Defects in liquid crystals: homotopy theory and experimental studies

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The fundamental concepts of the homotopy theory of defects in liquid crystals and the results of experimental studies in this field are presented. The concepts of degeneracy space, homotopy groups, and topological charge, which are used for classifying the topologically stable inhomogeneous distributions in different liquid-crystalline phases are examined (uni and biaxial nematics, cholesterics, smectics, and columnar phases). Experimental data are given for the different mesophases on the structure and properties of dislocations, disclinations, point defects in the volume (hedgehogs) and on the surface of the medium (boojums), monopoles, domain formations, and solitons. Special attention is paid to the results of studies of defects in closed volumes (spherical drops, cylindrical capillaries), and to the connection between the topological charges of these defects and the character of the orientation of the molecules of the liquid crystal at the surface. A set of fundamentally new effects that can occur in studying the topological properties of defects in liquid crystals is discussed.

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1. INTRODUCTION

The physics of defects of order is traditionally one of the most important fields of the physics of condensed media. This is explained by the importance of the role of defects in the course of different processes (phase transitions, plastic deformations, electronic processes, etc.). Defects in liquid crystals (LCs) are no exception in this respect, as they affect the manifestation of a number of optical, field, hydrodynamic, and other effects.

The variety of inhomogeneous distributions in LCs is extremely large. Here one can observe singular and nonsingular features, linear (dislocations, disclinations) and point defects (in the bulk: hedgehogs, and at the surface: boojums), monopoles and solitons, and domain walls. Their nature is closely connected with the character of the ordering of the LC. Hence it is not surprising that historically the deciphering of the structure of the fundamental types of LCs was based on the polarizing-microscope study of structural defects[1]; in individual cases such an approach is even more informative than x-ray diffraction.[2,3] Defects in LCs attracted especial attention in the '70s, when sufficient experimental material had been amassed for generalizations, and it turned out that the standard theoretical methods (like the Volterra process) clearly do not suffice—irresolvable paradoxes arise.[4] Also the problem of classification of defects proved extremely complex for the traditional methods in another class of condensed media, namely, the superfluid anisotropic "liquid-crystalline" phases of helium-3 discovered in 1972.

As was first systematically shown by Volovik and Mineev[5–7] and by Toulouse, Kléman, and Michel,[8–10] an adequate description of defects in liquid crystals and in other condensed media requires introducing a new mathematical apparatus. The theme here is topology, or more exactly, homotopy theory.[1)]

Precisely in the language of topology it became possible for the first time to associate the character of the ordering of a medium and the types of defects arising in it, to solve the problems of the structure of the defects, their stability with respect to relaxation to a homogeneous state, of the laws of decay and merger, and of behavior in phase transitions and under the action of external fields. The key point in this approach is occupied by the concept of topological charge, which is inherent in every defect. The stability of the latter is guaranteed by the conservation of its topological charge. The laws of conservation of such charges, analogously to the

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laws of conservation of electric and other physical charges, regulate the decay and merger of defects, their creation, annihilation, and mutual transformation.

The topological methods are being intensively applied at present in the most varied fields of the physics of inhomogeneous distributions: in field theory, biophysics, astrophysics, in studying superfluid liquids, magnetics, glasses, liquid crystals, and other media. However, among all the listed fields, a detailed experimental study of ordering defects is currently possible mainly only for LCs. On the one hand, this enables one to test experimentally the key tenets of topological theory applicable in physics as a whole and to pose new problems for it, and on the other hand, to use defects in LCs as models in studying other, less accessible media or fields. In particular, studying the effect of nonseparation of disclinations in biaxial nematics[14] can facilitate solving the problem of confinement of quarks in hadrons; monopole structures in LCs[15] make it possible to model the properties of magnetic monopoles; there is much in common between the processes of slipping of phase with participation of defects in nematics and the non-steady-state Josephson effect.[16] The importance of the study of defects in LCs also for understanding processes in biosystems is indubitable.[17]

We should consider the theory of defects in LCs based on the topological approach to be a science already established on the whole. A number of review[18–28] and popular[29,30] articles have been devoted to it. Despite the quantitative growth of the experimental studies, the individual results of which are presented in the well known monographs of Refs. 31–37, they as yet encompass far from all the interesting and fundamental questions (the existence and properties of solitons in LCs, chaining of disclinations, the defect structure of the blue phase, the transformations of defects of differing symmetry into one another, etc.).

Major attention is paid in this review to the connection between the topological transformations and the experimentally observable structural properties of defects in LCs. Section 2 describes the general principles of classification of defects as well as the fundamental methods of studying them experimentally. Further on, defects for different media are discussed, namely, Section 3 discusses uniaxial nematic LCs (NLCs), Section 4 discusses biaxial NLCs, Section 5—cholesteric LCs (CLCs), Section 6—smectic LCs of A- and C-types (SLC-A, SLC-C), and Sec. 7—columnar (nonsmectic) hexagonal LCs.

2. GENERAL CONCEPTS OF TOPOLOGICAL DEFECTS

2.1. Homotopy classification

The key concepts for classifying ordering defects are the order parameter, the degeneracy space of the order parameter, the homotopy groups of the degeneracy space, and finally, the topological charge of a defect. The first two actually describe the structure of the medium itself and the character of its order. Thus, the order parameter can be defined as a field (scalar, vector, tensor) fixed at each point of the system and describing its state at this point. The region of possible values of the order parameter that do not alter the thermodynamic potentials of the system is called the degeneracy space.[6]

In the general case the order parameter is a function of the coordinates and maps the points of real space occupied by the medium into the degeneracy space $\mathscr{R}$. If the value of the order parameter is the same at all points of the medium (corresponds to one point of the space $\mathscr{R}$), then the medium contains no disturbances of order and is called homogeneous. But inhomogeneous distributions of the order parameter can be of two types: those containing singularities and those without them. For a three-dimensional medium the singular regions are either zero-dimensional (points) or one-dimensional (lines) or two-dimensional (walls). These are the defects. Whenever a defect cannot be eliminated by continuous variations of the order parameter (i.e., one cannot arrive at the homogeneous state), it is called topologically stable, or simply a topological defect. But if the inhomogeneous state does not contain singularities, but nevertheless is not deformable continuously into a homogeneous state, one says that the system contains a topological soliton.[6,38]

The topological stability of defects is governed by the form of the homotopy groups $\pi_i(\mathscr{R})$ of the degeneracy space, whose elements serve as the mapping of i-dimensional spheres enclosing the defect in real space into the degeneracy space. The defects of dimensionality t in a t'-dimensional medium are classified by the group $\pi_i(\mathscr{R})$ with $i = t' - t - 1$. On the one hand, each element of the homotopy group corresponds to a class of stable defects equivalent to one another apart from continuous deformations, and on the other hand, to a certain topological invariant, which is the topological charge of the defect. The homogeneous state corresponds to a unit element and zero topological charge.

We shall illustrate the principles of the homotopy classification of defects with examples for two-dimensional systems having orientational (two-dimensional NLCs) and translational (two-dimensional SLCs) ordering.

2.1.1. Defects in a two-dimensional nematic

As we know, a nematic amounts to a medium having orientational order: it consists of axially symmetric molecules oriented along some common direction $\mathbf{n}$—the director. Owing to the nonpolarity of NLCs we have $\mathbf{n} \equiv -\mathbf{n}$.

In our model of a two-dimensional NLC the centers of gravity of all the molecules lie in one plane, while the director $\mathbf{n}$ makes the angle $0 \leqslant \alpha \leqslant \pi/2$ with the normal $\mathbf{v}$ to it. The order parameter can be chosen either in the form of the unit vector $\boldsymbol{\tau}$ of the projections of the axes of the molecules on the plane, or in the form of the wave function $\Psi = \alpha \exp(i\varphi)$, where φ is the azimuthal angle of the tilt of the molecules. The free energy f of the system depends only on the modulus α of the wave function and is degenerate in φ:

$$f = A \mid \Psi \mid^2 + B \mid \Psi \mid^4. \tag{2.1}$$

The region $\mathscr{R}$ of all possible values of φ for which the energy f takes on a minimum value is the degeneracy space of the two-dimensional NLC. The form of $\mathscr{R}$ substantially depends on the value of the modulus α.

In fact, if $0 < \alpha < \pi/2$, then the phase φ can vary from 0 to 2π and the space $\mathscr{R}$ is the circle S^1, each point of which corresponds to a certain value of φ. When $\alpha = \pi/2$, the axes of all the molecules lie in one plane and any two diametrically opposite points of S^1 become identical owing to the nonpolarity of the NLC; such a circle is written in the form S^1/Z_2, where Z_2 is the group of residues modulo 2, i. e., the group of the two numbers 0 and 1: $0 + 0 = 0$, $0 + 1 = 1$, $1 + 0 = 1$, $1 + 1 = 0$. Finally, if $\alpha = 0$, the space contracts to a single

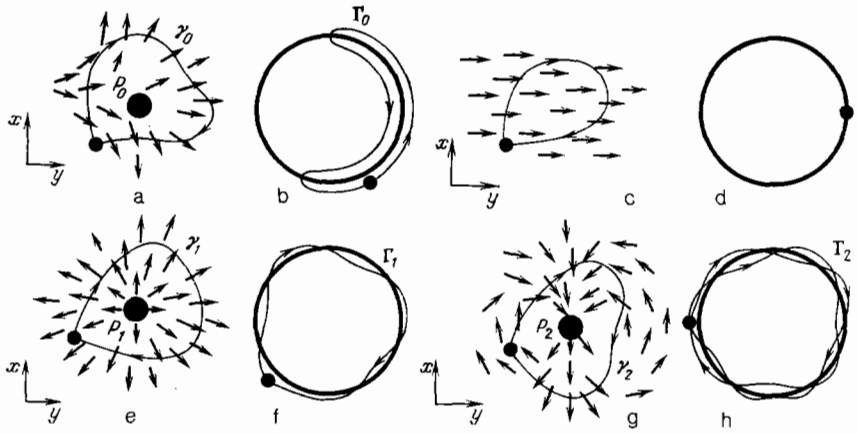

FIG. 1. Point defects in a two-dimensional NLC with $0<\alpha_0<\pi/2$ with different topological charges $m.m = 0$ (a,c), 1(e), 2(g). The arrows indicate the field τ of the projections of the molecules on the plane. b, d, f, h—Contours corresponding to the defects in the degeneracy space S^1.

point. Inhomogeneities in the orientation of the molecules in the layer of the two-dimensional NLC having a certain equilibrium value of the angle of inclination $\alpha = \alpha_0$ give rise to an additional gradient term in the expression for the free energy:

$$f = A\,|\Psi|^2 + B\,|\Psi|^4 + \frac{1}{2}K\,|\nabla\Psi|^2. \tag{2.2}$$

Here K is Frank's elastic modulus. If the characteristic scale of inhomogeneity is much greater than the coherence length $\xi = (K/|A|)^{1/2}$, then the angle α deviates little from the equilibrium value α_0 and the inhomogeneity involves only the variations of the function $\varphi(x, y)$ of the point (x, y) that maps real space into the degeneracy space $\mathscr{R}$. The study of the character of such mappings enables one to determine whether a defect is stable or not. As an example let us elucidate the stability of the defect at the point P_0 marked in Fig. 1a for $0<\alpha_0<\pi/2$.

Let us surround the point P_0 with the closed, oriented contour γ_0; it is mapped by the function $\varphi(x, y)$ into the space S^1 in the form of a contour Γ_0 that is also closed and oriented (Fig. 1b). As we can easily see, the contour Γ_0 is homotopic to zero: it can be contracted by continuous deformations into a point on S^1 (Fig. 1d). Correspondingly the inhomogeneous distribution (see Fig. 1a) is continuously deformable into a homogeneous distribution (Fig. 1c) having a smaller energy of elastic distortions. The defect under test proved to be removable, or topologically unstable.

The situation differs for the distribution shown in Fig. 1e. The contour, Γ_1 corresponding to it (Fig. 1f) runs around the entire circle S^1, and it can be contracted to a point only if we allow either a breakdown of the condensed state along an entire line starting at the point P_1 or a separation of the contour Γ_1 from the circle S^1 (i.e., allow an appreciable deviation of α from α_0). Of course, both cases require overcoming a considerable energy barrier that exceeds the energy of the defect by many times. In other words the defect in Fig. 1e is topologically stable. The defect in Fig. 1g, whose contour Γ_2 runs twice around S^1, is also stable.

On the whole, the set of all point singularities is divided into classes, each of which corresponds to its own class of homotopically equivalent contours Γ_m that run around S^1 the same number of times m in a given direction. The set of classes of contours Γ_m forms the so-called fundamental, or first homotopy group of the space $\mathscr{R}$, denoted as $\pi_1(\mathscr{R})$. Each element of the group corresponds to a certain number m of traverses of S^1. This is the topological charge of the defect. It cannot be changed by any continuous deformations, and this determines the stability of the corresponding defect. Analytically we have

$$m = \frac{1}{2\pi}\oint_\gamma \nabla\varphi\,dl = 0,\ \pm1,\ \pm2,\ \ldots \tag{2.3}$$

We can easily see that the classification of defects in a two-dimensional NLC is radically altered even with changes in the space $\mathscr{R}$ that are insignificant at first glance. Thus, when $\alpha_0 = \pi/2$ the degeneracy space is the circle S^1/Z_2. That is, it differs from the "usual" S^1 only in the identity of antipodal points. Yet already this alone leads to doubling of the set of defects, which can now take on not only integral values of the charge m, but also half-integral.

But if $\alpha_0 = 0$, then $\mathscr{R} = 0$, and there are no defects at all ($\pi_1(0) = 0$).

The merger of defects is governed by the rules of multiplication operation acting in the homotopy group. Merger of defects in a two-dimensional NLC with $0<\alpha<\pi/2$ corresponds to simple addition of the charges m: the group $\pi_1(S^1)$ is isomorphic to the group Z of integers m, and the group operation is ordinary addition. Thus, for example, two defects having $m = 1$ and $m = -1$ annihilate to form a homogeneous state with $m = 0$.

The processes of annihilation and decay of point defects not accompanied by a change in the total value of the topological charge of the system are generally energetically favorable.

Actually the minimization of the energy of elastic distortions in (2.2) yields the equilibrium equations

$$\nabla^2\varphi = 0 \tag{2.4}$$

having the solutions

$$\varphi = m\,\mathrm{tg}^{-1}\frac{y}{x} + \mathrm{const}. \tag{2.5}$$

The latter imply the following expressions for the energy of an isolated defect

$$F = \pi m^2 K \ln\frac{R}{\rho} \tag{2.6}$$

(R is the characteristic dimension of the system, ρ is the radius of the core of the defect, i.e., the region in which

$\alpha \neq \alpha_0$) and for the energy of a pair of defects lying at a distance d from one another:

$$F = -2\pi m_1 m_2 K \ln \frac{d}{\rho}. \tag{2.7}$$

In line with Eqs. (2.6) and (2.7), it is favorable for defects with large charges m to split into several defects with smaller m, and for defects with opposite signs of m to attract one another and annihilate.

The result of merger of defects in a two-dimensional NLC is always unambiguous. However, whenever the medium is characterized by a non-Abelian homotopy group, the result of merger is ambiguous and depends on the path of merger. The simplest example of such a medium is a two-dimensional system of equivalent bands, a two-dimensional smectic.

2.1.2. Defects in a two-dimensional smectic

A good experimental model of a two-dimensional SLC is the lyotropic $P_{\beta'}$ phases of phospholipids in the form of thin films isolated in a large volume of water, resembling biomembranes. The $P_{\beta'}$ phase manifests two types of corrugated supermolecular structures—the λ-phase and the $\lambda/2$-phase[39,40] (Fig. 2). As the electron-microscopic studies of these phases show, numerous point defects exist in them, involving inhomogeneous distortions of the system of layers corresponding to the ridges and troughs of the membranes. Let us elucidate the features of the topologic behavior of such systems.[39]

To find the degeneracy space we shall employ the general rule according to which the degeneracy space of the medium is the complete symmetry group of the functional of the energy G factored by its subgroup H, whose transformations leave the order parameter invariant[10]:

$$\mathscr{R} = G/H. \tag{2.8}$$

As the group G for the λ and $\lambda/2$ phases we can choose the same complete Euclidean group E of all translations and rotations in a plane. In the λ phase, as we see from Fig. 2a, continuous translational symmetry exists along the layers, and discrete symmetry (with the scale λ) in the perpendicular direction, as well as rotational symmetry about the C_2 axis perpendicular to the plane of the system. Therefore the symmetry group H_λ has the form $(R \times Z) \square C_2$, or as is the same,

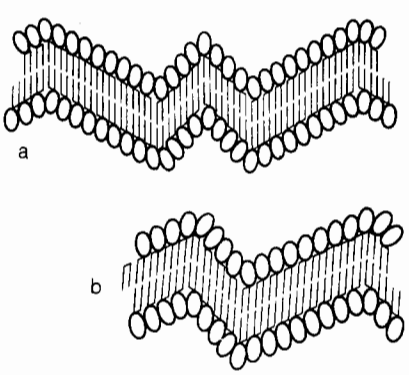

FIG. 2. Molecular order of the λ-phase (a) and the $\lambda/2$-phase (b).[39,40]

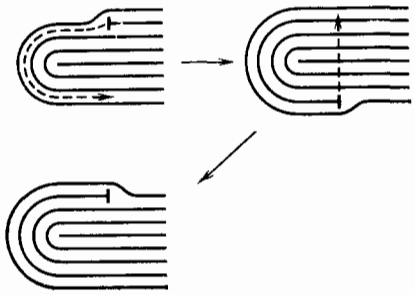

FIG. 3. Conversion of a dislocation having the charge (1,0) into an antidislocation (-1,0) on passing around a disclination (0,1/2) in the λ-phase. The lines denote the ridges of the phase.

$$H_\lambda = (R \times Z) \square Z_2. \tag{2.9}$$

Here R is the group of real numbers, while the symbols $\times$ and $\square$ respectively denote the direct and semidirect products of the groups. The fundamental group of the space $R_\lambda = E/H_\lambda$ is noncommutative and is isomorphic with the semidirect product of two groups of integers[39]

$$\pi_1(\mathscr{R}_\lambda) = Z \square Z. \tag{2.10}$$

Consequently every point defect in the λ-phase corresponds to a pair of integers (b, m). The elements of the form $(b, 0)$ describe point dislocations with the Burgers vector $b\lambda$, while elements of the form $(0, m)$ describe point disclinations of integral and half-integral strength. However, owing to the noncommutativity of $\pi_1(\mathscr{R}_\lambda)$, here every defect no longer corresponds to one element of the group, but to an entire class of coupled elements. Actually, a simple example (Fig. 3) shows that a (1,0) dislocation after passing around a (0, 1/2) disclination should now be characterized by the pair (-1, 0); in other words the elements (1, 0) and (-1, 0) describe the same defect. Therefore a (1, 0) dislocation and a (-1, 0) "antidislocation" upon merging either annihilate (Fig. 4b) or form a double dislocation (2,0), if the point (-1, 0) passed around the (0, 1/2) disclination on the path to the merger site (Fig. 4c). The ambiguity of the result of merger involves the fact that it is determined, not by the result of multiplication of individual elements of the homotopy group, as for "Abelian" media, but by the entire set of results of multiplication of classes of coupled elements.

The other variety of the $P_{\beta'}$ phase, the $\lambda/2$ structure,

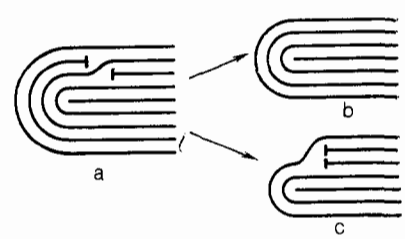

FIG. 4. Dependence of the result of merger of (1,0) and (-1,0) dislocations in the λ-phase (a) on the path of merger: above the disclination (0,1/2) (b) and below the disclination (c).

seemingly hardly differs from the λ structure (Fig. 2); only the twofold symmetry axis C_2 has disappeared, and the symmetry group has the form $H_{\lambda/2} = (R \times Z) \times Z$. However, now the group of point defects

$$\pi_1 (\mathscr{R}_{\lambda/2}) = Z \times Z \tag{2.11}$$

is commutative, and the result of merger of two defects is always unambiguous; moreover, in contrast to the λ phase, the $\lambda/2$ phase lacks isolated disclinations of half-integral strength, as is confirmed by experiment.[39]

Simple examples of λ and $\lambda/2$ phases demonstrate also some restrictions on the application of homotopy theory for classifying defects in media having broken translational symmetry. As we see from Eqs. (2.10) and (2.11), in a two-dimensional system of layers homotopy theory predicts the existence of disclinations with infinitely large values of m. At the same time, evidently, the creation of disclinations even with $m = 2$ requires introducing a large number of dislocations into the system owing to breakdown of equidistance of the layers, which is energetically unfavorable. Only the values $m = 1$, $1/2$, and 0 do not require varying the thickness of the layers.

The fundamental principles of the homotopic classification of topological defects were briefly examined with the example of two-dimensional systems. The nonsingular distributions—topological solitons—are described by an analogous scheme. They are characterized by the so-called relative homotopy groups.[6,24,38] The relative homotopy groups are also used for classifying defects on the surface of ordered media. Concrete examples will be presented in the following sections.

Now let us take up briefly the features of the experimental study of inhomogeneities in liquid crystals.

2.2. Methods of experimental study

As the simplest and most reliable method of experimental study of defects in liquid crystals, polarizing microscopy long ago proved advantageous. In studying in the polarizing microscope a thin layer of a LC placed, e.g., between two transparent plates, one sees a characteristic multicolored pattern, or texture. If one does not take special measures toward homogeneous orientation of the LC, then the specimen will contain a large number of varied defects, which determine the features of the birefringence in the medium, and hence, the character of the texture.

As a rule, the main feature is the presence of broad, dark bands, or extinction bands, which converge at individual sites in point centers. The extinction bands cover the regions in which the local optic axis lies in the plane of polarization of one of the Nicol prisms, and the light propagates in the form of a pure ordinary or pure extraordinary wave. Since, in turn, the distribution of the optic axis is strictly associated with the distribution of axes of the molecules (and the order-parameter field), then, by observing the position of the extinction bands for different positions of the specimen, one can establish the distribution of the molecules in the texture (for more details, see, e.g., Refs. 41–43).

In studying defects, in essence, all the methods of modern light microscopy are applied. Thus, objects are illuminated with linearly and circularly polarized light, and with white and monochromatic light. Dark-field,[11,44] phase-contrast,[44] and also interference[45–47] microscopy are used, and other special methods.[47–51] In particular, the method of dynamic light scattering has enabled measuring the mean velocity of disclinations in the convective flow of an NLC in a region of electrohydrodynamic instability from the magnitude of the Doppler shift in the frequency of the reflected light caused by moving scatterers—disclinations.[52] In a number of cases methods are useful of decorating the surface of an LC with various additives[53–55] and by adding dyes.[56]

In recent years the methods of electron microscopy have become ever more widespread in studying the textures of both lyotropic[57–59] and thermotropic[60–63] systems.

Fixing the boundary conditions and the geometry of experiment are of importance in studying defects in LCs. Without taking up in detail the specifics of the surface orientation of LCs (see the reviews of Ref. 64 and monographs of Refs. 31–36, 65), we shall point out that the choice of geometry of the experiment, as a rule, is dictated by the features of the defects being studied. Thus, specimens in the form of a wedge have been used for a long time in studying linear defects in CLCs and SLCs; the classical experiments were designed for cylindrical capillaries (pores) in studying disclinations in nematics, cholesterics, and smectics.[45,66–74]

Liquid-crystalline structures of spherical form are of especial interest. One can produce them by filling spherical bulbs with a liquid-crystal phase.[75] In a number of cases a more elegant solution is found that approaches the experiments of Plato: one can prepare drops of an LC freely suspended in a solution (see the studies on lyotropic systems[76–79]), in a melt (this especially pertains to carbonaceous phases[80]) or in a specially chosen transparent matrix that does not dissolve the LC. As the latter one can select polymeric liquids,[42,81,82] agar,[83] Canada balsam, immersion oil,[30] and even water.[84] Glycerol, traditionally used as a medium for embedding microobjects, is promising in this regard.[85] By using glycerol containing an admixture of lecithin, one can not only impose homogeneous boundary conditions on the surface of the drops (normal, tangential, conic), but vary them slightly over a broad range from strictly normal to strictly tangential, and vice versa, by varying the temperature.[86]

3. UNIAXIAL NEMATICS

Uniaxial nematics consist of molecules (or aggregates of them—micelles, as in the case of lyotropic phases[87,88]) having the symmetry of ellipsoids of revolution. Depending on whether the axis of rotation is the long or short axis of the molecule, one distinguishes cylindrical and discotic NLCs.[89] The interaction between the molecules tends to arrange them parallel to one another, whereby a defined direction of preferred orientation of the axes of rotation of the molecules arises in the bulk of the NLC, characterized by the director $\mathbf{n}$. One can choose the director as the order parameter of the NLC of either a cylindrical or a discotic phase.

Evidently any rotations of a nematic system as a whole in real space involving reorientation of $\mathbf{n}$ do not alter the energy of the system. Therefore the degeneracy space $\mathscr{R}_N$ is the two-dimensional sphere S^2 factored, owing to the condition $\mathbf{n} = -\mathbf{n}$ by the group Z_2 (projective plane)[6,8]:

$$\mathscr{R}_N = S^2/Z_2. \tag{3.1}$$

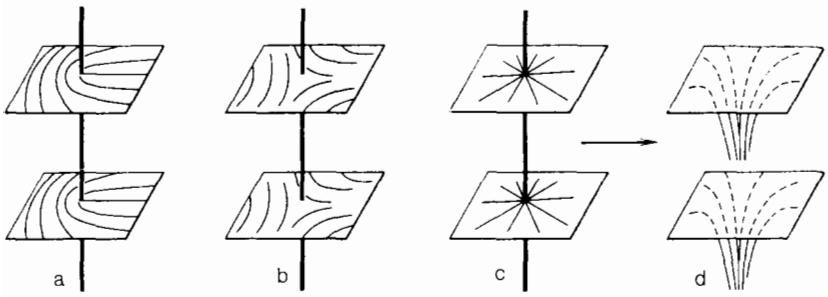

FIG. 5. Disclinations in the bulk of a uniaxial NLC having different topological charges N and strengths m. a—$N = 1$, $m = 1/2$. b—$N = 1$, $m = -1/2$. c,d—$N = 0$, $m = 1$. The lines denote the distribution of the field of the director **n**.

Now let us elucidate what types of linear defects allow such a form of the degeneracy space, i.e., what type has the group $\pi_1(S^2/Z_2)$.

3.1. Disclinations in the bulk

Only two classes of closed contours exist on the sphere S^2/Z_2: contours Γ_0 homotopic to zero, and contours Γ_1 linking antipodal points of the sphere S^2/Z_2, and hence not capable of contraction to a point. Consequently, $\pi_1(S^2/Z_2) = Z_2$ and the linear defects, disclinations, in the bulk of the NLC belong to only two classes: nonremovable, with charge $N = 1$ (Figs. 5a, b), and removable, with $N = 0$ (Figs. 5c, d). Transitions between the classes require breakdown of the structure on the whole half-plane Σ and the energy $\sim K\Sigma/\xi$, which is considerably greater than the energy $\sim KL$ of a disclination of length L itself.

Of course the existence of only two topological classes does not imply that the distribution of the field of the director around disclinations is manifested only in two variants of whatever kind. A great variety of disclinations exists within the bounds of a given class that differ among themselves in their symmetry or in the symmetry of the core, and hence, in physical properties (e.g., the magnitude of the charge caused by the flexoelectric effect on the core of the defect).[90] Since generally a given symmetry restricts the region of variation of the order parameter, we must introduce additional topological invariants to describe states of disclinations of differing symmetry. For example, if the disclination has a plane of symmetry perpendicular to its axis (such disclinations are called planar owing to the planar distribution of **n**), then this additional charge is the well known Frank index[91] or the strength m of the disclination, which is commonly considered equal to half the Frank index (see, e.g., Ref. 31). Actually the strength of a planar disclination is the topological charge of a point defect in a two-dimensional NLC with $\alpha_0 = \pi/2$ discussed in Sec. 2.1. The disclinations shown in Figs. 5a, b from the class $N = 1$ have different strengths and symmetries (respectively $m = 1/2$, D_{1h} and $m = -1/2$, D_{3h}). A remarkable result of the symmetry classification of disclinations proposed by Balinskiĭ, Volovik, and Kats[90] was the prediction of phase transitions between states of disclinations of differing symmetry and strength arising upon change of temperature or pressure, but not involving a change in the phase state of the NLC itself. For example, a first-order transition can occur between the states $m = 1/2$, D_{1h} and $m = -1/2$, D_{3h} in Figs. 5a, b. The existence of such transitions has been proved experimentally for point defects (see Sec. 3.2).

As we have already pointed out, transitions of disclinations between different topological classes require overcoming large energy barriers. Yet within a single class disclinations of different configurations can continuously transform into one another; the energy barrier, even if it exists for such deformations, is small (of the order of $K\xi$).[6] The question of locally stable types of disclinations or ensembles of them within the limits of each class is more complicated when one takes account of the concrete parameters of the NLC and the external conditions. Studies along this line—both theoretical (based on studying the energy of elastic distortions[66,67,91–99]) and experimental[11,66–71,96,100]—had been intensively conducted even before the rise of homotopy classification. The most detailed theoretical solution was given by Dzyaloshinskiĭ and Anisimov,[94] who used the general expression for the energy density of elastic distortions of the orientation of the director:

$$f = \frac{1}{2}[K_{11}(\operatorname{div}\mathbf{n})^2 + K_{22}(\mathbf{n}\operatorname{rot}\mathbf{n})^2 + K_{33}[\mathbf{n}\operatorname{rot}\mathbf{n}]^2] \quad (3.2)$$

(K_{11}, K_{22}, and K_{33} are respectively the Frank constants for splay, twist, and bend). They showed that, in addition to planar disclinations, "bulk" disclinations can exist (the director does not lie in a single plane). Planar disclinations are stable when $2K_{22} > K_{11} + K_{33}$, while bulk disclinations are so when $2K_{22} < (K_{11} + K_{33})$. Here, for close-lying values of the constants K, only elementary disclinations with $m = 1/2$ are stable. Disclinations with larger values of m become stable when $K_{22} \gg K_{11}$, K_{33} (planar) and when $K_{33} \gg K_{11}$, K_{22} (bulk).

The conclusions of the theory as a whole have been confirmed experimentally. A number of authors have been able to observe instability of a plane disclination having $m = 1$ in cylindrical capillaries, consisting in the reorientation of the director along the axis of the cylinder (the so-called effect of outflow of the disclinations into the third dimension)[11,45,66,71] (see Fig. 5c, d). The outflow corresponds to contraction of the contour Γ_0 from the equator of the sphere S^2/Z_2 to a point at the pole and is accompanied by a monotonic decrease in the energy of the disclination. One can show the latter within the framework of the single-constant approximation $K_{11} = K_{22} = K_{33}$. In this case the energy per unit length of a plane disclination with $m = 1$ is determined by Eq. (2.6) and is $\pi K \ln(R/\rho)$, while for the "outflowing" configuration of Fig. 5d it amounts to $3\pi K$: hence, in a specimen of real dimensions ($R \gtrsim 20\rho$) such a nonsingular configuration is energetically more favorable. We note that often the experimental situation looks somewhat more complicated than in Fig. 5d; since outflow "up" and "down" along the axis of the capillary are equally probable, the effect leads to

the appearance of breaks in the texture—point singularities localized in the bulk of the NLC[11,66,67,69-71] and bearing the name of "hedgehogs" (see Sec. 3.2).[86]

The absence of a singular core in a disclination with $m = 1$ is confirmed also by the so-called schlieren textures formed in plane layers of NLCs having tangential or conical boundary conditions.[11,36,67,96,101] The main feature of schlieren textures is the presence of two types of centers from which two or four extinction bands emerge. The centers with two bands have a singular core, insofar as can be seen, of molecular dimensions and corresponding to stable disclinations with $m = \pm 1/2$. The centers with four extinction bands are diffuse, at least at distances $\sim 1\ \mu$m. If one illuminates the specimen with monochromatic light, interference rings are distinctly visible near such nuclei, and are caused by the variation of the birefringence as the director flows out along the vertical axis.[67,96] The centers of the type being discussed do not correspond to linear, but to point singularities formed by outflow of disclinations with $m = 1$ in the bulk of the specimen and localized at the surface. Such defects are called boojums[86]; their properties substantially differ from those of point defects in the bulk, or hedgehogs (see Sec. 3.3).

The effect of outflow into the third dimension can be manifested not only on macroscopic scales for the entire structure of the disclination as a whole, as in the case with disclinations $m = 1$. As Lyuksyutov[102] first showed, in a range of distances that does not exceed $\rho_c \approx 2\times 10^{-8}$ m for classical NLCs, the order parameter is degenerate not on S^2/Z_2, but on a four-dimensional sphere S^4, for which $\pi_1(S^4) = 0$. It seems that on small scales disclinations with $N = 1$ are also nonsingular. Since different types of "outflow" can occur, we should expect phase transitions among them inside the core.[90] One can conveniently seek such transformations near the uniaxial-biaxial NLC transition, where ρ diverges.[90] However, their manifestation is not ruled out in light-scattering experiments on liquid crystals in micropores.[103]

As we see from the homotopy classification, a law of conservation of topological charges N should be fulfilled in merger of disclinations in the form

$$1 + 1 = 0,\quad 1 + 0 = 1.$$

And actually, Nehring and Saupe[96] observed merger of two singular disclinations with $N = 1$ into a nonsingular one with $N = 0$. The inverse process of dissociation of a line with $N = 0$ into two with $N = 1$ is also known.[69] Theoretical calculations of the interaction of disclinations have been presented in Refs. 69, 96, 104, 105. In particular, they imply that two identical disclinations can not only repel, but also attract one another, depending on the values of the Frank constants and the geometry of the specimen.

The overwhelming majority of experimental studies on disclinations have been performed on classical thermotropic NLCs of the type of MBB or PAA having molecules of cylindrical form. Naturally, they do not manifest the entire variety of possible properties of defects. In line with the need of elucidating the details of the relation between the features of molecular structure of the medium and the character of the defects, interest has recently risen in new nematic systems: polymeric NLCs, both thermotropic[106,107] and lyotropic,[108] thermotropic and lyotropic disconematics,[109,110] carbonaceous phases,[62,80] and finally, different mixtures of mesogenic and nonmesogenic substances.[101] Precisely for such mixtures, composed of classical NLCs (of the type of octylcyanobiphenyl) and a nonmesogenic substance with molecules of platelike shape (1, 4, 9, 10-tetrahydroxyanthracene), Madhusudana and Pratibha[101] first observed disclinations with $m = \pm 2$ and $m = \pm 3/2$ in schlieren textures. They were able to show that defects with $m = \pm 3/2$ are singular and can dissociate into pairs with $m = \pm 1/2$ and $m = \pm 1$ (by the scenario for N: $1 \to 1 + 0$). Probably the obtained results are explained by the sharp change in the elastic constants of the NLC upon introducing the stated additive—e.g., by an increase in the constants K_{22} or K_{33}, which, according to theory,[94] should lead to stability of disclinations with large m.

Unusual results have been obtained also for lyotropic NLCs in the form of acid solutions of rigid-chain polymers.[108] The predominant type of disclinations in these media proved to be lines of strength $m = 1$ with a thin singular core. In all appearance, this involves the fact that the constant K_{33} for bend of the system of rigid polymer chains must appreciably exceed the constants K_{11} and K_{22}. As is implied by Ref. 94, when $K_{33} > K_{11}, K_{22}$, disclinations with $|m| \geqslant 1$ become stable and possess a bulk structure.

The conclusions of Ref. 108 stand in a certain contradiction to the observations in thermotropic polymeric NLCs[106,107] of lines with $m = 1$ having a diffuse, nonsingular core and lines with $m = 1/2$ having a singular core. Although the textures in these systems externally differ little from those of classical NLCs, the cores of defects can have their own features, in particular, in containing many ends of polymeric macromolecules.[107,108]

The elucidation of the influence of the specifics of molecular structure of NLCs on the features of the disclination is also shown in the carbonaceous phases. Carbonaceous NLCs consist of large, platelike multinuclear aromatic molecules with a molecular weight of 1500–2000 packed parallel to one another and actually forming plane layers. Therefore the outflow into the third dimension of disclinations with $m = 1$ becomes unfavorable. Electron micrographs of sections of the solid modifications of carbonaceous phases confirm the presence of singular cores of lines, both with $m = 1$ and with $m = 1/2$ (see, e.g., the reviews of Ref. 62).

3.2. Point defects—hedgehogs

As was pointed out above, a consequence of the effect of outflow of disclinations with $m = 1$ in round capillaries can be the appearance of point singularities—hedgehogs in the bulk of the NLC. A somewhat more convenient experimental geometry for producing hedgehogs in a system is presented by spherical drops of NLCs with normal boundary conditions. There is also a proposal[111] that hedgehogs can arise in the form of polarization deformation coats around ions implanted into the NLC.

The topological classification of hedgehogs is based on examining the mapping of a closed surface σ surrounding the point defect into degeneracy space.[6] The image of σ in degeneracy space will be the surface Σ, which either can be contracted to a point and corresponds to an unstable configuration, or is wrapped $N \neq 0$ times around the sphere S^2/Z_2 and corresponds to a hedgehog having the charge N. The classes of surfaces Σ homotopic to one another form the second homotopy group $\pi_2(S^2/Z_2)$, which is isomorphic to the

group of integers Z. The topological charge of the hedgehog (the degree of mapping of the sphere σ onto the sphere S^2/Z_2) is

$$N = \frac{1}{4\pi} \oint_\sigma \mathbf{n} \left[\frac{\partial \mathbf{n}}{\partial \theta} \frac{\partial \mathbf{n}}{\partial \varphi} \right] d\theta \, d\varphi. \tag{3.3}$$

(Here θ and φ are arbitrary coordinates on σ.) This charge takes on only integral values. A very simple example of a point defect having $N = 1$, actually reminding one of a hedgehog, is shown in Fig. 6a. This is a singular point from which field lines of the director $\mathbf{n}$ diverge in all directions along the radii-vectors:

$$n(x, y, z) = (x, y, z)(x^2 + y^2 + z^2)^{-1/2}. \tag{3.4}$$

Figure 6b shows another hedgehog with $N = 1$, but now having a hyperbolic structure:

$$n(x, y, z) = (-x, -y, z)(x^2 + y^2 + z^2)^{-1/2}. \tag{3.5}$$

Here, as in the case of disclinations, a situation arises in which configurations of defects differing in symmetry corresponds to the same homotopic class, and phase transitions occur among them upon changing external conditions. To convince ourselves of this, let us substitute Eqs. (3.4) and (3.5) into (3.2) and find the energy of the two types of hedgehogs (respectively):

$$F_R = 8\pi K_{11} R,$$
$$F_H = 8\pi R \left(\frac{K_{11}}{5} + \frac{2K_{33}}{15} \right)$$

(R is the characteristic dimension of the system). We can easily see that either the radial structure (when $K_{33} > 6K_{11}$) or the hyperbolic structure (when $K_{33} < 6K_{11}$) can prove energetically favorable, depending on the relationship between the bending elastic constants K_{11} and K_{33}. Thus the transformation of the one hedgehog into the other can occur near the nematic-smectic phase-transition point, where K_{33} shows a critical increase, whereas K_{11} hardly varies.

Experimentally a phase transition with changing symmetry of hedgehogs has been discovered in spherical drops, at the surface of which a normal orientation of the molecules was imposed.[112] These boundary conditions unavoidably lead to the appearance in the bulk of the drop of a hedgehog with $N = 1$. Near the transition point the hedgehog has a radial structure, but on temperature increase it transforms into a combination of a hyperbolic hedgehog and a ring nonsingular disclination surrounding it. The disclination enables a smooth coupling of the distribution of the director at the center and the periphery of the drop (Fig. 7). The phase transition is accompanied by a change of symmetry $K_h \to C_{\infty h}$ and is a second-order transition.[112]

The overwhelming majority of experimental studies of point features in the bulk of NLCs have been performed with capillaries with normal boundary conditions.[11,66,67,69,71] Radial and hyperbolic hedgehogs arise in this geometry, just as in spherical drops. For capillaries with a tangential orientation of $\mathbf{n}$, Melzer and Nabarro[70] showed the existence of another type of hedgehog—with a spiral distribution of the field $\mathbf{n}$. This type of singularity corresponds to a "saddle-focus" singular point in the terminology of Poincaré,[113] whereas the radial hedgehog corresponds to a nodal singular point, and the hyperbolic to a saddle singular point. Nabarro[114] has analyzed in detail the relation between the different configurations of hedgehogs and Poincaré singular points.

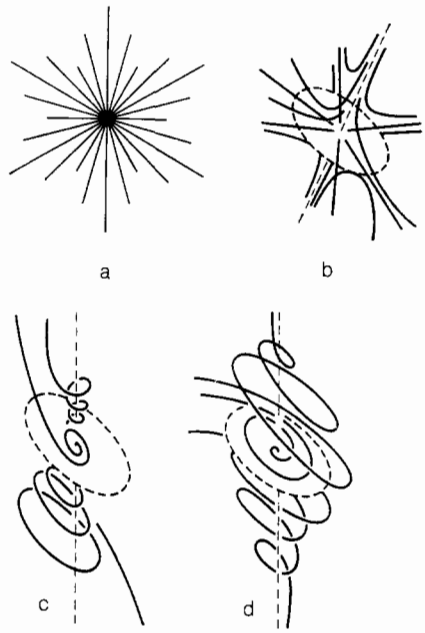

FIG. 6. Point defects—hedgehogs of various structures in the bulk of an NLC.[114]

Let us return to the general homotopy classification of hedgehogs. Within this framework Volovik and Mineev[6] have predicted the existence of a remarkable property of merger of hedgehogs, specifically the dependence of the result of merger on the path of merger. To explain the essence of this effect, we must first turn our attention to the fact that, in an NLC, the charge N of a hedgehog in (3.3) was defined only up to its sign. Therefore it is not clear *a priori* to what

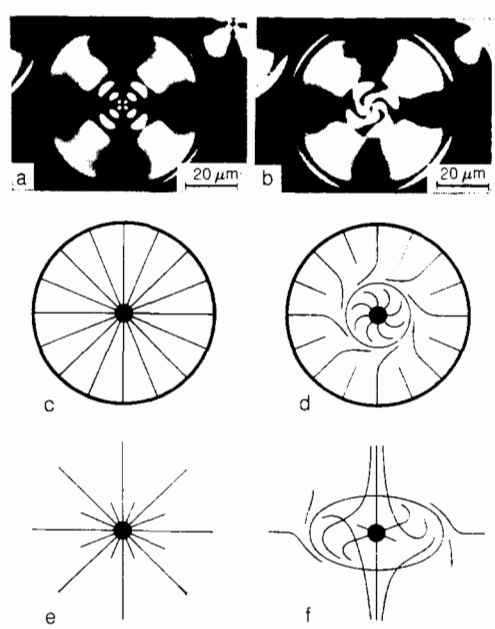

FIG. 7. Transformation of a radial (left) into a hyperbolic (right) hedgehog near the NLC-SLC transition in a spherical drop of an NLC. a,b—Textures of the drop. c,d—Cross section of the drop in the equatorial plane. e,f—Volume images of the hedgehogs.

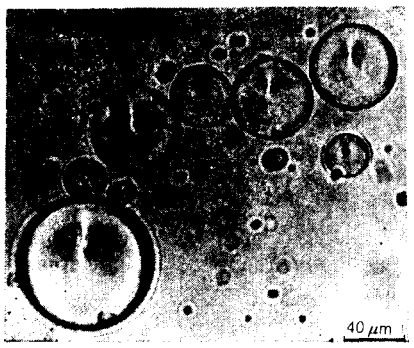

FIG. 8. Texture of spherical drops of a uniaxial NLC with strands linking a hedgehog inside each drop with a pair of boojums, or poles at its surface.

result the merger of two hedgehogs having the same N will lead: to annihilation or to forming a hedgehog with doubled N. It would seem that the paradox is simple to eliminate: One must for a certain time replace the field of the director $\mathbf{n}$ with the vector field $\mathbf{n}'$ for which both the charges N and the results of merger are defined unambiguously. This procedure solves the problem, but only if topologically stable disclinations are absent in the medium. Passage of a hedgehog around a disclination along a closed contour changes the direction of $\mathbf{n}'$, and hence the sign of the charge N, to their opposites. Now two hedgehogs having the same N in the presence of a disclination can either annihilate or give rise to a hedgehog with a doubled charge—depending on the path of merger with respect to the disclination. Owing to this feature, all hedgehogs in a system can be annihilated (or at least all but one with $N = 1$).

The effect being discussed is called the influence of the group $\pi_1(\mathscr{R})$ on the group $\pi_2(\mathscr{R})$ and arises from the nontriviality of $\pi_1(\mathscr{R})$. Unfortunately there are no experimental observations of merger of hedgehogs in the presence of disclinations in an NLC.

The problem of the interaction of hedgehogs in an NLC is of interest. Let us study an isolated hedgehog. Its elastic energy is proportional to the radius R of the volume under study (e.g., for a radial hedgehog we have $F = 8\pi K_{11}R$). It would seem that the energy of interaction of two hedgehogs is proportional to the distance between them, which recalls the interaction of quarks. Moreover, as Ostlund[115] showed, the field lines of $\mathbf{n}$ in the region between the hedgehogs collapse into a string. Strings can also link a hedgehog with boojums—surface defects (Fig. 8).

Disclination rings are defects close to hedgehogs in their topological nature. In the general case the annular singular lines are combinations of disclinations and hedgehogs and are characterized by two charges: N_L, an element of the group $\pi_1(S^2/Z_2)$, and N_P, an element of the group $\pi_2(S^2/Z_2)$.[10,24] To classify annular singularities one can use the so-called toroidal homotopy groups: an annular defect is not enclosed in a sphere, but in a torus, whereupon one studies the homotopy classes of the mapping of a torus into degeneracy space.[26,116] The dual character of these defects has the result that disclinations can emit (and absorb) hedgehogs in unbounded number (Fig. 9). The topological equivalence of a hedgehog with $N = 1$ and an annular disclination (a hedgehog "stretched" into a ring) has been demonstrated[86] with the example of defect structures in drops of NLCs.

3.3. Defects at the surface

3.3.1. Boojums

A three-dimensional NLC can contain defects not only in the bulk but also at the surface. Thus, the outflow of a vertical disclination with $m = 1$ in a plane capillary having a schlieren texture gives rise to point defects—boojums—localized at the surface and not coupled to any singularities in the bulk. This was first established by R. B. Meyer.[67] Boojums constitute a broad class of defects in various media (they were first identified in superfluid ^{3}He-A[117,118]). Their chief distinguishing feature is the impossibility of exit from the surface of the medium into the bulk: in such an operation the boojum proves to be linked to the surface by a linear

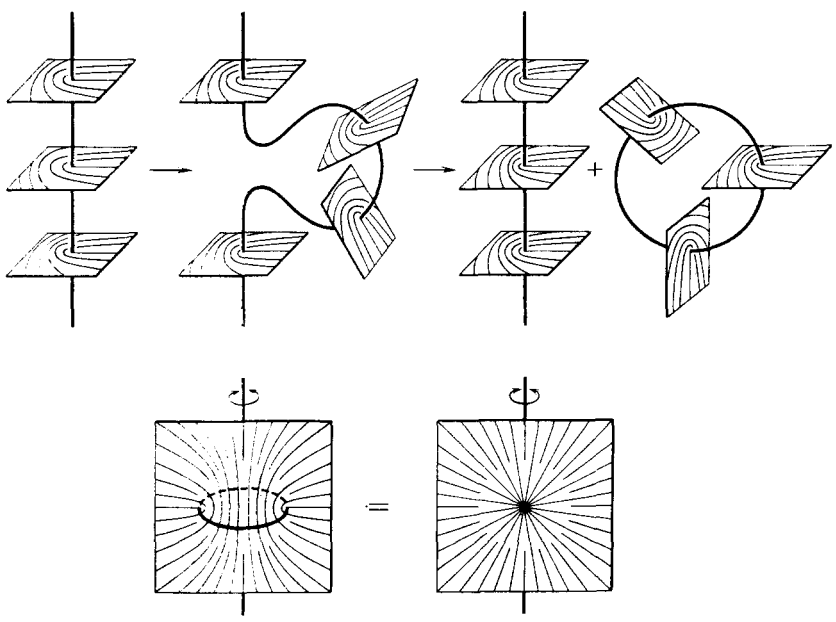

FIG. 9. Diagram of the emission of hedgehogs by a disclination line in a uniaxial NLC.[8]

defect, which is energetically unfavorable.

Boojums in NLCs have been observed also under other conditions[83,92,119]; the appearance was demonstrated[120] of an entire system of translationally ordered boojums at the phase boundary of an NLC with an isotropic melt; an analogous system is also established in the convective instability in a homeotropic layer of an NLC heated from above.[121] In Refs. 11 and 122, which described the merger of defects of strength $m = 1$, to all appearances, the merger specifically of boojums was observed.

The first attempt to give a homotopy classification of surface defects was undertaken in Ref. 123. However, the theory proved incomplete, since actually defects in two-dimensional NLCs were described (see Sec. 2.1 and Refs. 27 and 124), rather than at the boundary of a three-dimensional NLC. The flaw in this approach lies in the impossibility of distinguishing isolated point singularities and defects that are the ends of linear singularities localized in the bulk.

A systematic classification of defects at the boundary of ordered media has been proposed by Volovik.[125] According to Ref. 125, to elucidate the topological stability of a point defect at the surface, one should surround it not only with a contour on the surface, but also with a hemisphere $\tilde{\sigma}$ fitted onto this contour from the bulk side. The field $\mathbf{n}$ maps the hemisphere $\tilde{\sigma}$ itself into the space S^2/Z_2 of degenerate states of the system in the bulk and its edge (contour) into the space of states $\tilde{\mathscr{R}}_N$ that the system can adopt at the surface. As a result the relative homotopic group $\pi_2(\mathscr{R}_N, \tilde{\mathscr{R}}_N)$ is formed. Usually (as happens in NLCs) one can represent this group in the form of the product of two groups:

$$\pi_2(\mathscr{R}_N, \tilde{\mathscr{R}}_N) = P \times Q.$$

The elements of group P describe the point defects that exist only at the surface and cannot escape into the bulk owing to topological restrictions, i.e., boojums. The group P is the kernel of the homomorphism $\pi_1(\tilde{\mathscr{R}}_N) \to \pi_1(\mathscr{R}_N)$. This is, it consists of the elements of $\pi_1(\tilde{\mathscr{R}}_N)$ that transform into a single element of $\pi_1(\mathscr{R})$ under the homomorphism (this implies that boojums are not exit points at the surface of linear singularities). Let us take account of the fact that $\mathscr{R}_N = S^2/Z_2$, while $\tilde{\mathscr{R}}_N$ has the following forms, depending on the value of the angle α_0 between the director at the surface and the normal $\mathbf{v}$ to it (see Ref. 86 and Sec. 2,(a):

$$\begin{aligned} \tilde{\mathscr{R}}_N &= 0, && \text{if} \quad \alpha_0 = 0, \\ &= S^1, && \text{if} \quad 0 < \alpha_0 < \frac{\pi}{2}, \\ &= S^1/Z_2, && \text{if} \quad \alpha_0 = \frac{\pi}{2}. \end{aligned}$$

Then we find that the group P consists of the integers m when $\alpha_0 > 0$ and is trivial when $\alpha_0 = 0$. In other words, boojums exist under any conical boundary conditions with $\alpha_0 \neq 0$ and are described by the integral charges N of (2.3).

The group Q in an NLC coincides with the group $\pi_2(\mathscr{R}_N)$ and describes hedgehogs that have arrived from the bulk and did not disappear at the surface owing to the topological conditions at the boundary[125]; they are characterized by the integral charges N of (3.3).

In the general case a defect at the surface amounts to a combination of a hedgehog and a boojum, and hence is characterized by two charges—N and m. To determine the charge N of a defect at the surface, one must calculate the integral of (3.3) over the hemisphere $\tilde{\sigma}$. The quantity A obtained here is related to N, m, and the projection of $\mathbf{n}$ on the normal $\mathbf{v}$ by the following relationship[86]:

$$A = \frac{1}{4\pi} \int_{\tilde{\sigma}} \mathbf{n} \left[\frac{\partial \mathbf{n}}{\partial \theta} \frac{\partial \mathbf{n}}{\partial \varphi} \right] d\theta \, d\varphi = \frac{m}{2} (\mathbf{n}\mathbf{v} - 1) + N. \tag{3.6}$$

Here $\mathbf{n}$ is treated as a vector, rather than as the director, as occurs in the absence of disclinations in the bulk of the NLC. By using (3.6) one finds N from A, since the charge m is determined independently by Eq. (2.3).

The continuous topological charges A introduced in Ref. 86 are important characteristics of boojums. They enable describing the processes of topological evolution of defects, consisting in their creation, annihilation, and interconversion. Figure 10 shows the processes of smooth disappearance of a boojum having $A = \sin^2(\alpha_0/2)$ upon changing the boundary conditions from tangential to normal ($A \to 0$) and conversion of a boojum with $A = \cos^2(\alpha_0/2)$ into a hedgehog ($A \to 1$) under the same conditions. Now we shall examine the more complex and interesting problem of the evolution of defects in a closed system in which the total topological charge must remain invariant under any transformations of the defects.

3.3.2. Topological evolution of boojums and hedgehogs

The most perspicuous and convenient objects from the experimental standpoints are spherical drops of NLCs with regulatable boundary conditions. Under normal boundary conditions a drop of an NLC in equilibrium necessarily contains an elementary hedgehog with $N = 1$,[83,86,112] and with tangential conditions, two boojums $m_1 = m_2$ at the poles (Fig. 11a,e).[83,86,126] Under a smooth change in the boundary conditions, the equilibrium state in the drop must vary in such a way that the hedgehog vanishes, and boojums appear in its place. To describe the process, in addition to the relationships of (3.6), we must introduce restrictions on the charges N and m under the inclined conical conditions at the boundary. These restrictions are the Poincaré theorem (for $\alpha_0 \neq 0$):

$$\sum_{i=1}^{b} m_i = 2 \tag{3.7}$$

(the sum of indices m_i of the vector field fixed on the closed surface equals the Euler characteristic of this surface, i.e., two in the case of a sphere; see also Ref. 117), and the result of the Gauss theorem in the form[86,127]

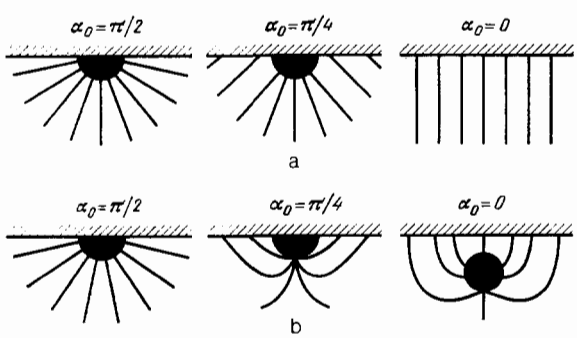

FIG. 10. Evolution of the structure of a boojum at the surface of a uniaxial NLC upon changing boundary conditions from tangential to normal. a—Disappearance of the boojum. b—Conversion of the boojum into a hedgehog.

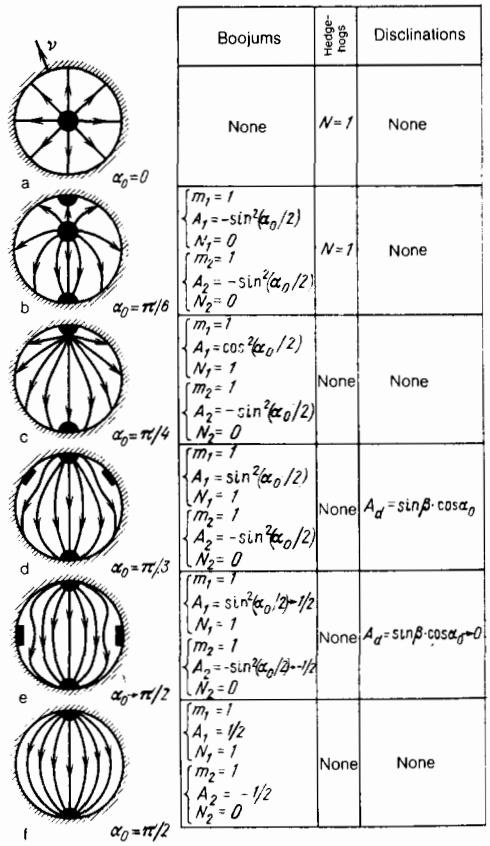

FIG. 11. Topological evolution of defects in a spherical drop of a uniaxial NLC upon changing boundary conditions, according to the experimental data of Ref. 86.

$$\sum_{j=1}^{b+h} N_j = 1\,. \tag{3.8}$$

(Here b is the number of boojums in the system, and h the number of hedgehogs.)

The relationships (3.6)–(3.8) enable one to describe the evolution of defects in a drop of an NLC under changing boundary conditions as a continuous redistribution of the charges A among the defects with overall conservation of the total charge. The theory predicts several most likely scenarios for rearrangement of the structure whose realization depends on the interplay of the energy parameters of the system. One can answer the question of the concrete pathway of evolution by experiment. Such an experiment has been performed for fine drops of NLCs freely suspended in an isotropic matrix whose composition varying the boundary conditions as a function of the temperature.[86] The dynamics of defects in a drop upon changing the conditions from normal to tangential is shown in Fig. 11. The essence of the process consists in the following.

As the vector **n** deviates from the direction of the normal in the drop, besides the hedgehog two boojums are created "from nothing" at the poles (Fig. 11b) with $m_1 = m_2 = 1$, $A_1 = A_2 = -\sin^2(\alpha_0/2)$ and, as (3.6) implies, $N_1 = N_2 = 0$. Both boojums play the role of sinks for the field of **n**. The source is the hedgehog, which moves toward one of the boojums and merges with it to form a new boojum source with $A = \cos^2(\alpha_0/2)$ and $N_1 = 1$ (Fig. 11c). However, the latter proves unstable and decomposes into a boojum with $A_1 = \sin^2(\alpha_0/2)$, $N_1 = 1$ and a disclination ring, which also has a continuously defined topological charge, $A_d = \sin\beta\cos\alpha_0$ (β is the width of the distribution of the disclination on the sphere) (Fig. 11d). On being repelled by the boojum, the disclination moves toward the equator dissipating gradually. Simultaneously with this, the boojums become strengthened according to the law $\pm\sin^2(\alpha_0/2)$ (Fig. 11e). Ultimately the disclination disappears smoothly and two boojums remain in the drop having the charges $A_1 = -A_2 = 1/2$, $N_1 = 1$, $N_2 = 0$ (Fig. 11f).

Thus in the described process defects of differing topological types (hedgehogs, boojums, disclinations) and different homotopy classes smoothly tranform into one another, accompanied by a smooth redistribution of the charges A with invariant total charge, as the theory predicts.

In closing this subsection we shall take up the treatment of another example of a phase transition in the structure of defects, this time involving boojums. In Fig. 11f the distribution of the director in a drop having a bipolar texture is shown in simplified fashion without taking into account possible twisting deformations. The structure in Fig. 11f is energetically favorable if $K_{11} \ll K_{22}, K_{33}$, i.e., near the NLC-SLC-A transition. However, as we go away from the transition point with decreasing values of K_{22} and K_{33}, a second-order phase transition occurs to a twisted structure, in which the director at the surface of the drop does not lie along the meridians, but along loxodromes—lines intersecting the meridians at a constant nonzero angle; upon approaching the axis of the drop this angle decreases to zero.[128,86] The mirror symmetry of the boojums disappears in the transition. The described structure with twisting has been observed experimentally (Fig. 12) and amounts to a simple example of appearance of twist of a uniaxial NLC in the equilibrium state not involving the presence of chiral additives. Here the twist is not propagated in one direction, as in ordinary CLCs, but in two, as in the blue phases (see Sec. 5).

3.3.3. Disclinations at the surface

According to Ref. 125 surface disclinations, as observed, e.g., at the boundary of NLC drops, are described by the elements of the relative homotopy group $\pi_1(\mathscr{R}_N, \tilde{\mathscr{R}}_N)$. For NLCs with continuously degenerate boundary conditions[86] we have

$$\pi_1(\mathscr{R}_N, \tilde{\mathscr{R}}_N) = \pi_1(\mathscr{R}_N) = Z_2, \quad \text{if} \quad \alpha_0 \neq \frac{\pi}{2}\,,$$
$$= 0, \quad \text{if} \quad \alpha_0 = \frac{\pi}{2}\,. \tag{3.9}$$

That is, disclinations at the surface are topologically stable under any boundary conditions but tangential, and are described by the elements of the same group $\pi_1(\mathscr{R}_N) = Z_2$ as disclinations in the bulk. Consequently, these are the lines that have arrived from the bulk and have not vanished owing to the boundary conditions. There are no linear disclinations-boojums at the surface of NLCs.

Most of the experimental studies and calculations of the energy parameters of surface disclinations in ordinary[51,83,86,129–136] and polymeric[107] NLCs have been devoted to studying the lines under tangential boundary conditions in plane cuvettes.[51,96,129–132,135] Their stability in this case is made possible by rubbing the substrates in one direction, which narrows the degeneracy space $\tilde{\mathscr{R}}_N$ at the surface to a single point. A common feature of surface disclinations is

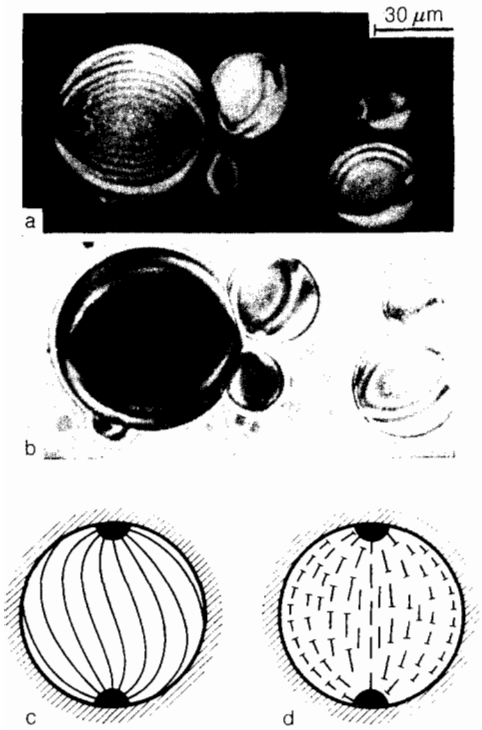

FIG. 12. Twisted bipolar structure of a uniaxial NLC in a spherical drop. a,b—Micrographs of drops with crossed and skew Nicols. c—Distribution of the field of the director at the surface of the drop. d—Distribution of the molecules in the meridional cross section.

the presence of a broad nonsingular core whose dimension ρ is related to the value of the cohesion energy W[130,132];

$$\rho \sim \frac{K}{W}. \tag{3.10}$$

This enables one to estimate the value of W experimentally.[131,135] The existence of a nonsingular core is understandable already from the fact that any disclination at the surface can be supplemented by a virtual disclination, apart from a line with $m = 1$.[132] These conclusions continue to hold for surface disclinations also in the case of inclined conditions at the boundary of the NLC with a solid substrate,[133] an isotropic matrix,[83,84,126] and air.[55]

3.4. Solitons

3.4.1. Planar solitons

Let us study an NLC placed in a plane capillary, both surfaces of which have been rubbed by the method of Chatelaine in one direction **h**. If the capillary is thin enough, the molecules throughout the bulk will be oriented along the direction of **h**:**h** $= \pm$ **h**. In other words, the interaction of the molecules with the walls of the capillary contracts the degeneracy space of the NLC to a single point. Let a vertical disclination of strength $m = \pm 1/2$ exist in the specimen. In its presence it is impossible to conserve a homogeneous distribution of the director **n** $= \pm$ **h**: at a certain surface supported by the disclination the director will rotate 180° (Fig. 13). The thickness of the wall is fixed and is determined by the balance of energy of elastic distortions and the energy of interaction of the molecules with the surface of the capillary. If we write the energy of the wall in the form

$$F = \frac{Kd}{\rho} + W\rho, \tag{3.11}$$

then its equilibrium thickness is

$$\rho_0 = \left(\frac{Kd}{W}\right)^{1/2}. \tag{3.12}$$

Here d is the thickness of the capillary. Such walls with an inhomogeneous, nonsingular distribution of the director are commonly called planar solitons[38,24] of topological type. In addition to stability and conservation of the characteristic dimension, topological solitons possess nontrivial values of the topological charges. Indeed, let us study the mapping of the line γ threaded through the wall into the degeneracy space of the NLC (see Fig. 13). The ends of the line are mapped into antipodal identical points **n** $= \pm$ **h** on S^2/Z_2, while the line γ itself is mapped onto the closed contour $\Gamma_{1/2}$ linking these points. This contour cannot be contracted to a point by any continuous transformations, and this determines the topological stability of a planar soliton.

In the general case the classes of homotopic mappings of the line γ threaded through the soliton form the relative homotopy group $\pi_1(\mathscr{R},\tilde{\mathscr{R}})$, where $\tilde{\mathscr{R}}$ is the region of possible values of the order parameter far from the core of the soliton, narrowed in comparison to $\mathscr{R}$ owing to the extra interaction (external field, boundary conditions, etc.).[38,24] If $\mathscr{R}$ consists of a single point, as in the case being studied, the group $\pi_1(\mathscr{R},\tilde{\mathscr{R}})$ coincides with the absolute group $\pi_1(\mathscr{R})$. Therefore, soliton walls in NLCs exist in a mutually single-valued correspondence with the disclinations that have produced them and are described by the same group $\pi_1(S^2/Z_2) = Z_2$; we can attribute to the planar soliton the charge of the disclination from which it breaks off.

In condensed media planar walls of another nature can exist, arising from the incoherence of the space $\tilde{\mathscr{R}}$. With an incoherent $\tilde{\mathscr{R}}$:$\pi_1(\mathscr{R},\tilde{\mathscr{R}})$ is no longer a group, and the transition layers between the regions characterized by different incoherent components of $\tilde{\mathscr{R}}$ are domain walls of the type of the Bloch and Néel walls, which Mineev has proposed to call "classical domain walls" to distinguish them from soliton walls ending at linear defects.[24] This terminological distinction has a physical basis: to remove walls associated with a linear singularity, it suffices to create a ring of disclinations in the plane of the wall. The latter, in expanding, "eats up" the wall; at the same time, to remove a classical wall requires overcoming a considerably larger energy barrier and perform a transformation of the order parameter over the entire half-space on one side of the wall.[24]

Solitons described by the group $\pi_1(S^2/Z_2) = Z_2$ were known in NLCs long before the development of the homotopy classification. Thus, the configuration shown in Fig. 13 amount to nothing other than inverse walls of the first type,

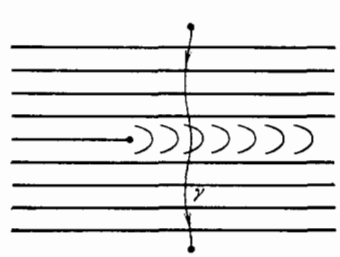

FIG. 13. Planar soliton in a uniaxial NLC.

which were studied in detail by Nehring and Saupe[96] and by others.[36] They contain not only disclinations with $m = \pm 1/2$, but also centers with $m = \pm 1$. Planar solitons also arise in specimens placed in a magnetic[137–143] or electric[143,144] field, and amount to transition layers between two differently oriented regions (parallel and antiparallel to the field) in the Freedericks effect. If the wall forms a closed loop, then according to the theory of Brochard[138] its form must be elliptical. Here one can determine the ratio of the elastic constants from that of the axes, as has been done for a thermotropic NLC by Léger.[139]

Brochard's theory dealt with walls with bending deformation. However, as recent studies have shown, in the general case one must also take into account twisting deformations,[141] which lead to experimentally observable features of the walls in lyotropic NLCs.[142]

3.4.2. Linear solitons

Just as a disclination in an external field can give rise to a planar soliton, a point defect can give rise to a linear soliton (Fig. 14). Linear solitons are described by the relative group $\pi_2(\mathscr{R},\tilde{\mathscr{R}})$; in the case of an NLC placed in an external magnetic field that orients the director along the field, we have $\pi_2(\mathscr{R}_N,\tilde{\mathscr{R}}_N) = \pi_2(\mathscr{R}_N) = \pi_2(S^2/Z_2) = Z$, and their classification coincides with that of hedgehogs.[6,38] We note that the nucleus of a linear soliton can contain point singularities differing from the singularity from which the soliton breaks off.[145] One might detect linear solitons experimentally by placing a drop of NLC containing a hedgehog at its center in an external magnetic field. We know of only one such design of an experiment.[83] However, the result was the formation of a ring disclination, rather than a soliton.

3.4.3. Particle-like solitons

The distribution of the order parameter in particle-like solitons depends on all three coordinates. They are described by the group $\pi_3(\tilde{\mathscr{R}},\mathscr{R})$ of homotopy classes of the mappings of the three-dimensional spherical volume D^3 containing the soliton into the space $\mathscr{R}$. Here the boundary of the spherical volume, the sphere σ, is mapped into the narrowed space $\tilde{\mathscr{R}}$.[6,24] If $\tilde{\mathscr{R}}$ consists of one point, then the particle-like soliton is described by the group $\pi_2(\mathscr{R})$. For an NLC we have $\pi_3(S^2/Z_2) = Z$, and the particle-like soliton amounts to an inhomogeneous distribution of the field of the director localized in a region of finite dimensions, outside of which the distribution is uniform.[24] As a rule, such solitons are unstable with respect to decrease in dimensions and subsequent disappearance on scales smaller than the coherence length ξ. Actually the decrease in dimension of the soliton $L \to L\mu\,(\mu < 1)$ entails an increase in the elastic-energy density of the soliton by a factor of $1/\mu^2$ and a decrease in its volume by a factor of μ^3, so that the total elastic energy decreases[24,26,146]: $F \to F\mu$. Stabilizations of particle-like solitons can be facilitated by any additional interaction, in particular, helical twisting of the structure[146] (in this regard see Ref. 147 on the role of solitons in an NLC-SLC transition).

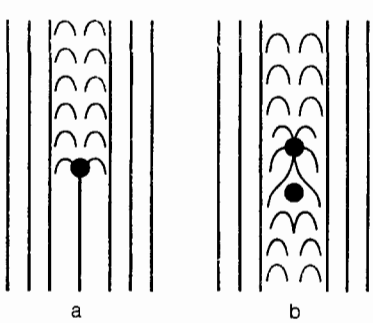

FIG. 14. a—Linear soliton in a uniaxial NLC arising at a hedgehog with $N = 1$ in the presence of a magnetic field.[24] b—Annihilation of a soliton owing to creation and separation of a pair of hedgehogs with $N = 1$ and $N = -1$.[24]

Bouligand[148,149] obtained a very interesting experimental result that confirms the presence in LCs of topologically stable structures described by the group $\pi_3(S^2/Z_2) = Z$. In a weakly twisted nematic-cholesteric mixture Bouligand observed two singly linked annular nonsingular disclinations of strength $m_1 = m_2 = 1$, each of which by itself is topologically unstable, whereby all points of the nucleus of the disclination are mapped into a single point of the degeneracy space S^2/Z_2. As he was able to show, in going from one ring to the other, the director undergoes a 180° rotation and one can represent the rings as inverse images of two diametrically opposite points on the sphere S^2 (in the absence of singularities in the configuration, one can replace the director **n** with the vector **n**′). Evidently one cannot convert the configuration into a homogeneous state because the rings are linked: upon trying to unlink the rings, they must intersect one another and singularities arise in the configuration. The degree of linking of the rings, equal in this case to unity, coincides with the Hopf invariant, which is an element of the group $\pi_3(S^2/Z_2) = Z$. Thus the stability of the configuration as a whole is guaranteed by the conservation of the Hopf invariant.

4. BIAXIAL NEMATICS

A biaxial nematic phase was found experimentally quite recently—in lyotropic systems, as an intermediate between uniaxial cylindrical and discotic phases.[110,150,151] Apparently the structural units of such media—micelles—have the symmetry of a parallelepiped, or in other words, the symmetry of point group D_2. The order parameter is the triad of directors $\mathbf{l} \equiv -\mathbf{l}$, $\mathbf{n} \equiv -\mathbf{n}$, $[\mathbf{n},\mathbf{l}] \equiv -[\mathbf{ln}]$, which corresponds to the orientational order of both the long and short axes of the micelles. Consequently the degeneracy space of a biaxial NLC is the space SO(3) of rotations of the triad **l**, **n**, [**ln**], factored by the point group D_2 of 180° rotations about the directions **l**, **n**, and [**nl**][14]:

$$R_{\mathrm{bx}} = \mathrm{SO}\,(3)/D_2, \tag{4.1}$$

or, as is the same, since $\mathrm{SO}(3) = S^3/Z_2$, we have

$$R_{\mathrm{bx}} = S^3/Q, \tag{4.2}$$

Here S^3 is a three-dimensional sphere in four-dimensional space, Q is the quaternion group $\{1, -1, i, -i, j, -j, k, -k\}$ with the following multiplication rules:

$$ij = -ji = k,\quad jk = -kj = i,\quad ki = -ik = j,$$

$$ii = jj = kk = -1. \tag{4.3}$$

Thus the degeneracy space of the biaxial NLC is the sphere S^3, each point of which has seven equivalent points obtained by inversion and 180° rotations of the triad **l**, **n**, and [**nl**].

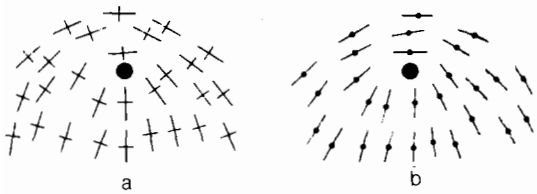

FIG. 15. Distribution of the fields of the directors **l** (long segments) and **n** (short) for disclinations of different types in a biaxial NLC. Cross sections in a plane perpendicular to the axis of the disclinations are shown. a—Disclination of strength $m = 1/2$, singular both in the field **l** and the field **n** (class C_z). b—Disclination with $m = 1/2$ singular only in the field **l** (class C_y).

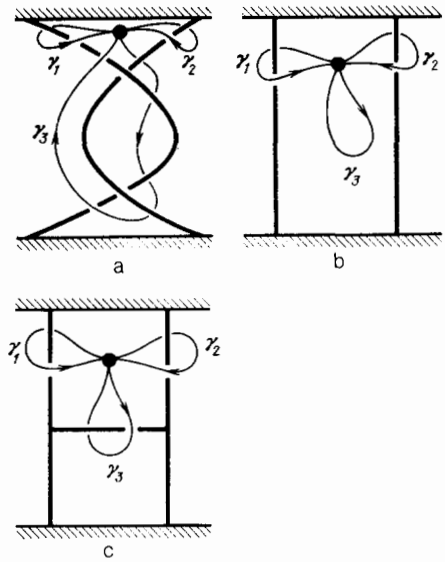

FIG. 16. Linkage of disclinations in a biaxial NLC (see the text).

4.1. Disclinations

4.1.1. Processes of merger-decay and linking

The fundamental group describing the disclinations in a biaxial NLC,[14]

$$\pi_1 (S^3/Q) = Q, \tag{4.4}$$

is noncommutative and consists of five classes of coupled elements. Because of this, the properties of disclinations in a biaxial NLC differ sharply from those of disclinations in a uniaxial NLC. Among them we should distinguish five, rather than one, classes of topologically stable lines, which correlate with the five classes of coupled elements of the group Q[6,14]:

$$C_0 = \{1\}, \quad \overline{C}_0 = -\{1\}, \quad C_x = \{i, -i\},$$

$$C_y = \{j, -j\}, \quad C_z = \{k, -k\}. \tag{4.5}$$

Correspondingly, the topological charge can acquire the values 1; -1; $(i, -i)$; $(j, -j)$; $(k, -k)$, with the multiplication rules of (4.3). The structure of the different disclinations is shown in Fig. 15. Analogously to the situation for the disclinations in a uniaxial NLC, the classification of the defect lines in a biaxial NLC is given not only by the element of the quaternion group Q, but also by the strength m, which can be integral or half-integral. In the sole experiment on defects in a biaxial NLC, precisely disclinations with $m = 1/2$ were observed.[152]

We should especially emphasize that the five classes of disclinations correspond specifically to the classes of elements of the group Q, rather than to the elements themselves. Actually disclinations corresponding to different elements, e.g., k and $-k$ of the same class C_z, can be converted into one another by continuous transformations, which implies their topological equivalence. A natural consequence of this is that the merger and decay of disclinations in a biaxial NLC obeys the multiplication rules specifically of the classes of elements, rather than the elements themselves.[14,22] The results of this multiplication[22] are given by the table. If two disclinations belonging to two different classes of the group Q merge, then a disclination is formed that belongs to the class of the product of the first two. The result of merger of disclinations of the same class from the set C_x, C_y, C_z is ambiguous: either a homogeneous distribution (class C_0) or a disclination from class $\overline{C}_0$ can be formed, depending on the path of merger with respect to other defect lines in the system.

The ambiguity of the results of multiplication of the classes of the group Q is also manifested in the decay of defects. Thus, any disclination from the classes C_x, C_y, of C_z can catalyze the disappearance of any disclination of the class $\overline{C}_0$. To do this, it suffices to unlink the latter into two that do not belong to the class of the catalyst line, and then bring them together again along paths that pass on opposite sides of the catalyst.

The cited features of the merger and decay of disclinations are a consequence of the noncommutativity of the group Q. Another consequence of this is the features of the processes of linking of disclinations in biaxial nematics,[10,14,22,153–155] which we shall now proceed to discuss.

Figure 16a shows two mutually linked disclinations. The question is whether they can be transformed by continuous variations of the field of the order parameter into an unlinked configuration (Fig. 16b), if we require that the

TABLE I.

	C_0	$\overline{C}_0$	C_x	C_y	C_z
C_0	C_0	$\overline{C}_0$	C_x	C_y	C_z
$\overline{C}_0$	$\overline{C}_0$	C_0	C_x	C_y	C_z
C_x	C_x	C_x	C_0 или $\overline{C}_0$	C_z	C_y
C_y	C_y	C_y	C_z	C_0 или $\overline{C}_0$	C_x
C_z	C_z	C_z	C_y	C_x	C_0 или $\overline{C}_0$

ends of the disclinations remain fixed.

To find the answer let us draw three contours γ_1, γ_2, and γ_3 from the point P of real space (see Fig. 16) whose images in degeneracy space will be the contours Γ_1, Γ_2, and Γ_3. Evidently the defects can be unlinked only when the contour Γ_3 is homotopic to zero. If this is not so, then separation of the disclinations will lead to appearance in the medium of a distinctive trace in the form of a third disclination (Fig. 16c). The result depends on the nature of the linked disclinations. Actually one can show[10,22] that the contour Γ_3 is homotopic to the product $\Gamma_1\Gamma_2\Gamma_1^{-1}\Gamma_2^{-1}$; an element of this form is called a commutator in the fundamental homotopy group. For Abelian groups the commutator always coincides with the identity element, since $\Gamma_2\Gamma_2 = \Gamma_2\Gamma_1$. This is not true for non-Abelian groups; in particular, for the group Q the contour Γ_3 can belong either to the class $C_0(\Gamma_1\Gamma_2\Gamma_1^{-1}\Gamma_2^{-1} = 1)$ or to the class $\overline{C}_0$ $(\Gamma_1\Gamma_2\Gamma_1^{-1}\Gamma_2^{-1} = -1)$. The latter situation correponds to linking of two disclinations belonging to different classes of the set C_x, C_y, C_z. Therefore, after drawing the lines through one another, they prove to be connected by a disclination belonging to $\overline{C}_0$. Since increasing the length of the bridge disclination requires an increase in elastic energy, as Toulouse noted,[14] a biaxial NLC must manifest a distinctive "topological stiffness" under mechanical deformations.

The single linkage that we have discussed has been generalized to p-fold linkage.[154] It turns out that all $2p$-fold linkages in a biaxial NLC reduce to the configuration shown in Fig. 16b, and all $(2p+1)$-fold to the configuration shown in Fig. 16c. Poenaru and Toulouse[153] and also Monastyrsky and Retakh[155] have conducted a generalized study of linkages of defects of different dimensionality.

4.1.2. Disclinations in phase transitions

As is known from the existing experimental data[110,150–152] a biaxial nematic phase arises in lyotropic systems as an intermediate between two uniaxial phases. The transitions occur under varying concentration and/or temperature. The question arises of how the set of topological defects changes hereby. Trebin[26] has studied this problem with the example of a biaxial-uniaxial NLC transition with cylindrical structural elements (the degeneracy space S^3/Q is transformed into S^2/Z_2). Let a disclination exist in a biaxial NLC. We shall assume that the order parameter is transformed in the phase transition in the same way at every point of this inhomogeneous system (apart from the core of the defect) as in a homogeneous medium. Let us surround the disclination with the contour γ, whose image in the space S^3/Q we shall denote as Γ. In the phase transition the contour Γ is transformed into the contour Γ_1 from the space S^2/Z_2. Evidently, if the contour Γ_1 is homotopic to zero, then the test disclination after the phase transition will become topologically unstable. On the whole, all the disclinations will become unstable that correspond to elements of the group $\pi_1(S^2/Z_2)$, i.e., those belonging to the kernel of the homomorphism

$$\pi_1(S^3/Q) \to \pi_1(S^2/Z_2). \tag{4.6}$$

The kernel of the homomorphism of (4.6) in the transition being studied corresponds to disclinations of the classes $\overline{C}_0$ and C_x. Consequently they lose topological stability in the process of transition to a calamitic and can continuously disappear. As regards disclinations of the classes C_y and C_z, they are transformed into topologically stable disclinations with $m = \pm 1/2$.

In the second biaxial-uniaxial discotic NLC transition, disclinations of the class C_x are now conserved, but disclinations of C_y disappear. It is useful to remember this property in the experimental identification of disclinations as belonging to the classes of the quaternion group Q.

The rules of transformations of disclinations in the reverse direction of transition, from a uniaxial to a biaxial phase, can be easily derived from what we have discussed above. The problem of transformation of point defects looks less trivial. Actually, hedgehogs can exist in the bulk of a uniaxial NLC. In a biaxial NLC, since $\pi_2(S^3/Q) = 0$, such defects do not exist. Then what are hedgehogs transformed into? It turns out that they cease to be isolated and are converted into monopoles—point centers from which defects of higher dimensionality—disclinations—emerge.[26] Such an effect was first predicted for superfluid ^{3}He-A[117] and for SLCs.[156] Experimental confirmation exists for the SLC-A—SLC-C transition in a spherical drop, where a point hedgehog is replaced by a monopole with one or two disclinations[157] (see also Sec. 6.3). However, in biaxial NLCs, monopoles must be unstable, since their stability in condensed media arises from one-dimensional translational order, which biaxial NLCs do not have. Therefore we must expect that the monopoles formed from hedgehogs in a biaxial NLC will move to the surface of the system (owing to contraction of the defect lines associated with them) and be converted into boojums—point surface singularities.

4.2. Boojums

The existence of boojums in a biaxial NLC arises from the nontriviality of the relative homotopy group $\pi_2(S^3/Q, \tilde{\mathscr{R}}_{bx})$. As is implied by Ref. 125, the latter is isomorphic with the nucleus of the homomorphism

$$\pi_1(\tilde{\mathscr{R}}_{bx}) \to \pi_1(S^3/Q) \tag{4.7}$$

($\tilde{\mathscr{R}}_{bx}$ is the degeneracy space of a biaxial NLC at the surface). It would seem that the problem of topological classification of boojums is reduced to finding the space $\tilde{\mathscr{R}}_{bx}$, whose form depends on the boundary conditions, and in calculating the kernel of the homomorphism (4.7).

For example, let the director $\mathbf{l}$ be oriented perpendicular to the surface, and the director $\mathbf{n}$ lie in the plane of the surface. Then we have $\tilde{\mathscr{R}}_{bx} = S^1/Z_2$ and

$$\operatorname{kern}(\pi_1(S^1/Z_2) \to \pi_1(S^3/Q)) = 2Z = \{0, \pm 2, \pm 4, \ldots\}. \tag{4.8}$$

This implies the existence of topologically stable boojums with a charge m_n equal to multiples of two (Fig. 17). The charge m_n is the number of turns of the director $\mathbf{n}$ in passing around the defect along a closed contour lying at the boundary.

We must also fix the topological charge N_l that characterizes the distribution of the field $\mathbf{l}$ and is defined as the degree of mapping of a hemisphere $\tilde{\sigma}$ surrounding the boojum on the sphere S^2 of possible orientations of $\mathbf{l}$ in the bulk:

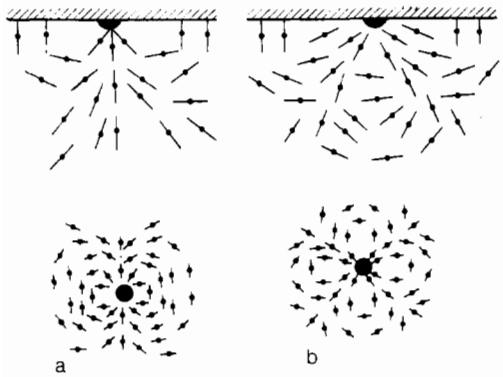

FIG. 17. Boojums in a biaxial NLC. Above—distribution of the field **l** in a cross section by a vertical plane along the symmetry axis; below—distribution of the field **n** at the surface of the NLC. a—Boojum with $m_n = 2$. b—Boojum with $m_n = 4$.

$$N_l = \frac{1}{4\pi} \int_\sigma \mathbf{l} \left[\frac{\partial \mathbf{l}}{\partial \theta} \frac{\partial \mathbf{l}}{\partial \varphi} \right] d\theta\, d\varphi = 0,\ \pm 1,\ \pm 2,\ \ldots, \tag{4.9}$$

The classification of boojums in a biaxial NLC looks somewhat more complicated under inclined conic boundary conditions. In addition to integral charges, we must assign also continuous charges, depending on the boundary conditions, analogously to the situation in a uniaxial NLC (see Sec. 3.3).

There are as yet no experimental confirmations of the existence of boojums in biaxial NLCs. In view of the Poincaré and Gauss theorems, an isolated boojum with $m = 2$ and $N = 1$ ought to be observed in spherical drops of a biaxial nematic. Interestingly, on changing the boundary conditions the dynamics of the defects in such a drop is restricted to the very same boojum.[27]

5. CHOLESTERICS

A cholesteric in equilibrium possesses a structure in which the director **n** describing the orientation of the long axes of the molecules is twisted into a helix:

$$\mathbf{n}(\mathbf{r}) = \mathbf{n}(\mathbf{r}_0) \cos\left[\frac{2\pi}{P} \mathbf{l}(\mathbf{r}_0)(\mathbf{r} - \mathbf{r}_0)\right] + [\mathbf{l}(\mathbf{r}_0)\,\mathbf{n}(\mathbf{r}_0)] \sin\left[\frac{2\pi}{P} \mathbf{l}(\mathbf{r}_0)(\mathbf{r} - \mathbf{r}_0)\right]$$

(**l** is the unit director of the axis of the helix, and P is the pitch of the helix). Just as in a biaxial NLC, the order parameter has the form of the triad **l**, **n**, [**nl**], while the degeneracy space[6] is $\mathscr{R}_{\rm ch} = S^3/Q$.

This conclusion is valid only for scales much greater than the pitch of the helix of the CLC; for scales comparable with the pitch of the helix or smaller we have

$$\mathscr{R}_{\rm ch} = \mathscr{R}_N = S^2/Z_2.$$

The classification of defects in CLCs in the large-scale approximation coincides with that of defects in biaxial NLCs owing to the coincidence of their degeneracy spaces[6]: there are no point singularities—hedgehogs, while the disclinations are described by the five classes C_0, $\overline{C}_0$, C_x, C_y, and C_z of the quaternion group Q. The first three classes describe linear defects lacking singularities in the distribution of the field **n**, since they belong to the kernel of the homomorphism[158] $\pi_1(S^3/Q) \to \pi_1(S^2/Z_2)$. The dimension of the core of such defects is comparable with the magnitude of the pitch of the helix of the CLC. The two other classes, C_y and C_z, describe disclinations with a singular core whose dimensions are of the order of molecular dimensions (or, as in the case of disclinations with a singular core in a uniaxial NLC, somewhat larger).

In describing defects in CLCs, it is accepted to use the long-established terminology of Kléman and Friedel,[159] according to which three types of disclinations are distinguished: $\lambda(m)$, $\tau(m)$, and $\chi(m)$. Their distribution among the classes of the quaternion group Q looks as follows[6]:

$$C_0\colon \lambda(2p),\ \tau(2p),\ \chi(2p),$$
$$\overline{C}_0\colon \lambda(2p+1),\ \tau(2p+1),\ \chi(2p+1),$$
$$C_x\colon \lambda\left(p+\tfrac{1}{2}\right),\quad C_y\colon \tau\left(p+\tfrac{1}{2}\right),\quad C_z\colon \chi\left(p+\tfrac{1}{2}\right);$$
$$p\text{—integer},$$

(the strength of the disclination is noted in parentheses). Here, in the λ-lines, the long axes of the molecules are parallel to the axis of the disclination, perpendicular in τ (respectively nonsingular and singular cores) (Fig. 18). In both cases the axis of the helix **l** is always perpendicular to the axis of the defect. In contrast to λ- and τ-lines, χ-lines can be oriented at different angles to **l**.

An extensive literature[11,44,53,72,81,106,148,159–171] has been devoted to experimental studies of disclinations in CLCs and their behavior in external fields. Most of these studies treated χ-lines (singular—of strength $\pm 1/2$ and nonsingular—of strength ± 1) in plane textures of a Kano wedge that were oriented perpendicular to the helical axis **l**. Calculations of the energy of such disclinations are given in Ref. 172. As a rule, χ-lines in a Kano wedge dissociate into disclination pairs $\lambda\lambda$, $\lambda\tau$, and $\tau\tau$.

Unpaired λ- and τ-disclinations of strength $\pm 1/2$ are observed in another geometry of experiment—in "fingerprint" textures. An unusual result here was obtained recently by Livolant,[173] who studied cholesteric structures of DNA in chromosomes of algae of the group of dinoflagellates obtained *in vitro* and *in vivo*.[2)] Just as in fingerprint textures, λ- and τ-lines were observed. Amazingly, "live" chromosomes contained only τ-disclinations, and "nonliving" only λ. Apparently this distinction is based on energy factors. We note also that λ-lines of strength $m = 1$ can be

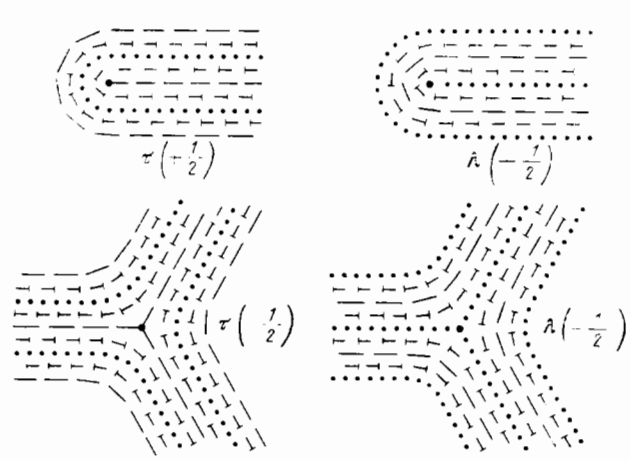

FIG. 18. λ and τ disclinations in a CLC.[159]

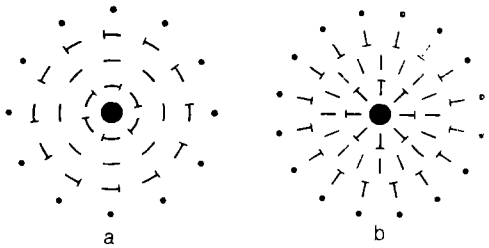

FIG. 19. Models of bubble domains in CLCs.

contained in bubble domains that arise in CLCs under the action of various external fields (temperature, ultrasound, electric[177–180]). A simple model of such a domain with a $\lambda(+1)$-disclination proposed by Akahane and Tako[181] is shown in Fig. 19a. In essence it is a transfer of the model of Cladis and Kléman[182] of the structure of band domains to the structure of bubble domains. However, as these same authors have recently shown on the basis of data of not only polarization but also holographic and interference microscopy, the model shown in Fig. 19b is more adequate to the experimental data.[183]

Now let us study disclinations whose axis coincides with the axis of the helix—vertical χ-lines. The properties of $\chi(+1)$-lines with $m=1$ have been most fully studied.[11–53,81,161,163,165–167,170–171] As is implied by polarizing-microscope observations, a model of the core of such a disclination has the following features (Fig. 20):

a) molecules in the core are oriented along the axis of the defect;

b) the dimensions of the core are comparable with the pitch of the CLC helix;

c) point and linear singularities can arise in the core.

As a rule, an isolated $\chi(+1)$-disclination has a straight shape. However, two paired $\chi(+1)$-disclinations always exist in a twisted state owing to the helical twist of the medium itself. Here the mutual repulsion tends to increase the distance between them. However, owing to the nonzero linear tension of the disclinations, the helicoidal configuration remains stable.[99] Yet if the disclinations are of unequal strengths, and hence, unequal values of the linear tension, then one of them (having the greater tension) remains straight, while the other wraps around the former. This has been actually observed experimentally for different situations: for a pair $\chi(+1)$, $\chi(-1)$[163,165] and for a system of one $\chi(+2)$ and two $\chi(-1/2)$ disclinations.[72]

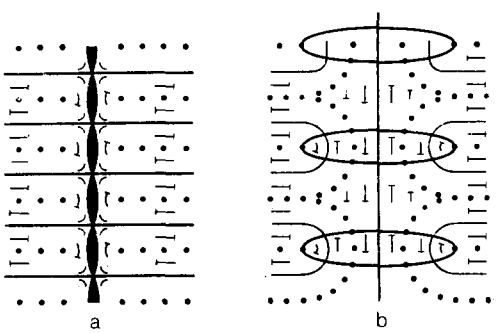

FIG. 20. A vertical $\chi(+1)$ disclination in a CLC containing point (a) and linear ring (b) defects in the core.[167]

In many substances in a narrow temperature range (~ 1 °C) one or several intermediate phases exist between the isotropic and cholesteric phases that are called blue phases (see the review of Ref. 184). It has been established experimentally that the so-called I and II blue phases have a periodic cubic structure. In particular, this is indicated by micrographs[185] of monocrystals of a blue phase I in which screw dislocations are distinctly visible that arose in the process of growth of the single crystal from the melt. However, more interestingly, the lattice itself of these phases is apparently nothing other than a periodic network of disclinations. The point is that, in the general case, chiral molecules are not constrained to form a structure twisted in only one direction, as in an ordinary CLC: twist in two directions is locally more favorable (see Fig. 12). However, double twist cannot propagate continuously to large volumes. Therefore a lattice of singularities arises in the system in the form of disclinations of strength $m=-1/2$ that is stable for a certain relationship of the parameters of the system (for more details see the review of Ref. 184).

6. A AND C SMECTIC PHASES

The main distinctive feature of smectic liquid crystals consisting of rod-shaped molecules is their layered order. The density function of SLCs of types A and C, in contrast to NLCs and CLCs, is modulated along the normal to the layers with a period of the order of the length of a molecule $u \sim 10^{-8}$ m. Within each layer the density is constant, and the molecules are oriented either normal to the layer (SLC-A) or are inclined (SLC-C). Such types of order are widespread, not only in thermotropic, but also in lyotropic and biological systems (lamellar structures, membranes, etc.).[17,89]

The orientational order of an SLC-A, just like an NLC, is described by the director **n**. Moreover, one must also take account of the translational order along the normal to the layers. To find the degeneracy space of an SLC-A, we can use the general formula (2.4); as Kléman and Michel[156] showed, we have

$$\mathscr{R}_A = R^3 \times \mathrm{SO}(3)/(R^2 \times Z) \,\square\, D_{\infty h}. \tag{6.1}$$

Analogously, for an SLC-C we have

$$\mathscr{R}_C = R^3 \times \mathrm{SO}(3)/(R^2 \times Z) \,\square\, C_{2h}. \tag{6.2}$$

We must choose the orientational part of the order parameter of an SLC-C in the form of the triad **n**, $\boldsymbol{\tau}$, $[\boldsymbol{\tau}\mathbf{n}]$, where $\boldsymbol{\tau}$ is the unit vector fixing the orientation of the projections of the molecules in the plane of the layer, and **n** is the normal to the layer.[186]

Also chiral SLC-C*'s are known, in which the direction of the long axes of the molecules precesses about the normal to the layers. The symmetry of the phase is reduced here to the group C_2, and we have $\mathscr{R}_{C^*} = R^3 \times \mathrm{SO}(3)/(R^2 \times Z) \square C_2$.

6.1. Dislocations and disclinations

To establish the types of topologically stable singular lines in SLC-A's and SLC-C's, we must calculate the groups $\pi_1(\mathscr{R}_A)$ and $\pi_1(\mathscr{R}_C)$. In view of the complexity of the degeneracy spaces of $\mathscr{R}_A$ and $\mathscr{R}_C$ (see (6.1) and (6.2)), the direct algebraic approach to the calculations is difficult.

Therefore we shall use a more graphic geometric scheme for calculation with the example of SLC-A.

We can represent the degeneracy space of an SLC-A in the form of a continuous torus $(S^2/Z_2)\times S^1$. The vertical cross sections of the torus in the form of two circles amount to hemispheres of S^2/Z_2 stretched into disks whose points characterize the orientation of the director **n**. The points lying along the large circles of the torus correspond to points along the segment $[0,u]$ closed into the circle S^1. Two types of elementary contours not homotopic to zero exist in the degeneracy space $(S^2/Z_2)\times S^1$: Γ_1, which joins diametrically opposite points of the disks S^2/Z_2 and which describes the disclinations, and Γ_2, which runs through the hole of the torus and describes the dislocations. The fundamental group of the degeneracy space of an SLC-A, $\pi_1(S^1/Z_2)\times S^1)$, therefore has the form

$$\pi_1(\mathscr{R}_A) = \pi_1(S^1)\times\pi_1(S^2/Z_2) = Z\times Z_2\,. \qquad (6.3)$$

It has the elements (b,p), where b is an integer, and p takes on the values 0 and 1. This presupposes the existence in the SLC-A of a single class of stable disclinations (elements (0,1)), an infinite number of classes of dislocations with different values of the Burgers vector that are multiples of u (elements $(b,0)$), and also combinations of them, or disgyrations.

For an SLC-C we can easily calculate the group $\pi_1(\mathscr{R}_C)$ by using the relationship $\mathscr{R}_A = \mathscr{R}_C/S^1$, which implies that each point of $\mathscr{R}_A$ corresponds in $\mathscr{R}_C$ to an entire family S^1 of points fixing the orientation of the vector $\boldsymbol{\tau}$ in the plane of the layer, owing to the inclination of the molecules in the layers of the SLC-C. Direct calculation shows that

$$\pi_1(\mathscr{R}_C) = Z\,\square\,Z_4. \qquad (6.4)$$

Here $Z_4 = (I,a,a^2,a^3)$ is the group of subtractions modulo 4 with the unit element I.

6.1.1. Dislocations in smectics-A

Just as in ordinary crystals, edge and screw dislocations are singled out in SLC-A's (Fig. 21a,b). We see from Fig. 21 that dislocations in SLC-A's are not associated with singularities of the field of the director, and thus are very simple examples of semidefects. The term "semidefect" was introduced recently[187] to denote disturbances of order that involve a singular distribution of not the entire order parameter, but only a part of it. Since the distribution of the director involves the distribution of the optic axis, the stated feature makes the direct observation of elementary dislocations in SLC-A's using the light microscope extremely difficult. It is relatively simple to observe dislocations or groups of them having large Burgers vectors[188,189]; here there are grounds for assuming that groups of dislocations enter into the composition of the so-called oily streaks.[48,58,59,190] However, despite the fact that oily streaks are very often found in the most varied layered media, the question of their detailed structure remains under discussion.[58,59,191,192] To all appearance, the wealth of models involves the very nature of oily streaks and the dependence of their structure on the concrete values of the parameters of the medium.

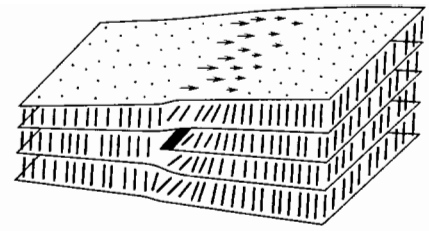

FIG. 22. SLC-A–SLC-C phase transition involving an edge dislocation in a wedge.

In recent years special experimental methods have been developed to detect isolated elementary edge dislocations.[58,59,193,194] In thermotropic smectics Meyer, Lagerwall, and Stebler have used the features of a second-order SLC-A–SLC-C phase transition in wedge-shaped cells with an angle $w\sim 10^{-4}$ radian and a normal orientation of the molecules at the surface (Fig. 22).[193] The geometry of the cell necessarily led to the formation of a system of edge dislocations separated from one another by the distance $w/u\sim 10$ μm. The idea of the experiment to visualize the dislocations was based on the fact that local stresses near defects in the region of a phase transition ($s=\pm u/d$, where d is the thickness of the specimen) either initiate the formation of an SLC-C ($s>0$), or hinder it ($s<0$). Actually, according to the theory of Landau, the free-energy density of the system

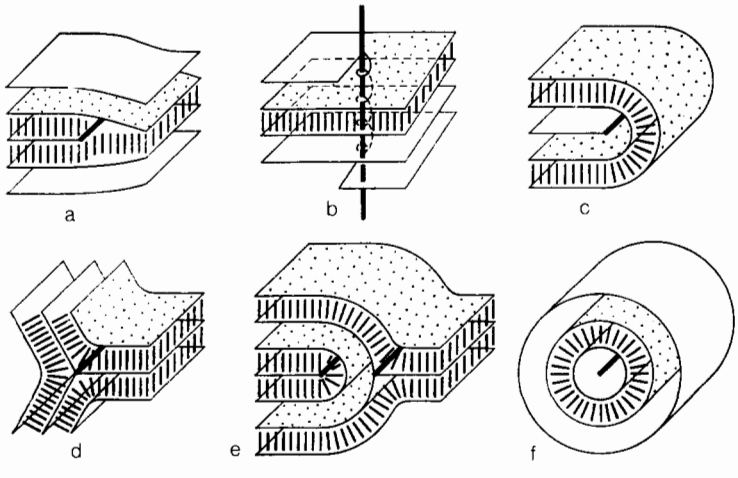

FIG. 21. Dislocations (a,b) and disclinations (c–f) in A-type SLCs.

has the following form near the transition point T_c with the imposed stress s:

$$f = f_0 + A(T - T_c)\alpha^2 + B\alpha^4 + C\left(s + \frac{1}{2}\alpha^2\right)^2. \tag{6.5}$$

Here α is the inclination angle of the molecules to the normal in the SLC-C. As the temperature is lowered to T_c in the geometry of Fig. 22, the A-phase is preserved to the left of the dislocation with $s < 0$, and the C-phase arises to the right with $s > 0$. One can easily observe the elementary edge dislocation separating the regions of the A- and C-phases in the microscope: optical contrast is made possible by the sharp change in the slope of the molecules (Fig. 22).

Chan and Webb[194] have used a similar geometry in studying a lyotropic lamellar phase L_α (lecithin in aqueous solution), a structural analog of an SLC-A. The elementary edge dislocations were detected by introducing fluorescent additives into the system. Measurement of the mobility of the dislocations ($q = 10^{-15}$ cm^{2}s/g) enabled determination of the permeation coefficient for the L_α-phase: $\eta = 10^{-30}$ cm^2/poise. Both quantities proved to be many orders of magnitude smaller than the analogous values for thermotropic SLC-A's[195] and lyotropic nonionic systems[196] ($q = 10^{-6}$–10^{-7} cm^{2}s/g and $\eta = 10^{-14}$ cm^2/poise). Apparently the differences involve the presence in the two latter systems of a large number of screw dislocations and pores, which facilitate permeation of the molecules across the layers and slip of the edge dislocations.

Dislocations in lyotropic L_α-phases have also been observed by the method of electron microscopy.[58,59,196,197] It turned out that edge dislocations are found much more rarely than screw dislocations unless special geometric conditions are fulfilled. Analogous data have also been obtained in studying thermotropic systems.[198–200] One can interpret the effect as a manifestation of the condition of equidistance of the smectic layers: in contrast to edge dislocations, screw dislocations do not alter the thickness of the layers in the first approximation, and have relatively low energies of formation.[201–202] It was shown in the theory of Loginov and Terent'ev[202] of dislocations of general form that the energy of a screw line in an SLC-A consists only of the energy of the core, while the energy of the elastic distortions outside the core vanishes. An interesting result of the theory was the prediction of an effect of combination of dislocations having a unit and doubled Burgers vector (one and two interlayer spacings) into one having a larger Burgers vector as the point of the SLC-A–NLC transition is approached.

We should mention another interesting question involving dislocations in SLC-A's. We are referring to the model of de Gennes of the SLC-A–NLC [203] (or CLC [204]) transition, based on the analogy with the superconductor-normal metal transition. Just like superconductors, SLC-A's are classified, depending on the magnitude of the ratio λ/ξ of the depth λ of penetration of deformations into the bulk and the distance ξ at which layered order breaks down, into two types—I ($\lambda/\xi < 1/\sqrt{2}$), and II ($\lambda/\xi > 1/\sqrt{2}$). Upon applying twist or bend deformations to a type II SLC-A, one should expect onset in the system of a system of dislocations that straighten the stresses in the medium (an analog of the Shubnikov phase). The known SLC-A's belong to type I (see, e.g., Ref. 205). However, it is not ruled out that cholesteryl pelargonate[206] and mixtures of it[175] form type-II SLC-A's.

6.1.2. Disclinations in a smectic-A

As a rule, disclinations in an SLC-A arise in the form of pairs of lines with $m = 1/2$ and $m = -1/2$, e.g., as a result of splitting of edge dislocations[189–191,58,59,207] (Fig. 21e). In round capillaries with a normal orientation of the molecules at the inner surface, disclinations of strength $m = 1$ were observed (Fig. 21f).[45,69,72,73,208] In contrast to the corresponding situation in NLCs, these disclinations are energetically stable; outflow into the third dimension is hindered by the condition of equidistance of the layers. In addition, another type of instability of disclinations having $m = 1$ in SLC-A's is known, namely, the appearance of a specific periodic structure near the core,[69,208] probably caused by compression of the smectic layers in the process of preparing the specimen or upon changing its temperature.[209]

6.1.3. Dislocations in a smectic-C

As a number of studies[186,210,211] have indicated, dislocations in SLC-C's are analogous in many ways in their structure to dislocations in SLC-A's. Therefore we shall not take up a detailed description of them.

6.1.4. Disclinations in a smectic-C

Disclinations in SLC-C's are classified into two types: m-lines in the distribution of the vector field $\boldsymbol{\tau}$ of the projections of molecules not involving distortions of the smectic layers, and l-lines in the distribution of the field $\mathbf{n}$ of normals to the layers.[186] Vertical m-lines are often found in schlieren textures of SLC-C's with horizontally arranged layers.[11,96,36,211,212] In contrast to nematic schlieren textures, only m-disclinations of integral strength exist, while lines of half-integral strength are not formed, which is explained by the vector and two-dimensional character of the field $\boldsymbol{\tau}$. A more convenient object for studying the features of m-lines is monopoles (see Sec. 6.3), which contain (0,1) and (0,a^2) disclinations of strength $m = 2$ and $m = 1$, respectively. As polarizing-microscope studies indicate, the cores of m-lines in monopoles are nonsingular and have a dimension of the order of 1 μm. Here, with change in the angle of inclination of the molecules to the layers, the thickness of the core changes correspondingly. The most favored model of the cores of m-disclinations is the model of a nematic core, in which the molecules are oriented along the axis of the defect (Fig. 23).

In contrast to m-lines, l-type disclinations can also have a half-integral strength. If such a disclination is not perpendicular to the plane of symmetry of the SLC-C, the distribution of the field $\boldsymbol{\tau}$ along each layer is inhomogeneous and reminds one of the distribution of spins in a Néel wall or contains a series of alternating point defects with $m = 1$ and $m = -1$.[186,213] By studying the behavior of such lines in a magnetic field, one can determine certain combinations of elastic constants of the SLC-C.[214]

6.1.5. Linear defects in chiral smectics-C

Owing to the presence of two translationally ordered one-dimensional sublattices in SLC-C*'s having a chiral twist, linear defects arise both in the distribution of the smectic layers proper and in the distribution of the "layers" of the chiral structure.[215] The different types of such defects have been studied experimentally in Refs. 200, 216.

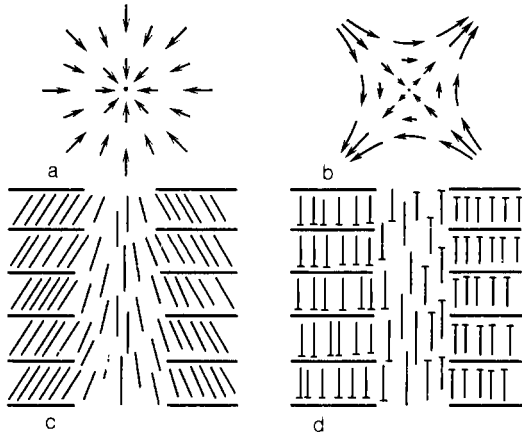

FIG. 23. Structure of disclinations in an SLC-C of strengths $m = 1$ (a,c) and $m = -1$ (b,d). Above—the field of the projections of τ of the molecules on the surface of the smectic layer (a,b); below—distribution of the molecules in a cross section by a vertical plane (c,d).

Usually the ptich of the SLC-C* helix is incommensurable with the thickness of the smectic layer; such an SLC-C* is a simple example of an incommensurable structure. If the incommensurable phase (SLC-C*) coexists with a commensurable one (SLC-C), a series of disclinations, or dechiralization lines, must arise at the phase boundary, and they separate the regions of the twisted and untwisted phases.[217] A similar situation arises in a plane cell with an SLC-C* whose helical axis is oriented along the cell under the condition that a planar orientation of the molecules has been fixed at the upper and lower surfaces of this cell—then the disclination separate the region of the SLC-C* in the bulk from an SLC-C region near the surfaces.[218–220] Movement and annihilation of dechiralization lines is one of the fundamental mechanisms of the SLC-C*–SLC-C transition in a planar specimen under the influence of an electric field.[218]

6.2. Hedgehogs and confocal domains in smectics-A

The homotopy classification of point hedgehogs in SLC-A's coincides with the classification of hedgehogs in uniaxial NLCs and predicts the existence of an infinite set of types of point singularities in the field of the director $\mathbf{n}:\pi_2(\mathscr{R}_A) = Z$. However, application of the method of homotopic groups to describing defects in smectics is restricted owing to the broken translational symmetry of these media[22,221] (in addition, see Ref. 222). Besides, this property facilitates the solution of problems of inhomogeneities of geometric constructions.[1,221,223] Since energy is required to change the thickness of a smectic layer considerably exceeding the bending energy of the layers, an SLC-A can be represented as a simple geometric image: a family of flexible, but everywhere equidistant surfaces. In particular, the geometric methods enable one to solve the rather difficult problem of filling space with a smectic. The problem is reduced to finding close packings of layers in a volume for which, first, the thickness of the layers remains invariant, second, the conditions of orientation of the molecules at the boundary are satisfied, and third, the total energy of distortions is close to minimal. Before we proceed to it, let us discuss what types of distortions are possible in principle in a system of layers.

Let us study the field of the normals to parallel smectic layers, which coincides with the field of the director in the case of an SLC-A. For a layered equidistant structure we have $\mathbf{n}\,\mathrm{curl}\,\mathbf{n} = 0$ and $\mathbf{n}\times\mathrm{curl}\,\mathbf{n} = 0$, which entails the requirement that the field lines of $\mathbf{n}$ should be straight: if a line $\mathfrak{N}$ is perpendicular to any layer $\mathfrak{M}$, then it remains perpendicular to any other layer that intersects it. The point of intersection of $\mathfrak{N}$ and $\mathfrak{M}$ is characterized by definite values of the two principal radii of curvature. The corresponding centers of curvature belong to $\mathfrak{N}$ and are also the centers of curvature for other points of intersection of $\mathfrak{N}$ with layers parallel to $\mathfrak{M}$.[221] Moreover, these centers are defects, since the radii of curvature approach zero in their vicinity.

When the normal $\mathfrak{N}$ passes through all points of the surface $\mathfrak{M}$, both centers of curvature describe a two-sheet surface $\mathfrak{E}$, which is called the focal surface or evolute of the surface $\mathfrak{M}$.[221] We can logically expect that situations are energetically favorable in which the two-dimensional defect $\mathfrak{E}$ degenerates into a zero-dimensional (point) or one-dimensional (line, pair of lines) defect.

The only surfaces with zero-dimensional evolutes are spheres. Correspondingly the only point singularities that do not alter the thickness of smectic layers will be radial hedgehogs (Fig. 24a). Their existence in SLC-A's has been shown unequivocally only recently in experiments with spherical drops, at the surface of which a normal orientation of the molecules was fixed.[43] However, in numerous experimental studies of smectic textures in plane specimens, such point defects have not been revealed in isolated form. The most characteristic structural defects of "planar" textures are linear singularities in the form of an ellipse or a hyperbola that are regular in shape and form the distinctive frames of confocal domains. One can represent an individual domain in the form of a cone of rotation whose base is an ellipse, while the vertex lies on a hyperbola (Fig. 24b). The ellipse and hyperbola are linear evolutes, to which, as is known from geometry, corresponds a single class of surfaces, namely the so-called Dupin cyclides.[224] Surfaces in the form of Dupin cyclides constitute the structure of the confocal domains. In particular, the Dupin cyclides are the cylinder, the torus, and the cone of rotation.[224] On the whole one distinguishes three types of Dupin cyclides with evolutes in the form of: (1) pairs of an ellipse and a hyperbola lying in mutually perpendicular planes so that each curve passes through the focus of the other (i.e., confocal); (2) pairs of confocal parabolas; (3) pairs of a circle and a line passing through the center of the circle.

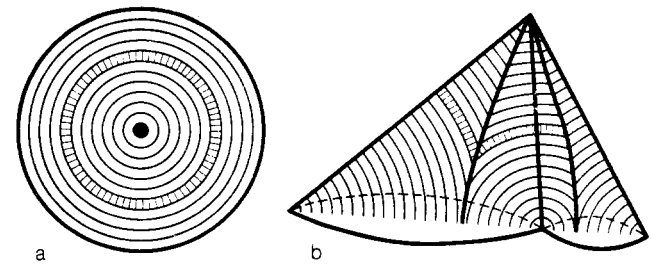

FIG. 24. Family of equidistant smectic surfaces having a zero-dimensional evolute point (radial hedgehog in the field of the normal to the layers) (a) and with a linear evolute in the form of confocal lines of an ellipse and a hyperbola (confocal domains) (b).

All three types of evolutes-linear defects have been observed experimentally (see respectively: (1) Refs. 1, 189, 225, 225 in SLC-A's, Refs. 227, 228 in SLC-C's and SLC-C*'s, Refs. 197 and 198 in lyotropic lamellar phases; (2) Refs. 229, 46 in SLC-A's, Refs. 48, 192, 230 in lyotropic phases; (3) Ref. 231 in SLC-A's, Ref. 232 in SLC-C*'s, and Refs. 58, 59, 199 in lyotropic phases).

The predominance of confocal domains over spherical and smectic textures arises from several causes: the effect of the boundary conditions, the conditions of growth and relaxation of SLCs, and finally, the balance of energy of local distortions.[233,234,148] which involve the values of the principal radii of curvature R_1 and R_2. In the general case the energy of the distortions of the system of layers of an SLC of invariant thickness is calculated by the formula

$$F=\frac{1}{2}\int K_{11}(\operatorname{div}\mathbf{n})^2\,\mathrm{d}V=\frac{1}{2}K_{11}\int\left(\frac{1}{R_1}+\frac{1}{R_2}\right)^2\mathrm{d}V \tag{6.6}$$

(V is the volume of the domain.) For each point $\mathfrak{P}$ on the surface $\mathfrak{M}$, we must take the quantities R_1 and R_2 with a definite sign that depends on whether the point $\mathfrak{P}$ is a point of elliptic ($R_1R_2>0$) or hyperbolic ($R_1R_2<0$) curvature. For a spherical system of layers we have $R_1=R_2=R>0$, and $F_{\mathrm{sph}}=8\pi K_{11}R$. However, when $R_1R_2<0$, which is realized in part of the volume of the confocal domain, the energy can be even smaller. In particular, as Kléman[234] has shown, the energy of a toroidal domain with Dupin cyclides of type (3) amounts to

$$F_{(3)}=2\pi^2K_{11}R\left(\ln\frac{2R}{\rho}-2\right). \tag{6.7}$$

Here R is the radius of the circle. An "ordinary" confocal domain with Dupin cyclides of type (1) can have an even smaller energy:

$$F_{(1)}=\pi K_{11}(1-e^2)\,p\ln\frac{a}{\rho}. \tag{6.8}$$

Here e, p, and a are the parameters of the ellipse: respectively the eccentricity, the perimeter, and the semimajor axis.

Usually in textures one observes not isolated domains, but entire groups of confocal domains in contact. Here no two-dimensional defects, or walls, are formed. The question arises: how do the layers fill space without creating defects of a dimensionality higher than unity? For a long time the only model was that of iterational filling,[235] in which the interstices between large domains are occupied by smaller domains, etc., down to molecular scales. Such iterations are actually manifested in many textures. However, as a rule, the process is interrupted at scales much larger than molecular. As we see from Fig. 25, regions exist between the large domains that are free from smaller domains, and hence are filled with layers of a special form.

The second model, which was studied by Sethna and Kléman,[221] explains the filling of the intermediate regions between the confocal domains by the appearance of systems of concentric spherical layers. The model is rather simple.

Let us study a sphere with a spherical concentric system of layers (Fig. 26a) and dissect from it several spherical sectors along the surfaces of circular cones of normals $\mathfrak{N}$ with vertices at the center of the sphere. We shall fill the inner regions of the cones with layers with a configuration of Dupin cyclides, i.e., individual confocal domains. Since at the surface of "joining" the lines $\mathfrak{N}$ are common normals for the layers of both domains–both the spherical and the confocal—we can easily see that such a construction is what enables a smooth transition of the layers between the confocal domains owing to the regions of the spherical domain filling the interstitial regions. One can see the possibility of such a filling with the example of spherical drops of an SLC-A (Fig. 26b).[27,236]

FIG. 25. Texture with confocal domains in an SLC-A.

It was shown recently[236] that in other experimental geometries the filling of space with smectic layers of invariant thickness can be attained exclusively by combination of spherical and focal domains. The overall scheme of the filling proposed in Ref. 236 consists in the following (Fig. 27).

On large scales comparable with the charactertistic dimension L of the system, the filling is carried out with confo-

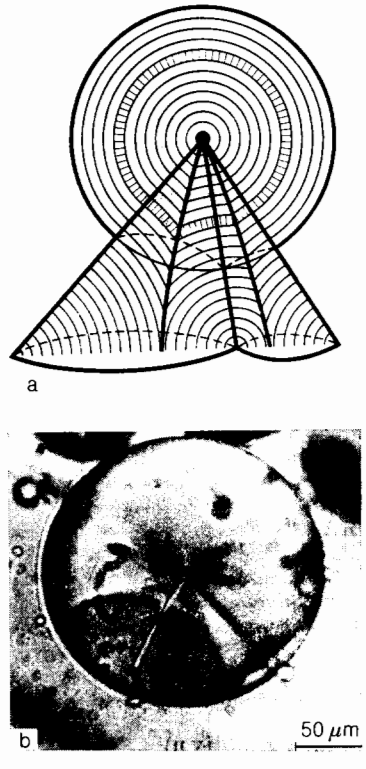

FIG. 26. Filling of the interstices between confocal domains with layers of spherical form. a—Model of Sethna and Kléman.[221] b—Micrograph of a spherical drop of an SLC-A having a structure analogous to that shown in Fig. a.

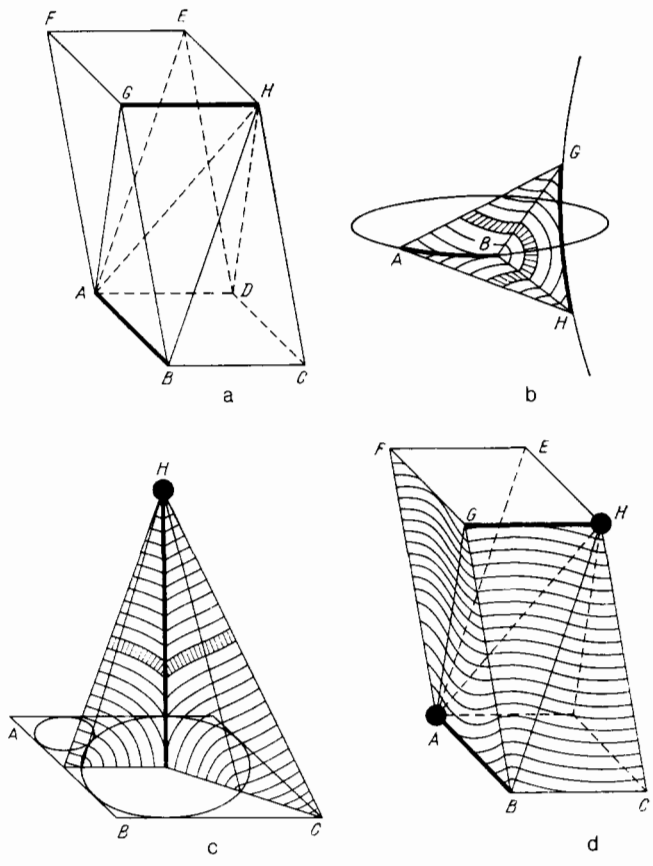

FIG. 27. Overall diagram of the filling of space by smectic layers. a—Subdivision of a parallelepiped with which space can be filled by parallel transport into a pair of pyramids H ($ABCD$) and A ($EFGH$) and a pair of tetrahedra $ABGH$ and $ADEH$. b—Filling of the tetrahedron $ABGH$ with a unitary family of cyclides of Dupin intersecting its faces at a right angle. c—Filling of a pyramid with a unitary family of spherical layers into which confocal domains have been smoothly incorporated. d—Diagram of the smooth transition of layers from a pyramid to a tetrahedron within the limits of a single parallelepiped.

cal domains of dimension $\sim L$. The interstices between them are occupied by smaller confocal domains, etc., until the dimensions of the bases (ellipses) of the smallest domains reach some critical scale ρ^* determined by the balance of bulk and surface energy. In the general case we have

$$\rho^* = L\left(a + \frac{bL\Delta\sigma}{K_{11}}\right)^{-1}.$$

Here a and b are numerical constants that depend on the geometry of the system, $\Delta\sigma = \sigma_\perp - \sigma_\parallel$, and $\sigma_\perp$ and $\sigma_\parallel$ are the values of the surface tension for orientations of the molecules normal and tangential to the boundary, respectively.

On scales smaller than ρ^*, the hierarchy of confocal domains is replaced by a packing of layers of spherical form that enable a smooth transition between the confocal domains and completely fill all the free interstices.

Generally speaking, the described hierarchy of structures is realized in a limited part of the space in the form of pyramids; each pyramid is associated with one family of contiguous confocal domains with a common vertex and one family of spherical concentric layers (the center is at the vertex of the pyramid) (see Fig. 27c). The lateral faces of each pyramid, whose base can be any polygon, are adjoined by tetrahedra completely filled with layers of one single confocal domain (see Fig. 27b). In turn the tetrahedra are adjoined by pyramids rotated by 180° with respect to the initial one, etc. One can trace how the linkage of the layers among all the stated polyhedra is brought about smoothly, without creating walls (for more details see Ref. 236). Thus the only defects in the system are point hedgehogs and linear defects.

In real experiments the structure of the spherical and confocal domains can be distorted, first, by the breakdown of the conditions of equidistance of layers $\mathbf{n}\cdot\mathrm{curl}\mathbf{n} = 0$ and $\mathbf{n}\times\mathrm{curl}\mathbf{n} = 0$, which implies the appearance, respectively of edge and screw dislocations,[223,162] and second, by tendency of the Dupin cyclides to adopt the form of minimal surfaces ($R_1 = -R_2$), which perhaps has been observed in certain cases for lyotropic[59] and cholesteric thermotropic[162] phases. However, on the whole these distortions do not introduce substantial changes into the large-scale pattern of filling.

6.3. Monopoles and confocal domains in smectics-C

Isolated point singularities are absent in SLC-C's: $\pi_2(\mathscr{R}_C) = 0$. The question arises of how the structure of a radial hedgehog is transformed in a system of spherical concentric layers in an SLC-A–SLC-C transition.

If the smectic layers keep their spherical packing in the process of the phase transition, a point hedgehog with $N = 1$ exists in the field of the normal $\mathbf{n}$ in the C-phase, just as in the A-phase. However, in the SLC-C this defect is no longer isolated. Actually, owing to the inclination of the molecules at the surface of each layer of the SLC-C, a tangential field $\boldsymbol{\tau}$ of the projections of the molecules arises, and in view of the Poincaré theorem, the radial hedgehog proves to be associated with disclinations in the field $\boldsymbol{\tau}$. This can be a single line of strength $m = 2$ or two with strength $m_1 = m_2 = 1$ (respectively (0,1) and $(0,a^2)$ disclinations).[156] The structure that is produced in the form of a hedgehog, from whose center one or two disclinations emerge, is a monopole in the SLC-C. Topologically the formation of a monopole in the SLC-A–SLC-C transition is analogous to the formation of a boojum from a hedgehog in the uniaxial-biaxial NLC transition. Actually a monopole is a boojum drawn from the surface into the bulk and linked to this surface by a disclination. The stability of such a structure is enabled by the conservation of the distance between the smectic layers.

A representation of monopole structures first arose in 1931, when Dirac predicted the existence of isolated magnetic charges in the form of a hedgehog in a magnetic field with a linked linear singularity in the field of the vector potential.[237] Despite a set of weighty arguments favoring the real existence of monopoles, experimental searches for these objects (see, e.g., Ref. 238) have yielded no unambiguous positive results. In this regard, especial interest is aroused by the study of structural analogs of monopoles in various condensed media, including liquid-crystalline–cholesterics,[239,15,81,170,171,240] and smectics-C.[156,157,241] As Volovik[239] first showed, one can introduce variables for them that directly describe the distribution of the molecules, and which coincide in their analytic expression with the form of the vector potential of a monopole of Dirac. Let us show this with the example of a monopole in an SLC-C.[157]

The order parameter of an SLC-C can be assigned not only in the form of the triad $\mathbf{n}$, $\boldsymbol{\tau}$, $[\boldsymbol{\tau}\mathbf{n}]$, but also by using the wave function $\Psi = \alpha\exp(i\varphi)$. A change in the phase of the wave function $\varphi \to \varphi + \beta$ has the meaning of a rotation of the

vectors τ and $[\tau \mathbf{n}]$ with respect to $\mathbf{n}$. The following spatial derivatives are defined for the quantity β at each point of the system:

$$\varkappa_x = \frac{\partial \beta}{\partial x}, \quad \varkappa_y = \frac{\partial \beta}{\partial y}, \quad \varkappa_z = \frac{\partial \beta}{\partial z}. \tag{6.9}$$

Since the quantity β is not a complete differential of any function (the rotations of the triad $\mathbf{n}$, τ, $\tau \times \mathbf{n}$ are noncommutative, $\partial^2\beta/\partial x \partial y \neq \partial^2 \beta/\partial y \partial x$, etc.), in the general case we have curl $\varkappa \neq 0$. For an SLC-C the quantity $\varkappa$ is the field of distortions of the orientation of the projections of the molecules on the surface of the layers. If the layers form a spherical concentric system, then in spherical coordinates we have

$$\operatorname{rot} \varkappa = \frac{\mathbf{r}}{|\mathbf{r}|^3}. \tag{6.10}$$

The solution of Eq. (6.10) will be, e.g.,

$$\varkappa_r = \varkappa_\theta = 0, \quad \varkappa_\varphi = \frac{1}{2} \operatorname{tg} \frac{\theta}{2}. \tag{6.11}$$

Equation (6.11), which contains a linear singularity lying along the negative part of the OZ axis, coincides with the solution for the vector potential of the Dirac monopole,[237] and also with the expression for the field of distortions of the Volovik monopole in a CLC.[239]

Experimental studies of freely suspended drops of SLC-C's confirm the possible existence of monopole structures.[157] They actually have the form of concentric spherical systems of smectic layers from whose center emerge one, as in the solution (6.11), or two m-type disclinations (Fig. 28).

The described radial monopoles can transform into hyperbolic ones upon changing temperature. The structure of the latter recalls toroidal confocal domains (see Sec. 6.2). In such a monopole a point defect of the field $\mathbf{n}$ has the form of a hyperbolic hedgehog (Fig. 7d,f), while the disclinations associated with it are characterized by the strength $m_1 = m_2 = -1$.[241]

Monopoles have also been found in cholesteric drops[15,81,170,171,240]; they are stable if the pitch of the CLC helix is much smaller than the dimensions of the drop. In contrast to SLC-C's, in CLCs, depending on the type of helical twist (right- or left-handed), one can distinguish monopoles with $N = 1$ and antimonopoles with $N = -1$. By using compensated binary mixtures of cholesteric materials that change the direction of twist upon changing temperature, it has been possible experimentally to conduct a continuous monopole-antimonopole transition.[240] In the inversion region the untwisting of the cholesteric helix gives rise in the drop to the defects inherent in the nematic phase–hedgehogs, boojums, and surface disclinations. In other words, here again a topological dynamics of defects prevails that is caused by a change in the degeneracy space.

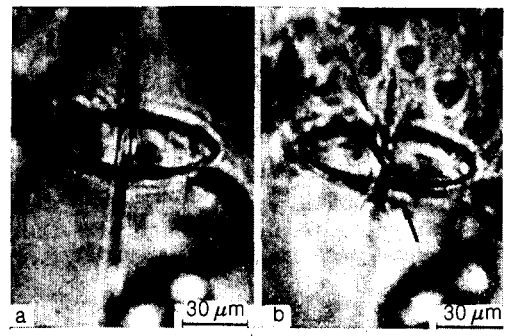

FIG. 29. Appearance in a SCL-A (a) to SLC-C (b) phase transition of a pair of m-disclinations of strength $m = -1$, each in a confocal domain.

Monopoles can be formed also in other condensed media if these media fulfill the following two requirements: the existence of an order parameter in the form of an orthonormalized triad of vectors (directors) and the existence of a one-dimensional periodic structure with equidistant layers along one (and only one) of these vectors. In such media as superfluid ^{3}He-A or a biaxial NLC, monopoles are unstable and relax into boojums, since they do not fulfill the second of these conditions. In an ordinary solid crystal monopoles also are not formed owing to the large energy of the deformations involving breakdowns of the three-dimensional periodic lattice. The listed requirements are fulfilled, in particular, by chiral smectics-C.

As was shown above, an isolated radial hegehog is converted in the SLC-A–SLC-C transition into a monopole with disclination lines. Confocal domains also undergo similar changes: in the SLC-C the ellipse and hyperbola prove to be bound together by two disclinations of strength $m = -1$ (Fig. 29). In its topological nature, this effect, which was discovered by Perez *et al.*[227] and studied in detail in Refs. 232 and 228, is analogous to the effect of transformation of a hedgehog into a monopole, and involves the appearance of the field τ in the SLC-A–SLC-C transition.

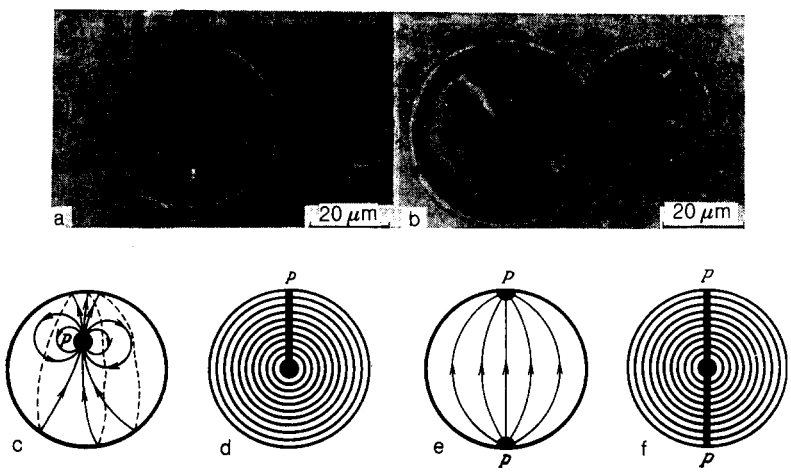

FIG. 28. Monopoles in SLC-C's. a,b—Micrographs of spherical drops of SLC-C's containing monopoles with one and two disclinations. c,e—The corresponding distributions of the field τ on spherical surfaces of the smectic layers. d,f—Distribution of layers of an SLC and disclinations inside the drop.

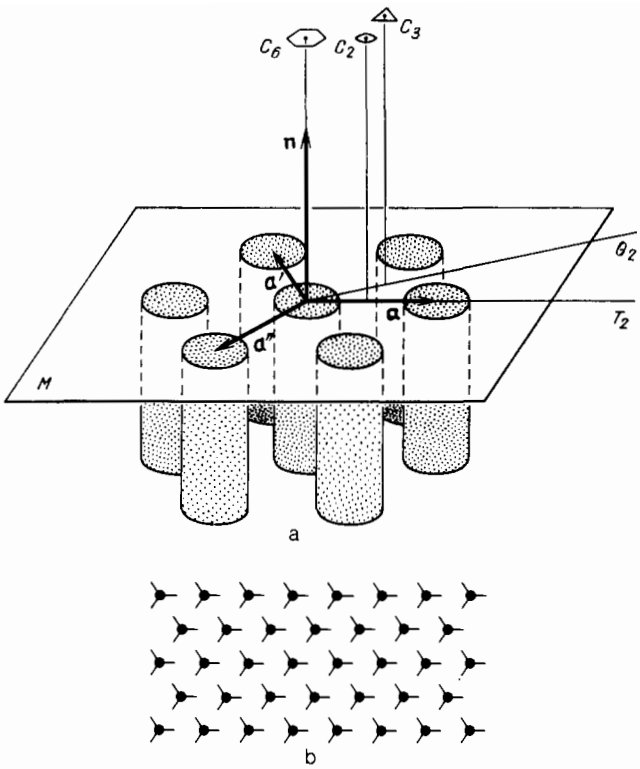

FIG. 30. Hexagonal lattice of liquid columns whose orientation is given by the director **n**.[3] a—Translation vectors **a**, **a**′, and **a**″ perpendicular to **n**. Symmetry axes of the structure: C_2, θ_2, T_2—twofold; C_3—threefold; C_6—sixfold. b—Example of a hexagonal structure not possessing C_6, C_2, and θ_2 axes.

7. COLUMNAR SYSTEMS WITH HEXAGONAL ORDERING

Up to now hexagonal ordering has been found in numerous liquid-crystalline media. They are, e.g., the thermotropic smectics-*B* with translational hexagonal ordering of the molecules within the limits of each layer[242] and their lyotropic analogs.[88] In essence, the defects in such media are classified in the same way as the defects in ordinary solid crystalline three-dimensional lattices[3)] (see Ref. 243 in this regard), and they have similar physical properties.[244] Therefore we shall not treat them.

The nonsmectic columnar phases are more interesting from the standpoint of topological properties. They are formed either by long cylindrical micelles,[88] or by liquid columns of disklike molecules[89] and have two-dimensional translational order—hexagonal (Fig. 30) or rectangular.

To find the degeneracy space of the medium depicted in Fig. 30, Bouligand[245] proposed the following pictorial scheme. Let us donote by **n** the unit director that fixes the orientation of the axes of the liquid columns. The region of variation of **n** is the sphere S^2/Z_2, which can be represented in the form of a hemisphere or disk. Diametrically opposite points on the boundary of the disk are mutually equivalent. We must also fix the orientation of the vector **a** (see Fig. 30), e.g., by using a continuous parameter that varies on the linear segment from 0 to $\pi/3$ (or to $2\pi/3$, if C_6 symmetry axes are absent in the structure). Then the orientational part of the degeneracy space amounts to the solid torus $(S^2\times Z_2)\times S^1$. We must supplement it with the translational part, which has the form of the hollow torus $S^1\times S^1$ for a

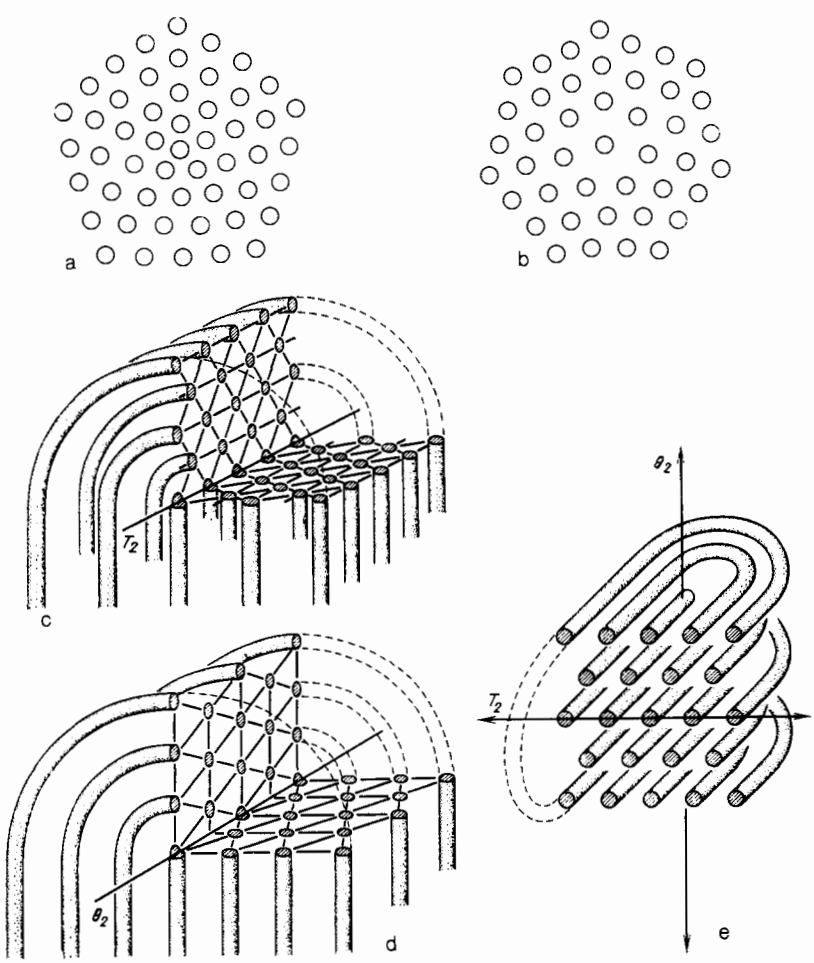

FIG. 31. Disclinations in a hexagonal structure.[27] a,b—Longitudinal disclinations $\pi/3$ and $-\pi/3$ oriented along the C_6 axis. d—Transverse disclinations oriented along the axes T_2 and θ_2, respectively. e—Two transverse, mutually perpendicular disclinations lying along the T_2 and θ_2 axes.

two-dimensional lattice. Consequently the complete degeneracy space of the hexagonal liquid is a complex five-dimensional manifold and allows the existence of dislocations[4)] having the Burgers vector $\mathbf{b} = l\mathbf{a} + m\mathbf{a}'$ and disclinations (Fig. 31) whose axis can be oriented either along the columns or perpendicular to them. Transverse disclinations are energetically more favorable, since they do not require a change in the distances between the columns.

If the medium has a C_6 symmetry axis, then transverse disclinations are formed both along the T_2 axis and along the θ_2 axis (Fig. 31c,d). In the absence of a C_6 axis the θ_2 axis is also absent (an example is shown in Fig. 30b), and this means that disclinations along θ_2 are also absent. This feature permitted an unambiguous proof of the existence of a C_6 axis in the hexagonal phase of hexapentoxytriphenylene. Oswald[2] was able to observe specific defect formations in the form of two mutually perpendicular disclinations, which is possible only when one of them is formed by rotations of the columns about the T_2 axis, and the other about the θ_2 axis. The existence of the latter implies the existence of a C_6 axis. Interestingly, x-ray structure analysis does not allow one to make such an identification.

The structure of hexagonal phases also allows formation of singular domains, which, like the confocal domains in smectics, do not fit in an obvious manner into a homotopy classification, but are described by geometric constructions. We have in mind the so-called developable domains first studied by Bouligand[245] and by Kléman.[247] Similarly to the situation with confocal domains in layered media, in developable domains in the presence of longitudinal bending deformations of the field $\mathbf{n}$ (and only of them), the columns keep both their thickness and their hexagonal (or rectangular) packing. The construction of such domains involves the concept of developable surfaces[224] and reduces to the following.

Let us distinguish the axis of a bent column—the space curve $\mathfrak{N}$. We shall set each point $\mathfrak{P}$ on $\mathfrak{N}$ in correspondence with the plane $\mathfrak{M}$ perpendicular to $\mathfrak{N}$ at the point $\mathfrak{P}$. In the absence of twist and splay deformations ($\mathbf{n}\cdot\mathrm{curl}\,\mathbf{n} = 0$, $\mathrm{div}\,\mathbf{n} = 0$), the axes of adjacent columns of the hexagonal lattice parallel to $\mathfrak{N}$ also intersect the plane $\mathfrak{M}$ at a right angle. Shifting the point $\mathfrak{P}$ along the line $\mathfrak{N}$ generates a single-parameter family of planes $\{\mathfrak{M}\}$ whose common envelope is a certain surface $\mathfrak{D}$ (Fig. 32). The surface $\mathfrak{D}$ consists of straight lines $\{g\}$ that are the limiting lines of intersection of two adjacent planes of the family $\{\mathfrak{M}\}$. Thus the surface $\mathfrak{D}$ has everywhere zero Gaussian curvature and by bending it one can develop it into a plane ("developable" surface). The columns intersect the developable surface $\mathfrak{D}$ at a right angle and actually can exist only on one side of it (where one can arrange at least one tangent to the plane of the family $\{\mathfrak{M}\}$). The family of straight lines $\{g\}$ has a common envelope—the curve E in the form of the cuspidal edge of the surface $\mathfrak{D}$.[224] The curve E and the developable surface $\mathfrak{D}$ itself are singular regions in the distribution of $\mathbf{n}$. Moreover, one can show that the families of columns themselves that form one row of the lattice (e.g., along the vector $\mathbf{a}$; see Fig. 30a) also have the form of developable surfaces.

Depending on the concrete form of the developable surface $\mathfrak{D}$, one can distinguish developable domains of different types. The surface $\mathfrak{D}$ can be a Riemann surface if E is a screw line; a conical surface if E is a point; a cylinder if E is a point

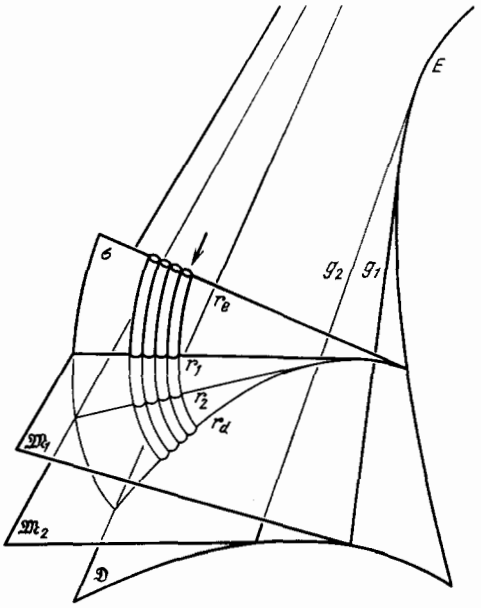

FIG. 32. Construction of the developable surface $\mathscr{D}$ and the cuspidal edge E corresponding to the space curve $\mathfrak{N}$ (arrow)—axes of the column (notation: r_e is $\Delta\mathscr{R}_0$, $r_{1,2}$ is $\mathscr{R}_{1,2}$, r_d is $\mathscr{R}_3$).[3]

removed to infinity. The distribution of the columns in the latter case is shown in Fig. 33. Each column describes a plane spiral, all turns of which intersect at a right angle one of the two tangents to the circle—the cross section of the cylinder $\mathfrak{D}$. Here the segment of the tangent between the two last turns has a constant length equal to the length of this circle. The domain that we are studying has the form of a disclination of strength $m = 1$. Similar structures have been observed in Ref. 248, and here it turned out that disclinations of strength $m = 1/2$ most often arise, and amount to half of the developable domain. We mention here also Ref. 249 on the study of the flexoelectric properties of developable domains.

8. CONCLUSION

As we see from the content of the preceding sections, the set of defects in liquid crystals is very numerous and varied—from "ordinary" dislocations and disclinations to boojums, monopoles, and solitons. Therefore it is not surprising that a unitary approach to describing and classifying all these objects was only recently developed via application

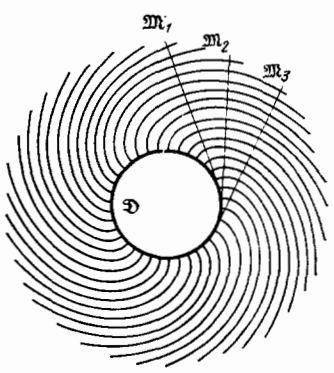

FIG. 33. Cylindrical developable domain in a hexagonal phase with a developable surface in the form of the cylinder $\mathfrak{D}$.[245]

of methods of homotopic topology. The very fact alone that this language of description is necessary also in solving a number of problems in other fields of physics indicates the general physical importance of studies of defects in liquid crystals.

Despite the evident progress in recent years, studies of defects in liquid crystals are far from completion. Above we tried to examine only a limited set of problems involving classification of the macrostructures of isolated defects. However, even on this level both the theory (primarily owing to applying homology theory together with homotopy) and experiment are being developed. This has arisen from the discovery of ever newer types of liquid-crystalline phases. Even more problems awaiting solution are concerned with elucidating the influence of defects on such physical properties of liquid crystals as viscosity and elasticity, on processes of phase transitions and "self-organization" in restricted volumes. It is also evident that the physics of topological defects is closely associated with the processes of formation of different modulated structures in dissipative and nondissipative instabilities, which apparently are the most popular objects of the science of liquid crystals of the past decade.[34]

Thus we should expect that defects in liquid-crystalline media even in the future will attract the attention of investigators to discover new, interesting properties, and will serve as a convenient model for solving general physical problems.

[1)]For some earlier applications of the topological approach for classifying defects in condensed media, see Refs. 11 and 12. The formalism of homotopy groups in physics was first employed in field theory.[13]

[2)]In their structure these chromosomes remind one of drops of ordinary CLCs,[173-175] and perhaps the division effect known for the latter[175] can serve as a starting point for studying the mechanism of division of chromosomes. It is interesting to note that a disclination model of this division exists.[176]

[3)]An exception is the hexatic smectics-B,[242] in the layers of which translational order is absent, but order exists in the orientation of bonds between molecules.

[4)]For a calculation of the energies of different types of such dislocations, see Ref. 246.

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