections to $\tilde{U}_1$ that are defined by the diagrams in Figs. 1–3, after averaging over the angles and insertion of (A.6) give

$$\Delta\tilde{U}_1=-\frac{1}{T}\int\frac{d^3q}{(2\pi)^3}\tilde{U}_1^2\left(4\Delta_{\alpha\beta}\Delta_{\alpha\beta}+\frac{1}{2}\Delta_{\alpha\alpha}^2\right)+\frac{2}{T}\int\frac{d^3q}{(2\pi)^3}\frac{\tilde{U}_1U^2}{B}(3\Delta_{\alpha\beta}\Delta_{\alpha\beta}+\Delta_{\alpha\alpha}^2)-\frac{2}{T}\int\frac{d^3q}{(2\pi)^3}\frac{U^4}{B^2}(2\Delta_{\alpha\beta}\Delta_{\alpha\beta}+\Delta_{\alpha\alpha}^2). \tag{A.8}$$

Some of the terms in (A.8) have the form (A.1), and the others reduce to the integral

$$\int_0^{\infty}dq_\perp^2\int_{-\infty}^{\infty}dq_z\left(q_z^2+\frac{K_1}{K_3}q_\perp^2+\mu^2\right)^{-1}\left(q_z^2+\frac{K_2}{K_3}q_\perp^2+\mu^2\right)^{-1}$$
$$=\frac{\pi K_3}{K_1-K_2}\int_0^{\infty}\frac{dq_\perp^2}{q_\perp^2}\left[\left(\frac{K_2}{K_3}q_\perp^2+\mu^2\right)^{-1/2}-\left(\frac{K_1}{K_3}q_\perp^2+\mu^2\right)^{-1/2}\right]$$
$$=\frac{\pi K_3}{\mu(K_1-K_2)}\ln\frac{K_1}{K_2}. \tag{A.9}$$

Using this integral to calculate $\Delta\tilde{U}_1$, going over from $\Delta\tilde{U}_1$ to ΔU_1, expressing this quantity in terms of U_1, and differentiating with respect to μ, we find the expression in (19) for the derivative of U_1.

Expanding the smectic energy (the first term in (10)) to third order in u (see the definition (2)), we find

$$F_u^{(3)}=-{}^1\!/_2B\nabla_zu(\nabla u)^2. \tag{A.10}$$

Using the third-order vertex found in (A.10), we can construct the fluctuation correction contributed to the constant B in (16) by the diagram in Fig. 4 (here the pairing is performed in such a way that ∇_z remains on the external points):

$$\Delta B=-\frac{1}{2T}\int\frac{d^3q}{(2\pi)^3}B^2q^4\Delta^2. \tag{A.11}$$

Substituting the expression (17) into this and integrating over q_z, we find (28). In this integration we must keep in mind that

$$q_z\sim(K/B)^{1/2}q_\perp^2\ll q_\perp.$$

Therefore, in the integral (A.11) q^4 can be replaced by $q_\perp^4$.

We now consider the fluctuation corrections to the constant K. These corrections appear only in the two-loop approximation. An example of such a two-loop diagram is given in Fig. 5. Allowance for diagrams with intermediate smectic lines (diagrams of the type shown in Fig. 7) reduces, with the use of (A.6), to replacing the vertex $\tilde{U}_1$ by the vertex U_1 in the diagram of Fig. 5. This diagram is more easily calculated in the $\mathbf{r}$-representation. The corresponding expression for the correction to the free energy has the form

$$\Delta F(\mathbf{r}')=-\frac{\psi_\alpha(\mathbf{r}')}{T}\int d^3rU_1^2[\Delta_{\alpha\delta}(\mathbf{r})\Delta_{\beta\gamma}^2(\mathbf{r})+2\Delta_{\alpha\beta}(\mathbf{r})\Delta_{\beta\gamma}(\mathbf{r})\Delta_{\gamma\delta}(\mathbf{r})]\psi_\delta(\mathbf{r}'+\mathbf{r}). \tag{A.12}$$

In (A.12) we expand $\psi_\delta(\mathbf{r}'+\mathbf{r})$ to second order in r; the terms with the first two quantities in the free energy drop out

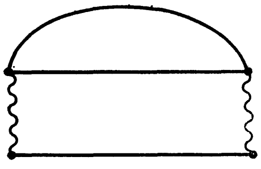

FIG. 7

upon regularization, and the second-order term gives the desired corrections to the constants K. Averaging over the angles, we find

$$\Delta K_1=\frac{U_1^2}{8T}\int d^3r\,r_\perp^2[3(\Delta_{\alpha\alpha}\Delta_{\beta\gamma}^2+2\Delta_{\alpha\beta}\Delta_{\beta\gamma}\Delta_{\gamma\alpha})-2(n_\alpha\Delta_{\alpha\delta}n_\delta\Delta_{\beta\gamma}^2+2n_\alpha\Delta_{\alpha\beta}\Delta_{\beta\gamma}\Delta_{\gamma\delta}n_\delta)],$$

$$\Delta K_2=\frac{U_1^2}{8T}\int d^3r r_\perp^2[\Delta_{\alpha\alpha}\Delta_{\beta\gamma}^2+2\Delta_{\alpha\beta}\Delta_{\beta\gamma}\Delta_{\alpha\gamma}]+(2n_\alpha\Delta_{\alpha\delta}n_\delta\Delta_{\beta\gamma}^2+2n_\alpha\Delta_{\alpha\beta}\Delta_{\beta\gamma}\Delta_{\gamma\delta}n_\delta)],$$

$$\Delta K_3=\frac{U_1^2}{2T}\int d^3rz^2(\Delta_{\alpha\alpha}\Delta_{\beta\gamma}^2+2\Delta_{\alpha\beta}\Delta_{\beta\gamma}\Delta_{\gamma\alpha}),\qquad n_\alpha\equiv r_\alpha/r_\perp. \tag{A.13}$$

In the calculation of the expression (A.13) we shall need the explicit form of the correlator $\langle\psi_\alpha\psi_\beta\rangle$ in the **r**-representation. Fourier-transforming (15) (with an introduced intermediate cutoff μ), we find

$$\Delta_{\alpha\beta}(r)=\frac{T}{4\pi K_3\mu}\left\{\frac{\mu_2}{r_2}\exp(-\mu_2r_2)\frac{r_\alpha r_\beta}{r_\perp^2}+\frac{\mu_1}{r_1}\exp(-\mu_1r_1)\left(\delta_{\alpha\beta}-\frac{r_\alpha r_\beta}{r_\perp^2}\right)+\frac{1}{r_\perp^2}[\exp(-\mu_1r_1)-\exp(-\mu_2r_2)]\left(\delta_{\alpha\beta}-2\frac{r_\alpha r_\beta}{r_\perp^2}\right)\right\}. \tag{A.14}$$

Here we have introduced the notation

$$\mu_1^2=\frac{K_3}{K_1}\mu^2,\quad \mu_2^2=\frac{K_3}{K_2}\mu^2,\quad r_1^2=r_\perp^2+\frac{K_1}{K_3}z^2,\quad r_2^2=r_\perp^2+\frac{K_2}{K_3}z^2.$$

After substitution of (A.14) into (A.13) the integration over the angle in the plane perpendicular to the z axis is trivially carried out. We also introduce the dimensionless variable $\xi=z/r_\perp$. The integral over $r_\perp$ is taken explicitly. As a result we find expressions for ΔK_{1-3}, which, after differentiation with respect to μ, give (29) with the following functions:

$$j_1=\frac{3^3}{2^3}\frac{K_1K_2}{K_3(K_1+K_2)}\int\limits_0^\infty d\xi\left\{\frac{\sigma_1^3}{\xi_1^2}+\frac{\sigma_1^2\sigma_2}{(2\xi_1+\xi_2)^2}+\frac{3\sigma_1\sigma_2^2}{(2\xi_2+\xi_1)^2}+\frac{\sigma_2^2}{3\xi_2^2}+26\sigma_1^2\left(\frac{1}{3\xi_1}-\frac{1}{2\xi_1+\xi_2}\right)-4\sigma_1\sigma_2\left(\frac{1}{2\xi_1+\xi_2}-\frac{1}{2\xi_2+\xi_1}\right)-6\sigma_2^2\left(\frac{1}{\xi_1+2\xi_2}-\frac{1}{3\xi_2}\right)+28\sigma_1[-\ln 3\xi_1+2\ln(2\xi_1+\xi_2)-\ln(\xi_1+2\xi_2)]+4\sigma_2[-\ln(2\xi_1+\xi_2)+2\ln(2\xi_2+\xi_1)-\ln 3\xi_2]+24[\xi_1\ln 3\xi_1-(2\xi_1+\xi_2)\ln(2\xi_1+\xi_2)+(\xi_1+2\xi_2)\ln(\xi_1+2\xi_2)-\xi_2\ln 3\xi_2]\right\}, \tag{A.15}$$

$$j_3=\frac{3^3}{2^2}\frac{K_1^2K_2^2}{(K_1+K_2)^2K_3^2}\int\limits_0^\infty d\xi\xi^2\left\{\frac{\sigma_1^3}{3\xi_1^2}+\frac{\sigma_1^2\sigma_2}{(2\xi_1+\xi_2)^2}+\frac{\sigma_1\sigma_2^2}{(\xi_1+2\xi_2)^2}+\frac{\sigma_2^2}{3\xi_2^2}+8\left[\sigma_1^2\left(\frac{1}{3\xi_1}-\frac{1}{2\xi_1+\xi_2}\right)-\sigma_2^2\left(\frac{1}{\xi_1+2\xi_2}-\frac{1}{3\xi_2}\right)\right]+8\sigma_1\ln\frac{(2\xi_1+\xi_2)^2}{3\xi_1(\xi_1+\xi_2)}+\sigma_2\ln\frac{(2\xi_2+\xi_1)^2}{3\xi_2(2\xi_1+\xi_2)}\right\}.$$

Here we have introduced the notation

$$\xi_1^2=\xi^2+\frac{K_3}{K_1},\qquad \xi_2^2=\xi^2+\frac{K_3}{K_2},\qquad \sigma_1=\frac{K_3}{K_1\xi_1},\qquad \sigma_2=\frac{K_3}{K_2\xi_2}.$$

The expression for j_2 differs from that for j_1 by interchange of the indices 1 and 2. The results of a numerical calculation of the quantities j are given in Fig. 6.

For $K_1=K_2=K_0$ the form of the function (A.14) is simplified considerably:

$$\Delta_{\alpha\beta}=\frac{T}{4\pi(K_0K_3)^{1/2}R}\exp\left[-\mu\left(\frac{K_3}{K_0}\right)^{1/2}R\right]\delta_{\alpha\beta}, \tag{A.16}$$
$$R^2=r_\perp^2+(K_0/K_3)z^2.$$

We substitute the expression (A.16) into (A.13) and go over to integration over R. The integration over the angular variables is trivial, and the integral over R is also taken simply; as a result, we obtain expressions which, after differentiation with respect to μ, give (31) with $j_1=j_2=j_3=1$. We now consider a weak deviation from the regime $K_1=K_2$:

$$K_1=K_0(1+\varkappa/2),\qquad K_2=K_0(1-\varkappa/2). \tag{A.17}$$

It is easy to see that the introduction of $\varkappa$ in the linear approximation does not effect the equations for U_1 and K_3, since these equations are symmetric under the interchange $K_1\leftrightarrow K_2$ and, consequently, are even in $\varkappa$, so that it will be sufficient to take account of the presence of $\varkappa$ in the equations for K_1 and K_2. Linearizing the expressions (A.13) for ΔK_1 and ΔK_2 in $\varkappa$, we find

$$\Delta K_1-\Delta K_2=-\frac{2}{T}\int d^3rU_1^2\,\Delta_{\alpha\beta}\Delta_{\beta\alpha}\,\delta\Delta_{\gamma\delta}r_\gamma r_\delta. \tag{A.18}$$

Here,

$$\delta\Delta_{\alpha\beta}=\frac{T\varkappa r_\perp^2}{16\pi(K_0K_3)^{1/2}R^3}\exp\left[-\mu\left(\frac{K_3}{K_0}\right)^{1/2}R\right]\left[1+\mu\left(\frac{K_3}{K_0}\right)^{1/2}R\right](\delta_{\alpha\beta}-2n_\alpha n_\beta). \tag{A.19}$$

We substitute the expression (A.16) into (A.18) and go over to integration over R. The angular integrals reduce to averaging over the angles, and the integral over R is also taken. Differentiating the resulting expression with respect to μ and substituting $\varkappa=(K_1-K_2)/K_0$, we find the expression (33).

[1)] We note that temperature $|T-T_c|\sim10^{-4}$ K, i.e., $|\tau|\sim10^{-6}$, are fully accessible experimentally.

[2)] To avoid confusion we note that we are using τ to denote a quantity which, in accordance with (7), is expressed in terms of the bare (unrenormalized) quantities.

[3)] Of course, this integral becomes logarithmic on the large scales (outside the fluctuation region) to which the analysis of Refs. 4 and 5 applies.

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Translated by P. J. Shephard