PLANE PROBLEMS IN ELASTICITY THEORY OF NEMATIC LIQUID CRYSTALS

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The mechanical equilibrium equations for nematic liquid crystals are solved for both the case of equal elastic moduli and the case when one of the moduli greatly exceeds the other. The structure of a liquid crystal near two close disclinations (with Franck indexes equal to 2) is found for the case of arbitrary moduli.

As is well known, certain organic substances, whose molecules have an elongated form, are in a definite temperature interval in a liquid-crystal state, the description of the properties of which can be found in Chistyakov's review[1]. In this state, the substance (which is thermodynamically stable) is anisotropic, and at the same time has a fluidity characteristic of ordinary (isotropic) liquids. From the microscopic point of view, this is due to the existence of long-range order in the molecule orientation (while there is no long-range order in the arrangement of their centers of gravity, i.e., there is no crystal lattice). The direction of the preferred orientation of the molecules is conveniently described with the aid of a single vector $\mathbf{n}$, called the director (in this case $\mathbf{n}$ and $-\mathbf{n}$ are equivalent).

Nematic liquid crystals are characterized by the fact that in the ground state the vector $\mathbf{n}$ is the same at all points (we are considering an infinite medium). On the other hand, if external forces act on the liquid crystal, then the field of the directions is, generally speaking, no longer homogeneous, and the stresses due to the deformation of the field $\mathbf{n}$ balance out the action of the external forces.

However, compared with ordinary materials, liquid crystals are unusually "soft", i.e., they are greatly deformed by rather small external actions. The reason can be readily understood. Drawing a parallel between the deformation of a liquid crystal and that of a solid, we note that the readily observed (as a result of the anisotropy of the optical properties) rotations of the liquid-crystal molecules through an angle on the order of unity correspond to displacements of the atoms of a solid on the order of interatomic distances: such small deformations in a solid are difficult to observe (but are produced under very small forces).

By way of an example, we can point to the experimentally well known fact that the walls of a vessel containing a liquid crystal exert an orienting action. Namely, because the surface energy depends on the angle between the director and the wall, the orientation of the liquid crystal near the surface is uniquely determined.

In the present paper we solve the problem of determining the field $\mathbf{n}$ in the planar case, when $n_z \equiv 0$ and n_x and n_y do not depend on z. We consider the case when the only cause of the deformation of the field $\mathbf{n}$ is the above-described orienting influence of the vessel walls.

As is well known, in the case when $\mathbf{n}$ changes noticeably only over macroscopic distances, the addition to the free energy as a result of the inhomogeneity of $\mathbf{n}$ is given by[2] (the entire discussion that follows pertains to the planar case)

$$\delta F = \int dV (K_{11}(\mathrm{div}_2 \mathbf{n})^2 + K_{33}(\mathrm{rot}_2 \mathbf{n})^2), \tag{1}$$

where K_{11} and K_{33} are the standard symbols for the elastic moduli of the liquid crystal[1)] and div_2 and rot_2 are the two-dimensional divergence and curl, while integration is carried out over the volume of the liquid crystal (actually, over the plane of the vessel cross section).

The problem thus consists of finding the field $\mathbf{n}$ that minimizes the functional (1) under given boundary conditions, and for concreteness it is assumed that $\mathbf{n}$ is directed tangent to the boundary.

In order not to take into account the condition $\mathbf{n}^2 = 1$, we can introduce an angle φ such that $\mathbf{n} = \{\cos\varphi, \sin\varphi\}$. Substituting this in (1), we obtain

$$\begin{aligned}\delta F = \int dV \Big[&(K_{11}\sin^2\varphi + K_{33}\cos^2\varphi)\left(\frac{\partial\varphi}{\partial x}\right)^2 \\ &+ (K_{11}\cos^2\varphi + K_{33}\sin^2\varphi)\left(\frac{\partial\varphi}{\partial y}\right)^2 \\ &+ 2(K_{33}-K_{11})\sin\varphi\cos\varphi\frac{\partial\varphi}{\partial x}\frac{\partial\varphi}{\partial y}\Big].\end{aligned} \tag{2}$$

As is well known, the problem is greatly simplified if it is assumed that $K_{11} = K_{33}$. We first consider just this case. Then (2) is transformed into

$$\delta F = K\int dV(\nabla\varphi)^2, \tag{3}$$

where $K = K_{11} = K_{33}$.

Varying (3), we obtain an equation for φ

$$\Delta\varphi = 0. \tag{4}$$

This equation must be solved under the condition that on the boundary of the region we have

$$\varphi = \chi,$$

where χ is the angle between the tangent to the boundary and the x axis, specified on the boundary.

We note that φ need not be a unique function, and is defined accurate to $\varphi \to \varphi + m\pi$, where m is an integer (we recall that $\mathbf{n}$ and $-\mathbf{n}$ are indistinguishable). Therefore $\int \nabla\varphi\, dl$ along a certain contour does not vanish in general:

[1)] In accordance with the statements made above, these moduli are of the order of 10^{-8} dyne.

$$\oint \nabla\varphi\, dl = m\pi. \tag{5}$$

This means that the function φ can have branch points, and φ changes by $m\pi$ when these points are circled. Such points correspond to the so-called disclinations. The structure of the field n near a disclination was investigated (at $K_{11} = K_{33}$) by Frank[3] and is described by the equation $\varphi = m\vartheta/2 + \text{const}$, where ϑ is the polar angle (the disclination is the pole of the polar coordinate system). The number m is called the Frank index. Inasmuch as the boundary Γ of the region is a closed curve, we have

$$\oint_\Gamma \nabla\varphi\, dl = 2\pi,$$

on the other hand

$$\oint_\Gamma \nabla\varphi\, dl = \pi \sum_i m_i,$$

where m_i are the Frank indices of the disclinations, and the summation is carried out over all the disclinations. This indicates that the ground state of a liquid crystal bounded on all sides by vessel walls is a state with one or several disclinations, with $\sum_i m_i = 2$.

Therefore, in order to find the minimum of the functional (3), it is first necessary to specify the positions of the branch points (and also their types, i.e., the Frank indices), find the solution of (4), then substitute this solution in the functional (3) and calculate the free energy at the given arrangement of the disclinations, followed by determination of the disclination arrangement (and type) at which this energy is minimal.

In order to avoid difficulties connected with the nonuniqueness of φ, we can change over to the conjugate function f (such that $f \neq i\varphi$ is an analytic function). In the calculation of the energy we can use the fact that $(\nabla\varphi)^2 = (\nabla f)^2$. The boundary condition for the function f can be obtained from the Cauchy-Riemann conditions

$$\partial f/\partial n = \partial\varphi/\partial s = \varkappa(s). \tag{6}$$

Here n is the coordinate normal to the boundary and s is the coordinate along the boundary, so that κ is the curvature of the boundary. Near the disclination (with index m), f has a singularity $f = (1/2)m \ln r$, where r is the distance to the disclination. We can readily see from this that if the distances between the disclinations are small (compared with the dimension of the region), so that the influence of the boundary conditions can be neglected, then their interaction is the same as in two-dimensional electrostatics, where m plays the role of the charge[2]. Nonetheless, there is no formal identification with electrostatics, owing to the different type of boundary condition (6).

Let us consider the interaction of the disclinations with the boundary. At small distances, the boundary can be regarded as plane and we can put in (6) $\kappa = 0$. The resultant problem coincides with the problem of a point source of current in a conducting medium near a nonconducting boundary (the function φ plays the role of the current function). The solution can readily be obtained with the aid of the method of images, wherein the sign of the image source of current remains unchanged. If we change over to the function f and to the language of electrostatics, then from the fact that the image charges are of the same sign it follows that the disclination is repelled from the wall. In the case of a simple, geometry, say a circle, we easily obtain a solution in explicit form. Namely, in a circle of radius R the ground state of a liquid crystal corresponds to the presence of two disclinations with m = 1, repelled from each other and from the walls, so that the distance between them is $2R/\sqrt{5}$. The corresponding picture is shown in Fig. 1.

We consider now the situation when $K_{11} \neq K_{33}$. All the topological considerations whereby the disclinations must exist remain in force. On the other hand, the derivation of the explicit solutions is much more difficult. Direct variation of Eq. (2) leads to an unwieldy nonlinear equation for φ, which is difficult to solve in the two-dimensional case. (Even if we set one of the K, say K_{11}, equal to zero, we gain very little in the sense of simplifying the equation.)

There is, however, a method of obtaining simpler equations (which, under certain conditions, lead to solutions), by using a more convenient coordinate system. Namely, assume that we have the solution of our problem, i.e., we know the field n. We can then construct the "force lines" of this field. It is clear that the most convenient coordinate system would be a "natural" one (x^1, x^2) such that the lines $x^2 = \text{const}$ coincided with the "force lines" of the field n, and the lines $x^1 = \text{const}$ were perpendicular to them.

We write down first δF in an arbitrary curvilinear system of coordinates. It is convenient to introduce a unit vector m orthogonal to n. Then (1) can be written in the form

$$\delta F = \int [K_{11}(n_{,i}^{i})^2 + K_{33}(m_{,i}^{i})^2]\sqrt{g}\, dx^1\, dx^2. \tag{7}$$

(We took into account the fact that $\text{curl}_2\mathbf{n} = \text{div}_2\mathbf{m}$ and used tensor notation.)

Varying (7) and integrating by parts, we obtain

$$K_{11}n_{,ik}^{i}\delta n^k + K_{33}m_{,ik}^{i}\delta m^k = 0. \tag{8}$$

Here, however, δn^k and δm^k are not arbitrary but obey the relations

$$\mathbf{n}\delta\mathbf{n} = 0, \quad \mathbf{m}\delta\mathbf{m} = 0, \quad |\delta\mathbf{n}| = |\delta\mathbf{m}|. \tag{9}$$

Let us write down Eq. (8) in a "natural" system of coordinates. In this system

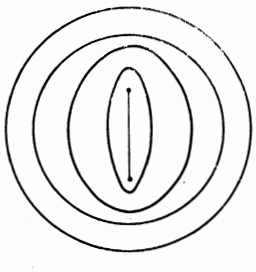

FIG. 1. Two disclinations with m = 1 in a circle, $K_{11} = K_{33}$.

[2]It can be proved that the time within which two disclinations with indices ~1 approach each other from a distance r until they "annihilate" is given, according to rough estimates, by $\tau = ar^2$, where $a \sim 10^6$ sec/cm^2. In experiments with liquid crystals, such an "annihilation" is actually observed.

$$n^1 = 1/\sqrt{g_{11}},\quad n^2 = 0,\quad m^1 = 0,\quad m^2 = 1/\sqrt{g_{22}},$$
$$\delta n^1 = 0,\quad \delta n^2 = |\delta \mathbf{n}|/\sqrt{g_{22}},\quad \delta m^1 = -|\delta \mathbf{n}|/\sqrt{g_{11}},\quad \delta m^2 = 0. \quad (10)$$

Using the known identity $A^i_{,i} = (1/\sqrt{g})(\partial(\sqrt{g}A^i)/\partial x^i)$, we obtain from (8), taking (10) into account

$$K_{11}\frac{1}{\sqrt{g_{22}}}\frac{\partial}{\partial x^2}\left(\frac{1}{\sqrt{g_{11}g_{22}}}\frac{\partial\sqrt{g_{22}}}{\partial x^1}\right) = K_{33}\frac{1}{\sqrt{g_{11}}}\frac{\partial}{\partial x^1}\left(\frac{1}{\sqrt{g_{11}g_{22}}}\frac{\partial\sqrt{g_{11}}}{\partial x^2}\right). \quad (11)$$

Equation (11), together with the equation P = 0, where P is the curvature tensor expressed in terms of g_{11} and g_{22}, constitutes a complete system, from which it is possible in principle to determine g_{11} and g_{22}, which in turn can be used to reconstruct the direction field.

We note, however, that the quantities $(1/\sqrt{g_{11}g_{22}})(\partial\sqrt{g_{22}}/\partial x^1)$ and $(1/\sqrt{g_{11}g_{22}})\cdot(\partial\sqrt{g_{11}}/\partial x^2)$ have a simple geometric meaning. Namely, it is easily seen from Fig. 2 that

$$\frac{1}{\sqrt{g_{11}g_{22}}}\frac{\partial\sqrt{g_{22}}}{\partial x^1} = \varkappa_2, \quad (12)$$

where κ_2 is the curvature of the line $x^1 = \text{const}$ ($\kappa_2 = (1/\sqrt{g_{22}})(\partial\varphi/\partial x^2)$. Analogously,

$$\frac{1}{\sqrt{g_{11}g_{22}}}\frac{\partial\sqrt{g_{11}}}{\partial x^2} = -\varkappa_1.$$

As a result we obtain from (11)

$$K_{11}\frac{1}{\sqrt{g_{22}}}\frac{\partial\varkappa_2}{\partial x^2} = -K_{33}\frac{1}{\sqrt{g_{11}}}\frac{\partial\varkappa_1}{\partial x^1}. \quad (13)$$

Let us consider the case $K_{11} = 0$. In this case we obtain from (13) that $\kappa_1 = \text{const}$ along the "force line" of the field n, i.e., these lines are circles (or straight lines). This result makes it possible in many cases to draw immediately the picture of the field, without solving any equations whatever. To calculate the free energy of the obtained solutions we can use the fact that the latter, as seen from (7), (10) and (12), can be written in the form

$$\delta F = \int K_{33}\varkappa_1^2 dS. \quad (14)$$

We present first the pictures of the disclinations (Fig. 3). These pictures correspond to the formulas obtained in[2] for $K_{11} = 0$. We note that the disclinations with m = 3, −1, −2, etc. have singular lines, near which it is possible to go over from one force line to another, with a different curvature. The conclusion given above is not valid here, since near these lines the coordinate system becomes degenerate. We present several examples illustrating the structure of a liquid crystal. We assume first that the boundary condition corresponds to n perpendicular to the boundary. Then for a square and a circle, in which there is a disclination with m = 2, we obtain the pictures shown in Figs. 4, 5, and 6. We note that the elastic energy for the case shown in Fig. 6 is equal to zero and is smaller than in the case shown in Fig. 5, corresponding to stability of the central position.

Figure 7 shows the structure in the presence of two disclinations with m = 1. When the two come closer together, the "force lines" straighten out and the energy decreases. Therefore the two disclinations in the circle merge. (Inclusion of small K_{11} makes the equilibrium distance between them small.)

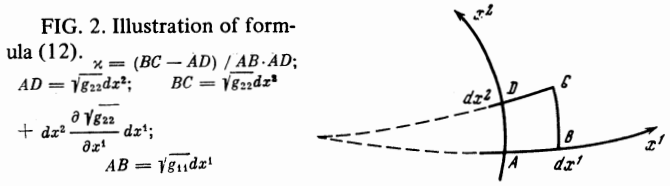

FIG. 2. Illustration of formula (12). $\varkappa = (BC - AD)/AB\cdot AD$; $AD = \sqrt{g_{22}}dx^2$; $BC = \sqrt{g_{22}}dx^2 + dx^2\frac{\partial\sqrt{g_{22}}}{\partial x^1}dx^1$; $AB = \sqrt{g_{11}}dx^1$

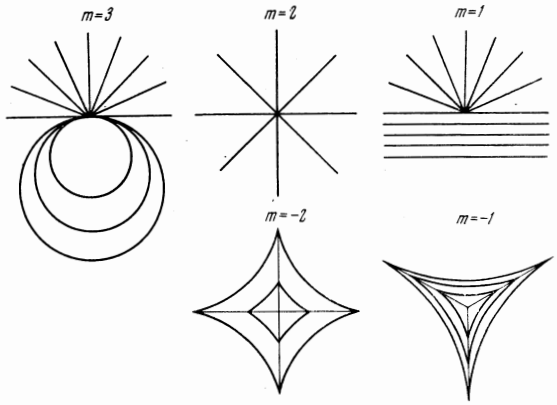

FIG. 3. Disclinations with different Frank indices for $K_{11} = 0$.

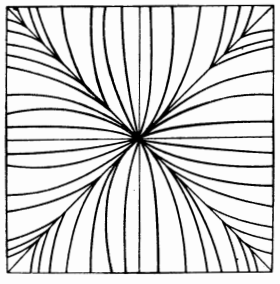

FIG. 4

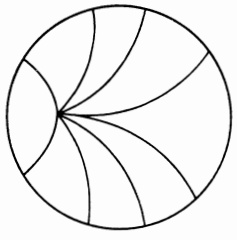

FIG. 5

FIG. 4. Disclinations with m = 2 in a quadratic region; n is perpendicular to the boundary, $K_{11} = 0$.

FIG. 5. Disclination with m = 2 in a circle; n is perpendicular to the boundary, $K_{11} = 0$.

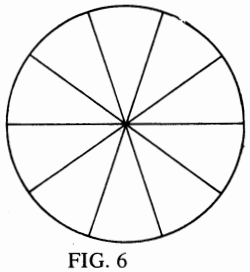

FIG. 6

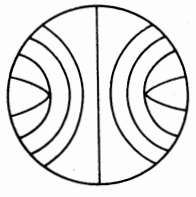

FIG. 7

FIG. 6. Disclination with m = 2 at the center of a circle; n is perpendicular to the boundary, $K_{11} = 0$.

FIG. 7. Two disclinations with m = 1 in a circle, n perpendicular to the boundary, $K_{11} = 0$.

Let us consider also several examples for the case when n is parallel to the boundary.

For a region in the form of a circle and a disclination with m = 2, the picture is shown in Fig. 8. A calculation of the energy as a function of the disclination position shows that the central position is stable.

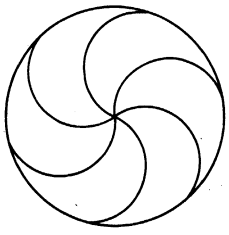

FIG. 8

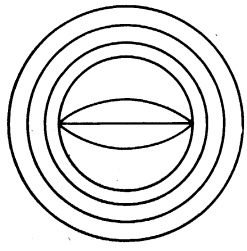

FIG. 9

FIG. 8. Disclination with m = 2 in a circle, n parallel to the boundary, $K_{11} = 0$.

FIG. 9. Two disclinations with m = 1 in a circle, n parallel to the boundary, $K_{11} = 0$.

Two disclinations with m = 1 are shown in Fig. 9. In this case the thermodynamic equilibrium corresponds to the position of both disclinations on the walls of the vessel. The number of examples of this type can easily be increased.

It turns out that the picture of the "force lines" near two close disclinations with m = 2 can be found in the general case when $K_{11} \neq K_{33}$. First of all, it is easy to show that when $K_{33} = 0$ the equilibrium configurations are such that the lines orthogonal to the "force lines" of the field n are arcs of circles.

At $K_{11} = K_{33}$ the picture of the lines near two disclinations with m = 2 corresponds to the picture of force lines and equipotential lines of two identical

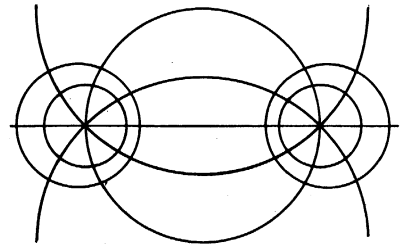

FIG. 10. Field structure near two disclinations with m = 2; K_{11} and K_{33} are arbitrary.

charges (Fig. 10). As is well known, both these families are circles. But this means that this picture remains in force both when $K_{11} = 0$ and when $K_{33} = 0$, i.e., it corresponds to a minimum of each of the terms in expression (1). But then it corresponds to a minimum of the functional (1) for arbitrary K_{11} and K_{33}.

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