Disclination symmetry in uniaxial and biaxial nematic liquid crystals

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Attention is drawn to the fact that, in general, the topological classification of linear singularities in nematic crystals gives incomplete information about the distribution of the order parameter. The symmetry of the director distribution in uniaxial nematics, or the triad of orthogonal unit vectors in biaxial nematics, also plays an important role. The symmetry groups of the distribution of the order parameter in the presence of disclinations are discussed. Possible phase transitions between the states of the liquid crystal, differing by disclination symmetry alone, are examined.

I. INTRODUCTION

Homotopic methods of investigation of disclinations in nematic crystals, and of other structural defects in condensed media,[1] have led to a simplification of the classification of these defects (see, for example, reviews.[2,3]) The entire set of defects turns out to be divided into classes with different topological indices. Thus, disclinations in the ordinary uniaxial nematic crystal form two topological classes with topological indices $N = 0$ and $N = 1$ and defect composition law

$$1+1=0, \quad 1+0=1. \tag{1}$$

Defects in one class can be continuously transformed into one another, whereas transitions between defects belonging to different classes involve considerable losses in producing a discontinuity in the order-parameter field, which necessarily arises in this process.

However, the topological classification is often too general and does not exhibit much of the detail of the distribution of the order parameter in the presence of defects. Thus, theoretical and experimental studies of vortex lines in superfluid He^3 have shown that a vortex belonging to a given topological class can exist in different states. In the B phase of He^3, a first-order phase transition is observed between different states,[4] but the properties of He^3-B itself do not change at the transition point. The states of the vortex differ by their symmetry[5] and by the physical properties of the vortex determined by this symmetry.[6,7]

Thus, the topological classification of defects must be augmented by the symmetry classification of the states of the defect that are possible within a given topological class. The symmetry classification of defects, i.e., essentially inhomogeneous states of the order parameter of an ordered medium, must differ from the usual classification based on the symmetry of ordered media themselves. In particular, the difference consists in the following. To enumerate the classes of ordered media, it is suffcient to find all the possible symmetry groups of the system, i.e., all the subgroups H of the general symmetry group G of its physical laws. For example, to enumerate all the possible crystal or liquid-crystal states, it is sufficient to find all the subgroups of the Euclidean group.

On the other hand, when the symmetry classification of defects is introduced, it is important in addition to take into account the fact that a given symmetry leads, in general, to a restriction on the range of variation of the order parameter, i.e., to a change in topology and hence to the appearance of new topological indices imposed by the symmetry.

Let us illustrate this point by considering the simple case of disclinations in a nematic crystal. When, for example, a symmetry plane perpendicular to the disclination line is given, the distribution of the order parameter (in this case, of the director $\mathbf{d}$) should be planar. As a result, we have a new symmetry-imposed topological invariant, namely, the disclination index m (the so-called Frank index), which is the index of a planar vector field (see Sec. II for further details).

Thus, the symmetry and topological factors are interrelated. Disclination states with different symmetry are possible within each topological class, and different subclasses are possible within given symmetry.

In this paper we shall illustrate the defect classification principle by considering the example of linear disclinations in uniaxial and biaxial nematic crystals. This classification predicts the existence of different disclination states between which (as also in superfluid He^3 phases) first-order phase transitions are possible on change of temperature and pressure, and are not accompanied by changes in the properties of the nematic crystal itself. Such transitions can be revealed, for example, by a discontinuous change in the optical properties of a given liquid crystal texture (see Sec. IV for further details).

II. DISCLINATIONS IN A UNIAXIAL NEMATIC CRYSTAL. STATES WITH MAXIMUM SYMMETRY

Consider a rectilinear disclination in a uniaxial nematic liquid crystal with order parameter

$$Q_{\alpha\beta}=\sqrt{3/2}\,s\,(d_\alpha d_\beta-1/3\,\delta_{\alpha\beta}) \tag{2}$$

specified by the director $\mathbf{d}(\mathbf{r})$ (s is the modulus of the order parameter). The Euclidean group defining the symmetry of this liquid crystal consists of rotations $O\,\mathbf{d}\equiv O\,\mathbf{d}(O\mathbf{r})$, inversion $I\,\mathbf{d}\equiv\mathbf{d}(-\mathbf{r})$, and translations $T\,\mathbf{d}\equiv\mathbf{d}(\mathbf{r}+\mathbf{a})$ ($\mathbf{a}$ is an arbitrary vector). This group reduces to the space subgroup consisting of translations T_z along the disclination line and the elements of the point group $D_{\infty h}$ containing all rotations around the disclination line, rotations of π around twofold

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axes perpendicular to this line, and inversion. For simplicity, we shall confine our attention to disclinations whose structure does not depend on the position coordinate along their axis. The classification of disclinations then reduces to the enumeration of the symmetry group, i.e., the subgroups of the group $D_{\infty h}$: D_∞, $C_{\infty h}$, $C_{\infty v}$, C_∞, D_{nd}, D_{nh}, D_n, C_{nh}, C_{nv}, C_n, S_{2n} (we are using the notation of Ref. 8), and to the enumeration of the topological subclasses within a given symmetry group.

Although this enumeration is straightforward, it is laborious and contains very little physical information. We shall therefore base our classification on the principle of maximum symmetry. By states with maximum symmetry, we shall understand states whose symmetry cannot be continuously increased without changing the topological subindex. It is clear that states with maximum symmetry are always the extrema of the free-energy functional F. This distinguishes them from states with lower symmetry. The latter become extrema only in definite ranges of the parameters of the energy functional that are bounded by the so-called catastrophe surface.[9] It is therefore more natural to begin by considering states with maximum symmetry for which there are always solutions of the Euler-Lagrange equations resulting from the minimization of the functional F. It is only then, and if these solutions turn out to be stable, i.e., correspond to saddles of the energy functional, that we must investigate states with lower symmetry. This procedure corresponds to the Landau scheme for second-order phase transitions.

Detailed direct analysis of all the symmetry subgroups of the group $D_{\infty h}$ shows that maximum symmetry states occur only for the groups D_{nh} with a symmetry plane perpendicular to the disclination line. We therefore begin with the groups D_{nh}.

To find the topological subclasses, let us consider the distribution of the director **d** on an arbitrary circle coaxial with the disclination (symmetry D_{nh}) and lying in the $z = 0$ plane. At each of the $2n$ points of intersection of this circle with the n perpendicular twofold symmetry axes, the director **d** must be invariant under rotations around the corresponding axis. Moreover, **d** must be symmetric with respect to the $z = 0$ plane. This means that, at these points, the director **d** can lie only along the following three directions:

I—along the z axis
II—along the radius of the circle
III—along a tangent to the circle.

For the purposes of our classification, it is sufficient to know the distribution of the director on an arc π/n joining two neighboring symmetry points on the circle, since the remaining distribution is obtained by applying the symmetry transformations in the group D_{nh} under consideration.

The director distributions on this arc form homotopic subclasses characterized by nonhomotopic paths connecting points I, II, and III in the space of states in different ways. The enumeration of these subclasses presents no difficulty since, apart from the I→I subclass (class of mutually homotopic paths connecting a point I to a point I), where **d** is parallel to the z axis, the director can vary only along the circle in all the remaining cases. There are only five such distinct subclasses:

$$1)\ \mathrm{I}\to\mathrm{I};\quad 2)\ \mathrm{II}\to\mathrm{II}(\pi/n+k\pi);\quad 3)\ \mathrm{III}\to\mathrm{III}(\pi/n+k\pi);$$
$$4)\ \mathrm{II}\to\mathrm{III}(\pi/n+\pi/2+k\pi);\quad 5)\ \mathrm{III}\to\mathrm{II}(\pi/n+\pi/2+k\pi). \tag{3}$$

The quantities in parentheses indicate the angle through which the vector **d** rotates between neighboring invariant points (k is an integer).

The first subclass corresponds to the homogeneous state (**d** parallel to the z axis), i.e., it belongs to the higher symmetry group $D_{\infty h}$.

In disclinations belonging to the second and third subclasses, the director **d** changes by $2\pi + 2nk\pi$ when the entire circle is traversed, i.e., the disclination index $m = 1 + nk$ is always an integer. It follows that these disclinations belong to the trivial homotopic class $N = 0$ for any n and k.

For disclinations in the fourth and fifth subclasses, which are equivalent since they are obtained by redesignation of the axes, the disinclination index is given by

$$m=1+nk+n/2. \tag{4}$$

These disclinations therefore correspond to the $N = 0$ class for even n and the homotopic class $N = 1$ for odd n.

We must now determine which of the above states are maximum-symmetry states, i.e., which of the groups D_{nh} cannot be continuously extended to a higher symmetry group without changing m.

It is readily seen that there are the following states with maximum symmetry: homogeneous state $m = 0$, $D_{\infty h}$; disclination with radial director distribution $m = 1$, $D_\infty^{(1)}$; disclination with tangential director distribution $m = 1$, $D_{\infty h}^{(2)}$ (the indices 1 and 2 are used to distinguish between these two types of disclination); $m = 1 - n/2$ $(n \neq 2)$, D_{nh}; $m = 1 + n/2$, D_{nh}. Figure 1 shows some distributions of the director around the disclination lines that have maximum symmetry. These disclinations can be distributed as follows over two homotopic classes of the subgroup $\pi_1(RP_2) = Z_2$ that describes linear defects in uniaxial nematic liquid crystals.

The trivial class $N = 0$ (topologically removable disclinations) includes the following maximal director distribution groups: $m = 0$, $D_{\infty h}$; $m = 1$, $D_{\infty h}^{(1)}$, $m = 1$, $D_{\infty h}^{(2)}$, $m \neq 0.1$, $D_{|2-2m|h}$. The nontrivial class $N = 1$ (disclinations that cannot be topologically removed) contains maximal groups, with m equal to a half-integer, and the symmetry group $D_{|2-2m|h}$. Of course, depending on the specific form of the free-energy functional F, not all these maximum-symme-

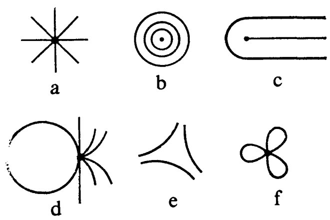

FIG. 1. Distribution of the director around maximum-symmetry disclination lines: a—$m = 1$; $D_{\infty h}^{(1)}$, b—$m = 1$; $D_{\infty h}^{(2)}$; c—$m = \frac{1}{2}$; D_{1h}, d—$m = \frac{3}{2}$; D_{1h}, e—$m = -\frac{1}{2}$; D_{3h}, f—$m = \frac{5}{2}$ D_{3h}.

try groups give stable director distributions. For example, Dzyaloshinskiĭ and Anisimov,[10] who have investigated the Frank energy functional for similar values of the elastic moduli, have shown that the planar disclination with $m = \pm\frac{1}{2}$ is unstable for $K_{22} < \frac{1}{2}(K_{11} + K_{33})$. The planar disclination with $m = 1$ is unstable when $K_{22} < 2K_{33}$ or $K_{33} < K_{11}$. Finally, all planar disclinations with high indices are definitely unstable for $K_{33} \gg K_{11}$, K_{22}. It is precisely this relationship between the Frank elastic moduli that obtains in classical nematic liquid crystals such as MBBA and PAA. However, many new systems have appeared in recent years,[11] in which this inequality may not be satisfied. Nematic liquid crystals formed in systems consisting of disk-shaped molecules[12] are promising in this respect.

Thus, when the conditions are favorable and the planar distribution of the director is stable, nontrivial disclinations have the maximum-symmetry group $D_{|2-2m|h}$, where m is a half-integer. Disclinations with different indices m can then have the same maximum-symmetry group. For example, the distributions of the director around the disclinations with $m = 1/2$ and $m = 3/2$ have the group D_{1h}, whereas the distributions around disclinations with $m = 5/2$ and $m = -1/2$ have the group D_{3h}. Phase transitions are possible, in principle, between these competing states when the temperature, pressure, or some other external parameter (for example, concentration in a mixture) is varied. These transitions should be of second order because they occur without a reduction or increase in symmetry.

The $N = 1$ class may also contain transitions between distributions of different symmetry. For example, from the state D_{3h} $(m = -\frac{1}{2})$ to the state D_{1h} $(m = \frac{1}{2})$.

Let us now examine the possible phase transitions associated with a change in the D_{3h} symmetry of a disclination within the framework of the Landau theory. This group[8] has four one-dimensional irreducible representations (we shall denote them by 1, u, v, and w) and two two-dimensional representations $(\psi, \tilde{\psi})$. The group D_{3h} can be written in the form of the direct product $D_{3h} = D_3 \times \sigma_h$ and, relative to action of the horizontal reflection plane σ_h we have (using the notation of Ref. 8),

$$\sigma_h u = u, \quad \sigma_h v = -v, \quad \sigma_h w = -w, \quad \sigma_h \psi = \psi, \quad \sigma_h \tilde{\psi} = -\tilde{\psi}.$$

It is readily seen that all the possible D_{3h} symmetry breakings are described by five parameters that are conveniently taken to be u, v, w and ψ. The remaining elements of D_{3h} $(C_3, C_3^2, U_2, U_2C_3, U_2C_3^2)$ operate on these parameters as follows:

$$C_3\psi = \exp(2\pi i/3)\psi, \quad C_3^2\psi = \exp(-2\pi i/3)\psi,$$
$$U_2\psi = \psi, \quad C_3 u = C_3^2 u = u, \quad U_2 u = -u, \quad C_3 v = C_3^2 v = v,$$
$$U_2 v = v, \quad C_3 w = C_3^2 w = w, \quad U_2 w = -w.$$

The free-energy functional that is invariant under D_{3h} depends on the following sixteen invariant combinations of the five parameters, of degree not higher than four;

$$u^2,\ v^2,\ w^2,\ u^4,\ v^4,\ w^4,\ u^2v^2,\ v^2w^2,\ w^2u^2,\ uvw,$$
$$|\psi|^2,\ \psi^3 + (\psi^*)^3,\ |\psi|^4,$$
$$u^2|\psi|^2,\ v^2|\psi|^2,\ w^2|\psi|^2.$$

One can also establish directly which nonzero parameters [out of the u, v, w, ψ] remain nonzero in the subgroups of D_{3h}:

$$D_3 - v,\ C_{3h} - u,\ C_{3v} - w,\ C_3 - u, v, w,$$
$$D_{1h} - \psi,\ U_2 - v, \psi,\ \sigma_h - u, \psi,$$
$$U_2\sigma_h - w, \psi,\ E - u, v, w, \psi.$$

Thus, the $D_{3h} \to D_{1h}$ transition is connected with the parameter ψ ($\psi \neq 0$ in a disclination with D_{1h} symmetry and $\psi = 0$ in a disclination with D_{3h} symmetry). This is a first-order phase transition because the Landau expansion for the free energy contains only the third-order terms $\psi^3 + \psi^{*3}$.

Other transitions can be described in an analogous manner.

Finally, for $K_{33} \gg K_{11}$, K_{22}, when planar disclinations are unstable, we must consider symmetry groups with non-planar director distribution. We need not then consider the low symmetry groups C_n, S_{2n}, I, E since, as the symmetry of the director distribution is lowered, the information that can be obtained from our analysis is also decreased. We shall therefore confine our attention to the groups D_{nd}, C_{nv}, D_n.

As before, it will be sufficient for the classification of states to know the distribution of the director on the arc π/n of a circle drawn around the disclination line. The only difference from the preceding analysis is that now we do not have the horizontal symmetry plane σ_h so that, without breaking the symmetry of the director distribution, we can rotate the director **d** in the vertical plane. Moreover, it must be remembered that, from the point of view of the degeneracy space RP_2 of the order parameter of the nematic crystal, the effect of a twofold symmetry axis (for example, the x axis) is equivalent to mirror symmetry relative to the yz plane. Consequently, the effect of D_n is obtained from C_{nv} by rotating through 90°, and it is sufficient to consider C_{nv} and D_{nd}.

It is readily verified that all distributions with the D_{nd} symmetry belong to the trivial topological class $N = 0$. On the other hand, distributions with the C_{nv} symmetry can be divided into two subclasses:

$$\mathrm{I} \to \mathrm{I}, \quad \mathrm{I} \to \mathrm{III}$$

where the director orientation of type II along the radius of the circle can be transformed into I without symmetry breaking. The subclass I→I always belongs to the trivial homotopic class $N = 0$, and the subclass I→III has $N = 0$ for even n and $N = 1$ for odd n.

As noted above, an analogous classification can be introduced when the distribution has the D_n symmetry. Thus, for odd n (i.e., for topologically stable disclinations) we have a possible competition between director distributions with C_{nv} and D_n symmetries, between which phase transitions are possible as the external parameters are varied (see Section IV for further details).

III. DISCLINATIONS IN A BIAXIAL NEMATIC LIQUID CRYSTAL

Biaxial nematic liquid crystals were discovered quite recently.[13] The order parameter in such cases is a tensor of rank two, of more general form than the uniaxial tensor (2) set by the director. It is convenient to parametrize it with aid of a triad of unit vectors $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ and some angle φ that specifies the degree of biaxiality of the tensor:

$$Q_{\alpha\beta}=\sqrt{2/3}\,s\,[e_{1\alpha}e_{1\beta}\cos(\varphi-\pi/3)+e_{2\alpha}e_{2\beta}\cos(\varphi+\pi/3)-e_{3\alpha}e_{3\beta}\cos\varphi], \qquad (5)$$

where $\sqrt{2/3}$ is a normalizing factor. It is readily seen that the tensor $Q_{\alpha\beta}$ in (5) is symmetric and $\mathrm{Sp}Q_{\alpha\beta}=0$.

When the angle φ is a multiple of $\pi/3$, the tensor $Q_{\alpha\beta}$ has uniaxial symmetry. For example, when $\varphi=\pi/3$, the tensor $Q_{\alpha\beta}$ is obtained directly from (2).

The tensor $Q_{\alpha\beta}$ can also be specified by its invariants:

$$I_2=\mathrm{Sp}\,Q_{\alpha\beta}{}^2=s^2,\quad I_3=\mathrm{Sp}\,Q_{\alpha\beta}{}^3=-6^{-1/2}s^3\cos 3\varphi. \qquad (6)$$

If we are in some equilibrium state, the tensor $Q_{\alpha\beta}$ will be defined in this state, and the values of temperature, pressure, and other parameters will determine I_2 and I_3.

Thus, in mathematical terms, we must find all the equivalent mappings of the space R^3 onto the space M of symmetric 3×3 matrices (for which $\mathrm{Sp}Q_{\alpha\beta}=0$, $\mathrm{Sp}Q^2_{\alpha\beta}=\mathrm{const}$ and $\mathrm{Sp}Q^3_{\alpha\beta}=\mathrm{const}$ under the action of the groups D_n, C_{nv}, D_{nd}, and D_{nh}). It is readily verified that it is sufficient to solve the problem for the mapping of a circle $S^1\to M$, since the continuation to R^3 occurs in the same way as in the problem of uniaxial nematic crystals, which was solved in the last section (where we required a description to within the invariant homotopic equivalence of the mapping of S^1 onto RP_2 under the action of the groups D_n, C_{nv}, D_{nd}, and D_{nh}).

It is well known[1-3] that the linear singularities of biaxial nematic crystals are determined by the group $\pi_1=Q$, where Q is the group of quaternion units. The topological index for the five different homotopic classes will also be denoted by the letter Q which can assume the following values:

$$Q=1,\quad Q=-1,\quad Q=(i,-i),\quad Q=(j,-j),\quad Q=(k,-k)$$

with the multiplication rules

$$(-1)^2=1,\quad i^2=j^2=k^2=-1,\quad ij=-ji=k. \qquad (7)$$

It is clear from the foregoing that the only difference from the uniaxial nematic crystal is that we must consider the triad $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ instead of the single unit vector $\mathbf{n}$. However, for the purposes of our classification, it is sufficient to solve only the plane problem, each time examining only the variation of one of the vectors $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ on the arc π/n. Accordingly, we shall use m_i as the disclination index that describes the orientation variation during rotation around $\mathbf{e}_i$.

As in the last section, we begin with the maximal subgroups. We take a homogeneous state with $m=0$ and D_{2h} symmetry. Next, for each of the vectors $\mathbf{e}_i$ there exist planar distributions in which the other two vectors of the triad are oriented along the radius or a tangent to the circle drawn around the disinclination line. The symmetry of these distributions is $D_{\infty h}$ and six types of such disclination may be present in a biaxial nematic crystal, namely, ($\mathbf{e}_1=\hat{\mathbf{r}}$; $\mathbf{e}_2=\hat{\boldsymbol{\varphi}}$), ($\mathbf{e}_1=\hat{\boldsymbol{\varphi}}$; $\mathbf{e}_2=\hat{\mathbf{r}}$), ($\mathbf{e}_3=\hat{\mathbf{r}}$; $\mathbf{e}_1=\hat{\boldsymbol{\varphi}}$), and so on, where $\hat{\boldsymbol{\varphi}}$ and $\hat{\mathbf{r}}$ are unit vectors along the tangent and the radius of the circle, respectively. Finally, we have the possible symmetry groups D_{nh}, where $m_i=1+n/2$ or $m_i=1-n/2$ ($n\neq 2$), each of which provides three cases for analogous reasons. To distribute these symmetry groups of the triad distributions among the topological classes (7) of the quaternion group, we need only find the angle through which any of the vectors in the triad is rotated as the complete circle is traced. The class $Q=1$ corresponds to rotation by 4π, the class $Q=-1$ corresponds to rotation by 2π, and any of the classes $(i,-i)$, $(j,-j)$, $(k,-k)$ corresponds to rotation by π. We thus obtain the following results. The trivial class Q_1 includes the following maximum-symmetry groups: D_{2h} with $m=0$, D_{nh} with $m_i=1+n/2$ (m_i even; three groups), and D_{nh} with $m_i=1-n/2$, where $m_i\neq 0$ is even (three groups).

The class $Q=-1$ includes six $D_{\infty h}$ groups with odd m_i. Finally, the classes $(i,-i)$, $(j,-j)$, $(k,-k)$ correspond to D_{nh} with half-integer m_1, m_2, or m_3.

If, for some energy reasons, the planar distributions with maximum-symmetry group are unstable, it is best to consider less symmetric (but still quite ample) symmetry groups D_{nd}, C_{nv}, and D_n, just as in the case of uniaxial nematic crystals. We shall use the letters A, B, C to denote the liquid-crystal states with vector $\mathbf{e}_1$, $\mathbf{e}_2$, or $\mathbf{e}_3$ tangential to the circle, and the letters A', B', C' to denote states obtained from A, B, C by rotation around a twofold axis (or by reflection in the vertical plane).

Thus, we find that there are the following nine subclasses for all the groups that we have considered: $A\to A$; $A\to A'$; $A\to B$ (and six additional subclasses obtained by permuting the letters A, B, and C). The first and second letters in the designation of a subclass correspond to the orientation of one of the vectors in the triad at the edges of the arc π/n.

Direct examination of the possible distributions shows that D_{nd} contains states $A\to A$ and $A\to A'$ with topological index $Q=1$ and the state $A\to B$ with $Q=-1$. (Of course, states obtained from these by permuting the letters A, B, and C will also belong to D_{nd}).

In C_{nv}, the $A\to A$ states have $Q=-1$ and the $A\to A'$ states have $Q=(-1)^n$, while the $A\to B$ states belong to the homotopic class $(i,-i)$ [and, correspondingly, $B\to C$ and $C\to A$ belong to $(j,-j)$ and $(k,-k)$].

In precisely the same way, and for the reasons noted above (Sec. II), the same classification can be introduced for the group D_n as well.

It is important to note that the $A\to A$ state with $Q=-1$ and the $A\to A'$ state with the same topological index (for odd n) can be extended to the higher D_{nd} symmetry (states $A\to B$ with $Q=-1$), but this extension does not take us outside the limits of the homotopic class $Q=-1$.

As above, structural phase transitions are possible within a given topological class. For example, for $Q=-1$, we have competition between disclinations with D_{nd}, C_{nv} ($A\to A$), and C_{nv} ($A\to A'$ for odd n) symmetries. For the classes $(i,-i)$, $(j,-j)$, $(k,-k)$, disclinations with C_{nv} and D_n symmetries are found to compete. Phase transitions between these disclination structures are possible in principle as the external parameters are varied.

IV. CONCLUSION

We shall now summarize the results of our symmetry analysis of disclinations.

We have shown for uniaxial nematic crystals that, for nontrivial topologically stable disclinations (i.e., $N=1$), the maximum symmetry groups of the director distribution are $D_{|2-2m|h}$, where m is a half-integer. This symmetry (for any half-integer m) cannot be increased without changing the topological index $N=1$). This extension of symmetry can only be achieved by overcoming a large energy barrier proportional to the area of the surface that rests on the disclination and on which nematic order has to be removed.

Next, lower-symmetry disclinations are possible when these planar distributions are unstable for energy reasons. The D_{nd} symmetry then always leads to the trivial homotopic class $N=0$, but nontrivial disclinations ($N=1$) with the C_{nv} or D_n symmetry are present for odd n.

Similarly, in biaxial nematic crystals, the classification of disclinations can be based on the indices Q of the quaternion group and the indices n_i which can be integers (even or odd) or half-integers. So far, we have always spoken of complete symmetry of the order-parameter distribution in the entire space surrounding a disclination. However, as was first noted by Lyuksyutov,[14] the order parameter is degenerate on the sphere S^4 at distances smaller than $R_c \sim (K/Bs^3)^{1/2}$ (K is the Frank modulus and B is the coefficient of $\mathrm{Sp}Q^3_{\alpha\beta}$ in the Landau expansion), and since $\pi_1(S^4)=0$, there are no topologically stable defects at all in the region $R<R_c$. For most ordinary nematic crystals,[11] we have $R_c \sim 10^{-7}$–10^{-6} cm, and the $R<R_c$ region is unimportant in the order-parameter distribution. We have therefore ignored structures differing by the type of this disclination outflow within the core. We note that, in contrast to our case, it is precisely transitions within the vortex core that were detected experimentally and studied theoretically in the case of the B phase of He^3.

In principle, liquid crystals are possible in which this disclination outflow region is much greater. For example, strictly speaking, R_c will at any rate diverge in the region of the transition from the uniaxial to the biaxial liquid crystal. In such disclinations with a wide core, the question of the type of disclination outflow is legitimate. We shall not consider this in detail here and will examine only some energy questions. The potential energy that must be overcome by the disclination outflow (and is, in fact, overcome by gradient energy) is determined by the Landau expansion in terms of the order parameter (5):

$$V(\varphi)=b\cos 3\varphi+c\cos^2 3\varphi, \tag{8}$$

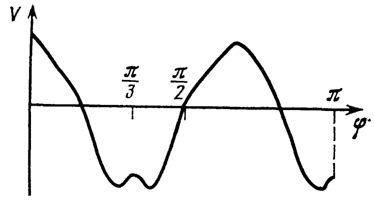

FIG. 2. Disclination outflow potential.

where b and c are related to the coefficients of $\mathrm{Sp}Q^3_{\alpha\beta}$ and $(\mathrm{Sp}Q^3_{\alpha\beta})^2$ in the Landau expansion.

The angle φ defines the latitude on the sphere from which the disclination outflow takes place. The function $V(\varphi)$ is shown in Fig. 2. As already noted in Sec. III, $\varphi=\pi/3$ in a uniaxial nematic crystal and the disclination outflow takes place toward the northern pole of the sphere $\varphi=0$. In biaxial nematic crystals, the angle φ is arbitrary. In the case of outflow at angles in the range $\pi/3<\varphi<\pi/2$ through the north pole of the sphere, we necessarily pass through the latitude $\varphi=\pi/3$, i.e., through the disclination structure of the uniaxial nematic crystal.

Finally, consider the possible experimental detection of first-order phase transitions between different disclination structures. A change in the order parameter is accompanied by a change in the optical characteristics (in particular, the transmission coefficient) of a liquid-crystal layer. The phase transition is in fact revealed by the rapid variation of these characteristics. We are thus able in principle to detect the structure of defects by observing the variation of the optical characteristics as functions of the wavelength and of the experimental geometry.

Other physical properties of disclinations may describe transitions in directly. For example, since the distribution of the order parameter is inhomogeneous in the presence of disclinations, the so-called flexoelectric effect[16] leads necessarily to dielectric polarization which, in turn, produces a charge on the disclination core. The value of this charge is determined by the integral of the flexoelectric dipole moment over the surface surrounding the disinclination. In principle this change can be determined, for example, by measuring the current transported by the disclinations, or simply by examining effect proportional to the first power of the electric field $\mathbf{E}$ (since the interaction between $\mathbf{E}$ and the director $\mathbf{d}$ is unrelated to the charge of the disclination core and is proportional to E^2). This charge depends in turn on the structure of the disclination and varies in the course of a phase transition between different structures.

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