

Topological Aspects of Liquid Crystals

Guo-Hong Yang,^{1,4} Hui Zhang,² and Yi-Shi Duan³

Received November 4, 2001

Using ϕ -mapping method and topological current theory, the properties and behaviors of disclination points in three-dimensional liquid crystals are studied. By introducing the strength density and the topological current of many disclination points, the total disclination strength is topologically quantized by the Hopf indices and Brouwer degrees at the singularities of the general director field when the Jacobian determinant of the general director field does not vanish. When the Jacobian determinant vanishes, the origin, annihilation, and bifurcation of disclination points are detailed in the neighborhoods of the limit point and bifurcation point, respectively. The branch solutions at the limit point and the different directions of all branch curves at the first- and second-order degenerated points are calculated. It is pointed out that a disclination point with a higher strength is unstable and will evolve to the lower strength state through the bifurcation process. An original disclination point can split into at most four disclination points at one time.

KEY WORDS: topological current; wrapping number; disclination point; bifurcation.

1. INTRODUCTION

A disclination is one of a class of what are called topological defects (Kléman, 1983; Kurik and Lavrentovich, 1988a,b; Mermin, 1979). It is defined by using the well-known Volterra process for the case of rotations (Friedel, 1964; Nabarro, 1967) in which the two lips of the cut surface are rotated with respect to each other. Gennes (1970) proposed another constitutive definition in which only the directors in liquid crystals of the cut surface are individually rotated around an axis passing through their centres of gravity. The two definitions are equivalent geometrically, except for a field of infinitesimal translation dislocations in the sense of Nye (Kléman, 1972, 1973). The disclinations have the property that no continuous distortion can make them disappear (i.e., return the system to its undistorted aligned

¹ Department of Physics, Shanghai University, Shanghai 200436, People's Republic of China.

² Department of Chemistry, Shanghai University, Shanghai 200436, People's Republic of China.

³ Institute of Theoretical Physics, Lanzhou University, Lanzhou 730000, People's Republic of China.

⁴ To whom correspondence should be addressed at Department of Physics, Shanghai University, Shanghai 200436, People's Republic of China; e-mail: yguohong@yahoo.com.

ground state). Their properties depend on the symmetry of the order parameter and the topological properties of the space in which the transformation variable resides (Lubensky, 1997). In liquid crystals, due to the equivalence of the general director fields \mathbf{n} and $-\mathbf{n}$ in physics, a disclination is labeled by the disclination strength of integer or half-integer.

Disclinations take a great part of liquid crystal physics and play important roles in the static structures and dynamic behaviors of liquid crystals (Holz, 1992). Because of the importance, their exploration has a long history and there were early attempts to classify them. As a branch of topology, homotopy theory provides the natural language for the description and classification of defects in a large class of ordered systems (Mermin, 1979). This work originated by papers of Finkelstein (1966), Rogula (1976), Toulouse and Kléman (1976), Volovik and Mineev (1976, 1977a,b), Shankar (1977), and Kléman *et al.* (1977), and was summarized by Mermin (1979), Anderson (1984), and Bray (1994). In the classification, a fundamental algebraic structure was discovered in the form of homotopy groups. These groups are discrete. Their elements, in essence, label the defects and constitute a generalization of the index of a defect (like the vorticity in a superfluid) or of the triple of indices (like the Burgers vector of a dislocation in three dimensions). Physical processes involving defects were recognized to correspond to algebraic operations: defect coalescence to the group product, defect transformation (for instance in a phase transition) to a group homomorphism, the crossing of defect lines to the commutator of group elements, the motion of a point defect about a line defect to a group action. Thus, via the homotopy theory, a deep relation between the symmetry group of the uniform medium and the defects of its distorted states becomes manifest (Trebin, 1982).

In 1976, Blaha proposed a quantization rule for point singularities in superfluid ^3He and liquid crystals, which was expressed in terms of the local symmetry axis of the order parameter. In this paper, we will discuss the topological quantization and bifurcation of disclination points in three-dimensional liquid crystals in terms of the general director field directly. This work is based on the so-called ϕ -mapping method and topological current theory (Duan *et al.*, 1997a; Yang and Duan, 1998, 1999).

This paper is organized as follows. In Section 2, the topological current of disclination points in three dimensions is introduced through the Volterra process. Then, the topological quantization of disclination points is achieved in Section 3 when the Jacobian determinant of director field does not vanish. When the Jacobian determinant vanishes, the origin and annihilation of disclination points are discussed at the limit point of director field in Section 4. The bifurcation processes of disclination points at the first- and second-order degenerated points of director field are studied in Sections 5 and 6, respectively. The conclusions of this paper are in Section 7.

2. TOPOLOGICAL CURRENT OF DISCLINATION POINTS

It is well known that a disclination can be produced by using the Volterra process for the case of rotations in which the two lips of the cut surface are rotated by angle Ω with respect to each other and some undistorted materials are inserted into or removed from the body of system. For the stable states, the rotation Ω must satisfy (de Gennes, 1974)

$$\Omega = 2\pi m, \quad m = \pm\frac{1}{2}, \pm 1, \pm\frac{3}{2}, \dots \tag{1}$$

due to the equivalence of the general director fields $\mathbf{n}(x)$ and $-\mathbf{n}(x)$ in physics, where m is defined as the disclination strength of integer or half-integer. A more general definition of the disclination strength is the winding number (Shankar, 1977) in two dimensions or wrapping number (Blaha, 1976) in three dimensions of the general director field $\mathbf{n}(x)$ around the disclination line or disclination point, respectively. In three-dimensional case, suppose there are N isolated disclination points in system and the l th disclination strength is

$$m_l = \frac{1}{4\pi} \oint_{\sigma_l} \epsilon_{ijk} n^i dn^j \wedge dn^k, \quad i, j, k = 1, 2, 3, \tag{2}$$

where σ_l is a closed surface around the l th disclination point and “ \wedge ” stands for the wedge product. Using the Gauss formula, (2) is changed into

$$\begin{aligned} m_l &= \frac{1}{4\pi} \frac{1}{2} \int_{V_l} \epsilon_{ijk} dn^i \wedge dn^j \wedge dn^k \\ &= \frac{1}{8\pi} \int_{V_l} \epsilon^{\alpha\beta\gamma} \epsilon_{ijk} \partial_\alpha n^i \partial_\beta n^j \partial_\gamma n^k dx dy dz, \quad \alpha, \beta, \gamma = 1, 2, 3, \end{aligned} \tag{3}$$

where V_l is the volume surrounded by σ_l . For the liquid crystals with a set of disclination points, the total disclination strength is

$$m = \sum_l m_l = \int_V \rho dx dy dz, \tag{4}$$

where

$$\rho = \frac{1}{8\pi} \epsilon^{\alpha\beta\gamma} \epsilon_{ijk} \partial_\alpha n^i \partial_\beta n^j \partial_\gamma n^k, \quad \alpha, \beta, \gamma, i, j, k = 1, 2, 3, \tag{5}$$

is called the strength density of the disclination points. In order to study the behavior of disclinations, we will extend the above density to the topological current of disclination points. In liquid crystals, it is well known that the general director field $\mathbf{n}(x)$ responds to some external factors, such as the magnetic field strength, electric field strength, pressure and temperature. If we let x^0 denote one of the

above factors, the director field is expressed by

$$\mathbf{n} = \mathbf{n}(x^0, \mathbf{x}). \tag{6}$$

In this case, taking account of the expression of ρ in (5), we introduce the topological current of disclination points as

$$j^\alpha = \frac{1}{8\pi} \epsilon^{\alpha\beta\gamma\delta} \epsilon_{ijk} \partial_\beta n^i \partial_\gamma n^j \partial_\delta n^k, \quad \alpha, \beta, \gamma, \delta = 0, 1, 2, 3, \quad i, j, k = 1, 2, 3. \tag{7}$$

It is obvious that

$$\partial_\alpha j^\alpha = 0, \quad j^0 = \rho, \tag{8}$$

i.e., the topological current is identically conserved and its 0-component is the strength density of the disclination points. In the following, we will study the inner structure and the topological quantization of the topological current using the so-called ϕ -mapping method.

3. TOPOLOGICAL QUANTIZATION OF TOPOLOGICAL CURRENT

Since the general director field \mathbf{n} in liquid crystals is a unit vector field,

$$n^i n^i = 1, \quad i = 1, 2, 3, \tag{9}$$

it can, in general, be further expressed as

$$n^i(x) = \frac{\phi^i(x)}{\|\phi(x)\|}, \quad \|\phi(x)\| = \sqrt{\phi^i(x)\phi^i(x)}, \tag{10}$$

where $\phi^i(x)$ is the order parameter of disclination points in three dimension. It is easily to see that the zeros of $\phi^i(x)$ are just the singularities of $n^i(x)$ at which the director field is indefinite. Here, we point out that the order parameter $\phi^i(x)$ is not arbitrary, its direction field must coincide with the director field $n^i(x)$ or, in other words, (9) and (10) are the limits of the choice of $\phi^i(x)$. In different conditions, the meaning of $\phi^i(x)$ is different. In solid state physics, $\phi^i(x)$ is the tangent stress field. For the case considered here, $\phi^i(x)$ can be taken as the molecular field $\phi^i(x) = \nabla^2 n^i(x)$ which is parallel to the director field $\mathbf{n}(x)$ (de Genes, 1974). Using (10) and

$$\partial_\alpha n^i = \frac{1}{\|\phi\|} \partial_\alpha \phi^i + \phi^i \partial_\alpha \left(\frac{1}{\|\phi\|} \right), \quad \frac{\partial}{\partial \phi^i} \left(\frac{1}{\|\phi\|} \right) = -\frac{\phi^i}{\|\phi\|^3}, \tag{11}$$

j^α in (7) can be rewritten as

$$j^\alpha = -\frac{1}{8\pi} \epsilon^{\alpha\beta\gamma\delta} \epsilon_{ijk} \partial_\beta \phi^j \partial_\gamma \phi^k \partial_\delta \phi^i \frac{\partial}{\partial \phi^j} \frac{\partial}{\partial \phi^k} \left(\frac{1}{\|\phi\|} \right). \tag{12}$$

If we define the general Jacobian determinants as

$$\epsilon^{ijk} J^\alpha \left(\frac{\phi}{x} \right) = \epsilon^{\alpha\beta\gamma\delta} \partial_\beta \phi^i \partial_\gamma \phi^j \partial_\delta \phi^k \tag{13}$$

and make use of the Green function relation

$$\Delta_\phi \left(\frac{1}{\|\phi\|} \right) = -4\pi \delta^3(\phi), \tag{14}$$

where $\Delta_\phi = (\partial^2 / \partial \phi^i \partial \phi^i)$ is the Laplacian operator in ϕ -space, we do obtain the δ -function like topological current of disclination points

$$j^\alpha = \delta^3(\phi) J^\alpha \left(\frac{\phi}{x} \right). \tag{15}$$

From (4), (5), and (15) we see that the total disclination strength, the strength density and the topological current of disclination points do not vanish only at the zeros of $\phi(x)$, i.e., at the singularities of the general director field $\mathbf{n}(x)$. So, let us concentrate on the zeros of $\phi(x)$.

Suppose that the order parameter $\phi^i(x)$ possesses N isolated zeros, according to the implicit function theorem, when the Jacobian determinant

$$J \left(\frac{\phi}{x} \right) \equiv J^0 \left(\frac{\phi}{x} \right) \neq 0, \tag{16}$$

the solutions of $\phi^i(x) = 0 (i = 1, 2, 3)$ can be expressed in terms of the external factor x^0 as

$$x^\alpha = z_l^\alpha(x^0), \quad \alpha = 1, 2, 3, \quad l = 1, \dots, N, \tag{17}$$

and the generalized velocity of the l th zero of $\phi^i(x)$ is given by

$$V^\alpha = \frac{dx^\alpha}{dx^0} = \frac{J^\alpha(\phi/x)}{J(\phi/x)} \Big|_{z_l^\alpha(x^0)}, \quad V^0 = 1. \tag{18}$$

Then, as we proved in Duan *et al.* (1997b), the δ -function $\delta^3(\phi)$ can be expanded by these zeros as

$$\delta^3(\phi) = \sum_{l=1}^N \frac{\beta_l}{|J(\phi/x)_{z_l}|} \delta(x^1 - z_l^1(x^0)) \delta(x^2 - z_l^2(x^0)) \delta(x^3 - z_l^3(x^0)), \tag{19}$$

where the positive β_l is called the Hopf index of $\phi^i(x)$ at \mathbf{z}_l and it means that, when the point \mathbf{x} wraps the zero \mathbf{z}_l once, the function $\phi^i(x)$ rotates β_l times of 4π , which is a topological number and relates to the wrapping number of $\phi^i(x)$. In liquid crystals, due to the equivalence of the general director field \mathbf{n} and $-\mathbf{n}$, β_l can be integers and half-integers, Substituting (18) and (19) into (15), the inner structure

of the topological current is formulated by

$$j^\alpha = \sum_{l=1}^N \beta_l \eta_l \delta(x^1 - z_l^1(x^0)) \delta(x^2 - z_l^2(x^0)) \delta(x^3 - z_l^3(x^0)) V^\alpha \quad (20)$$

which can also be looked upon as the topological quantization of the disclination points, where η_l is called the Brouwer degree of $\phi^i(x)$ at \mathbf{z}_l ,

$$\eta_l = \frac{J(\phi/x)}{|J(\phi/x)|} \Big|_{\mathbf{z}_l} = \pm 1 \quad (21)$$

according to the clockwise or anticlockwise rotation of $\phi^i(x)$ when \mathbf{x} wraps \mathbf{z}_l clockwise. Then, the topological quantizations of the strength density and the total strength of disclination points are

$$\rho = \sum_{l=1}^N \beta_l \eta_l \delta(x^1 - z_l^1(x^0)) \delta(x^2 - z_l^2(x^0)) \delta(x^3 - z_l^3(x^0)) \quad (22)$$

and

$$m = \sum_{l=1}^N \beta_l \eta_l. \quad (23)$$

Here, we stress that the total strength of disclinations in liquid crystals is not arbitrary, but is a topological invariant. From the Gauss–Bonnet–Chern theorem and the Hopf index theorem (Duan *et al.*, 1998; Yang, 1998), the total disclination strength equals the Euler characteristic of the material body. In liquid crystals, since the free energy is proportional to the square of the disclination strength, there exists in general the disclination lines of strength $\frac{1}{2}$ in two dimension and the disclination points of strength 1 in three dimension. In two-dimensional case, the general director \mathbf{n} rotates from 0 to π in a circle around a disclination line of strength $\frac{1}{2}$. Then, there must be two vertical directions, for example $\theta(0 \leq \theta < \frac{\pi}{2})$ and $\frac{\pi}{2} + \theta$, at which one can see two brushes when observed between the orthogonal Nicol prisms. While for a disclination point of strength 1 in three-dimensional case, the director \mathbf{n} rotates from 0 to 2π and there are four directions such as θ , $\frac{\pi}{2} + \theta$, $\pi + \theta$, and $\frac{3\pi}{2} + \theta$, which give four brushes. All these are the topological quantization and inner structure of disclinations in liquid crystals. In the following sections, we will study the bifurcation behavior of disclination points in terms of the external factor x^0 .

4. THE ORIGIN AND ANNIHILATION OF DISCLINATION POINTS AT THE LIMIT POINTS

In the above section, the topological quantization of disclination points is based on condition (16), which guarantees all of the zeros of $\phi(x)$ are regular

points. However, when the material body is distorted by some external factors from outside, the general director field \mathbf{n} inside the body and the order parameter ϕ of disclination are changed, and new disclinations might be created. In this case, condition (16) may not be satisfied any longer but becomes $J(\phi/x) = 0$, under which the kernel of $\phi^i(x)$ contains some branch points and, then, the consequences in Section 3 will change in some way. In the following, let us explore what will happen to the disclination points at the branch point $x^* = (x^{0*}, \mathbf{x}^*)$ determined by

$$\begin{cases} \phi^i(x^0, x^1, x^2, x^3) = 0, & i = 1, 2, 3 \\ \phi^4(x^0, x^1, x^2, x^3) = J\left(\frac{\phi}{x}\right) = 0. \end{cases} \tag{24}$$

In the ϕ -mapping $x \rightarrow \phi(x)$, there are usually two kinds of branch points, namely the limit points and bifurcation points satisfying

$$J^\alpha\left(\frac{\phi}{x}\right)\Big|_{x^*} \neq 0, \quad \alpha = 1, 2, 3 \tag{25}$$

and

$$J^\alpha\left(\frac{\phi}{x}\right)\Big|_{x^*} = 0, \quad \alpha = 1, 2, 3 \tag{26}$$

respectively, where the Jacobian determinants $J^\alpha(\phi/x)$ have been generally defined in (13). In this section, we consider case (25). The other case (26) is complicated and will be detailed in Sections 5 and 6. For simplicity and without loss of generality, we consider $\alpha = 1$ only.

Since the usual implicit function theorem is of no use when the Jacobian determinant $J(\phi/x) = 0$, for the purpose of using the implicit function theorem to study the branch properties of disclination points at the limit points, we use the Jacobian $J^1(\phi/x)$ instead of $J(\phi/x)$ to search for the solutions of $\phi^i(x) = 0$. This means we have replaced the role of the external parameter x^0 by x^1 . For clarity we rewrite the former equations of (24) as

$$\phi^i(x^1, x^0, x^2, x^3) = 0, \quad i = 1, 2, 3. \tag{27}$$

Considering condition (25) and making use of the implicit function theorem, the solution of (27) can be expressed in the neighborhood of the limit point $x^* = (x^{0*}, \mathbf{x}^*)$ as

$$x^0 = x^0(x^1), \quad x^2 = x^2(x^1), \quad x^3 = x^3(x^1) \tag{28}$$

with $x^{0*} = x^0(x^{1*})$. In order to show the behavior of the disclination points at the limit points, let us investigate the Taylor expansion of (28) in the neighborhood of $x^* = (x^{0*}, \mathbf{x}^*)$

$$x^0 = x^{0*} + \frac{dx^0}{dx^1}\Big|_{x^*} (x^1 - x^{1*}) + \frac{1}{2} \frac{d^2x^0}{(dx^1)^2}\Big|_{x^*} (x^1 - x^{1*})^2. \tag{29}$$

In the present case, from (18), (25), and the last equation of (24), one has

$$V^1 = \frac{dx^1}{dx^0} = \frac{J^1(\phi/x)}{J(\phi/x)}|_{x^*} = \infty, \tag{30}$$

i.e.,

$$\frac{dx^0}{dx^1}|_{x^*} = 0. \tag{31}$$

Then the Taylor expansion (29) can be further read as

$$x^0 - x^{0*} = \frac{1}{2} \frac{d^2x^0}{(dx^1)^2} |_{x^*} (x^1 - x^{1*})^2 \tag{32}$$

which is a parabola in $x^1 - x^0$ plane. From (32) we can obtain two solutions, $x_1^1(x^0)$ and $x_2^1(x^0)$, which give the branch solutions of disclination points at the limit point. If $(d^2x^0/(dx^1)^2)|_{x^*} > 0$, we have the branch solutions for $x^0 > x^{0*}$; otherwise, we have the branch solutions for $x^0 < x^{0*}$. These are related to the origin and annihilation of disclination points at the limit point. Since the topological current of disclination points is identically conserved, the strengths of the two generated disclination points must be opposite at the limit point, i.e.,

$$\beta_1 \eta_1 = -\beta_2 \eta_2, \tag{33}$$

or

$$\beta_1 = \beta_2, \quad \eta_1 = -\eta_2, \tag{34}$$

which is similar to the conservation law of Burgers vector in dislocation continuum. Furthermore, from the studies in this section, we can see that the origin and annihilation of disclination points are not gradual changes, but start at a critical value of external variable, i.e., sudden changes.

5. THE BIFURCATION OF DISCLINATION POINTS AT THE FIRST-ORDER DEGENERATED POINTS

Now, let us turn to consider the other case (26). In the present condition, we have the restrictions

$$J \left(\frac{\phi}{x} \right) |_{x^*} = 0, \quad J^\alpha \left(\frac{\phi}{x} \right) |_{x^*} = 0, \quad \alpha = 1, 2, 3, \tag{35}$$

i.e., the rank of the Jacobian matrix $[\partial\phi/\partial x]$

$$\text{rank} \left[\frac{\partial\phi}{\partial x} \right] |_{x^*} < 3. \tag{36}$$

The two restrictive conditions in (35) imply an important fact that the function relationship between x^0 and \mathbf{x} is not unique in the neighborhood of the bifurcation

point x^* . In the topological current form of disclination points, this fact can be seen easily from Eq. (18)

$$V^\alpha = \frac{dx^\alpha}{dx^0} = \frac{J^\alpha(\phi/x)}{J(\phi/x)} \Big|_{x^*}, \quad \alpha = 1, 2, 3, \tag{37}$$

which under (35) directly shows the indefiniteness of the direction of integral curve of (37) at x^* . This is why the very point $x^* = (x^{0*}, \mathbf{x}^*)$ is called the bifurcation point of disclination current.

Since the rank of the Jacobian matrix $[\partial\phi/\partial x]$ is smaller than 3, with the aim of finding the different directions of all branch curves at the bifurcation point, we suppose

$$\text{rank} \left[\frac{\partial\phi}{\partial x} \right] \Big|_{x^*} = 3 - 1 = 2 \tag{38}$$

and let

$$J_1 \left(\frac{\phi}{x} \right) \Big|_{x^*} = \begin{vmatrix} \frac{\partial\phi^1}{\partial x^2}, & \frac{\partial\phi^1}{\partial x^3} \\ \frac{\partial\phi^2}{\partial x^2}, & \frac{\partial\phi^2}{\partial x^3} \end{vmatrix} \Big|_{x^*} \neq 0, \tag{39}$$

which means x^* is a first-order degenerated point of $\phi^i(x)$. (The case that x^* is a second-order degenerated point will be treated in the next section.) From $\phi^1(x) = 0$ and $\phi^2(x) = 0$, the implicit function theorem says that there exists one and only one function relationship

$$x^2 = x^2(x^0, x^1), \quad x^3 = x^3(x^0, x^1). \tag{40}$$

Substituting (40) into $\phi^1(x)$ and $\phi^2(x)$, we have

$$\phi^j(x^0, x^1, x^2(x^0, x^1), x^3(x^0, x^1)) \equiv 0, \quad j = 1, 2, \tag{41}$$

which give

$$\sum_{\beta=2}^3 \phi_\beta^j x_0^\beta = -\phi_0^j, \quad \sum_{\beta=2}^3 \phi_\beta^j x_1^\beta = -\phi_1^j, \tag{42}$$

$$\sum_{\beta=2}^3 \phi_\beta^j x_{00}^\beta = -\sum_{\beta=2}^3 \left[2\phi_{\beta 0}^j x_0^\beta + \sum_{\gamma=2}^3 (\phi_{\beta\gamma}^j x_0^\gamma) x_0^\beta \right] - \phi_{00}^j, \tag{43}$$

$$\sum_{\beta=2}^3 \phi_\beta^j x_{01}^\beta = -\sum_{\beta=2}^3 \left[\phi_{\beta 0}^j x_1^\beta + \phi_{\beta 1}^j x_0^\beta + \sum_{\gamma=2}^3 (\phi_{\beta\gamma}^j x_0^\gamma) x_1^\beta \right] - \phi_{01}^j, \tag{44}$$

$$\sum_{\beta=2}^3 \phi_\beta^j x_{11}^\beta = -\sum_{\beta=2}^3 \left[2\phi_{\beta 1}^j x_1^\beta + \sum_{\gamma=2}^3 (\phi_{\beta\gamma}^j x_1^\gamma) x_1^\beta \right] - \phi_{11}^j, \tag{45}$$

where $j = 1, 2; \beta, \gamma = 2, 3$, and

$$x_0^\beta = \frac{\partial x^\beta}{\partial x^0}, \quad x_1^\beta = \frac{\partial x^\beta}{\partial x^1}, \quad x_{00}^\beta = \frac{\partial^2 x^\beta}{(\partial x^0)^2}, \quad x_{01}^\beta = \frac{\partial^2 x^\beta}{\partial x^0 \partial x^1}, \quad x_{11}^\beta = \frac{\partial^2 x^\beta}{(\partial x^1)^2}, \quad (46)$$

$$\phi_0^j = \frac{\partial \phi^j}{\partial x^0}, \quad \phi_1^j = \frac{\partial \phi^j}{\partial x^1}, \quad \phi_\beta^j = \frac{\partial \phi^j}{\partial x^\beta}, \quad \phi_{00}^j = \frac{\partial^2 \phi^j}{(\partial x^0)^2}, \quad \phi_{01}^j = \frac{\partial^2 \phi^j}{\partial x^0 \partial x^1}, \quad (47)$$

$$\phi_{11}^j = \frac{\partial^2 \phi^j}{(\partial x^1)^2}, \quad \phi_{\beta 0}^j = \frac{\partial^2 \phi^j}{\partial x^0 \partial x^\beta}, \quad \phi_{\beta 1}^j = \frac{\partial^2 \phi^j}{\partial x^1 \partial x^\beta}, \quad \phi_{\beta \gamma}^j = \frac{\partial^2 \phi^j}{\partial x^\beta \partial x^\gamma}. \quad (48)$$

From these expressions we can calculate the values of the first- and second-order partial derivatives of (40) with respect to x^0 and x^1 at the bifurcation point x^* .

In order to explore the behavior of the disclination points at the bifurcation point, as before, we will investigate the Taylor expansion of

$$F(x^0, x^1) = \phi^3(x^0, x^1, x^2(x^0, x^1), x^3(x^0, x^1)) \quad (49)$$

in the neighborhood of x^* , which according to (24) must vanish at the bifurcation point, i.e.,

$$F(x^{0*}, x^{1*}) = 0. \quad (50)$$

From (49) the first-order partial derivatives of $F(x^0, x^1)$ with respect to x^0 and x^1 can be expressed by

$$\frac{\partial F}{\partial x^0} = \frac{\partial \phi^3}{\partial x^0} + \sum_{\beta=2}^3 \frac{\partial \phi^3}{\partial x^\beta} x_0^\beta, \quad \frac{\partial F}{\partial x^1} = \frac{\partial \phi^3}{\partial x^1} + \sum_{\beta=2}^3 \frac{\partial \phi^3}{\partial x^\beta} x_1^\beta. \quad (51)$$

On the other hand, making use of (42), (51), and Cramer's rule, it is not difficult to prove that the two restrictive conditions in (35) can be rewritten as

$$J \left(\frac{\phi}{x} \right) \Big|_{x^*} = \left(\frac{\partial F}{\partial x^1} J_1 \left(\frac{\phi}{x} \right) \right) \Big|_{x^*} = 0, \quad (52)$$

$$J^1 \left(\frac{\phi}{x} \right) \Big|_{x^*} = \left(\frac{\partial F}{\partial x^0} J_1 \left(\frac{\phi}{x} \right) \right) \Big|_{x^*} = 0, \quad (53)$$

which lead to

$$\frac{\partial F}{\partial x^0} \Big|_{x^*} = 0, \quad \frac{\partial F}{\partial x^1} \Big|_{x^*} = 0 \quad (54)$$

by considering (39). The second-order partial derivatives of the function $F(x^0, x^1)$ are easily found to be

$$\frac{\partial^2 F}{(\partial x^0)^2} = \phi_{00}^3 + \sum_{\beta=2}^3 \left[2\phi_{\beta 0}^3 x_0^\beta + \phi_\beta^3 x_{00}^\beta + \sum_{\gamma=2}^3 (\phi_{\beta \gamma}^3 x_0^\gamma) x_0^\beta \right] \quad (55)$$

$$\frac{\partial^2 F}{\partial x^0 \partial x^1} = \phi_{01}^3 + \sum_{\beta=2}^3 \left[\phi_{\beta 0}^3 x_1^\beta + \phi_{\beta 1}^3 x_0^\beta + \phi_{\beta}^3 x_{01}^\beta + \sum_{\gamma=2}^3 (\phi_{\beta\gamma}^3 x_0^\gamma) x_1^\beta \right] \quad (56)$$

$$\frac{\partial^2 F}{(\partial x^1)^2} = \phi_{11}^3 + \sum_{\beta=2}^3 \left[2\phi_{\beta 1}^3 x_1^\beta + \phi_{\beta}^3 x_{11}^\beta + \sum_{\gamma=2}^3 (\phi_{\beta\gamma}^3 x_1^\gamma) x_1^\beta \right] \quad (57)$$

which at $x^* = (x^{0*}, \mathbf{x}^*)$ are denoted by

$$A = \frac{\partial^2 F}{(\partial x^0)^2} \Big|_{x^*}, \quad B = \frac{\partial^2 F}{\partial x^0 \partial x^1} \Big|_{x^*}, \quad C = \frac{\partial^2 F}{(\partial x^1)^2} \Big|_{x^*}, \quad (58)$$

where $\beta, \gamma = 2, 3$ and

$$\phi_{\beta}^3 = \frac{\partial \phi^3}{\partial x^\beta}, \quad \phi_{00}^3 = \frac{\partial^2 \phi^3}{(\partial x^0)^2}, \quad \phi_{01}^3 = \frac{\partial^2 \phi^3}{\partial x^0 \partial x^1}, \quad \phi_{11}^3 = \frac{\partial^2 \phi^3}{(\partial x^1)^2}, \quad (59)$$

$$\phi_{\beta 0}^3 = \frac{\partial^2 \phi^3}{\partial x^0 \partial x^\beta}, \quad \phi_{\beta 1}^3 = \frac{\partial^2 \phi^3}{\partial x^1 \partial x^\beta}, \quad \phi_{\beta\gamma}^3 = \frac{\partial^2 \phi^3}{\partial x^\beta \partial x^\gamma}. \quad (60)$$

Then, from (50), (54), and (58), we obtain the Taylor expansion of $F(x^0, x^1)$

$$F(x^0, x^1) = \frac{1}{2} A (x^0 - x^{0*})^2 + B (x^0 - x^{0*})(x^1 - x^{1*}) + \frac{1}{2} C (x^1 - x^{1*})^2 \quad (61)$$

that by (49) is the behavior of $\phi^3(x)$ in the neighborhood of the bifurcation point x^* . Because of (24), we have

$$A(x^0 - x^{0*})^2 + 2B(x^0 - x^{0*})(x^1 - x^{1*}) + C(x^1 - x^{1*})^2 = 0 \quad (62)$$

which is followed by

$$A \left(\frac{dx^0}{dx^1} \right)^2 + 2B \left(\frac{dx^0}{dx^1} \right) + C = 0 \quad (63)$$

or

$$C \left(\frac{dx^1}{dx^0} \right)^2 + 2B \left(\frac{dx^1}{dx^0} \right) + A = 0. \quad (64)$$

The different directions of the branch curves at the bifurcation point are determined by the solutions of (63) or (64). Some possible results are discussed and diagrammed in Duan *et al.* (1998) and Jiang and Duan (2000). The remaining components dx^2/dx^0 and dx^3/dx^0 can be deduced by

$$\frac{dx^\beta}{dx^0} = x_0^\beta + x_1^\beta \frac{dx^1}{dx^0}, \quad \beta = 2, 3 \quad (65)$$

in which the partial derivative coefficients x_0^β and x_1^β have been calculated in (42).

As before, since the topological current of disclination points is identically conserved, the sum of the strengths of the two split disclination points must be equal to that of the original disclination point at the bifurcation point, i.e.,

$$\beta_1 \eta_1 + \beta_2 \eta_2 = \beta \eta, \quad (66)$$

which is analogous to the conservation law of Burgers vector in dislocation continuum. Since the free energy is proportional to the square of the disclination strength, the result (66) indicates that in liquid crystals, a disclination point with a higher value of disclination strength is unstable and it will evolve to the lower value of disclination strength through the bifurcation process.

At the end of this section, we conclude that in our topological current theory of disclination points, there exists the crucial case of branch process due to the varying of external factors. This means when an original disclination point moves through the bifurcation point, it may split into two disclination points moving along different branch curves and reaches a stable state of lower value of disclination strength. The branch process of disclination point is also not a gradual change but a sudden change with the varying of external parameters.

6. THE BIFURCATION OF DISCLINATION POINTS AT THE SECOND-ORDER DEGENERATED POINTS

In the above section, we have studied the bifurcation of disclination points at the first-order degenerated points. In this section, we will discuss the branch process of disclination points at the second-order degenerated point $x^* = (x^{0*}, \mathbf{x}^*)$, at which the rank of the Jacobian matrix $[\partial\phi/\partial x]$ is

$$\text{rank} \left[\frac{\partial\phi}{\partial x} \right] \Big|_{x^*} = 3 - 2 = 1. \quad (67)$$

Suppose that

$$\frac{\partial\phi^1}{\partial x^3} \Big|_{x^*} \neq 0. \quad (68)$$

With the same reason of obtaining (40), from $\phi^1(x) = 0$ we have the function relationship

$$x^3 = x^3(x^0, x^1, x^2) \quad (69)$$

in the neighborhood of x^* . In order to determine the values of the first- and second-order partial derivatives of x^3 with respect to x^0 , x^1 , and x^2 , one can derive the system of equations similar to (41)–(48). Substituting the relationship (69) into

$\phi^2(x) = 0$ and $\phi^3(x) = 0$, we get

$$\begin{cases} F_1(x^0, x^1, x^2) = \phi^2(x^0, x^1, x^2, x^3(x^0, x^1, x^2)) = 0 \\ F_2(x^0, x^1, x^2) = \phi^3(x^0, x^1, x^2, x^3(x^0, x^1, x^2)) = 0. \end{cases} \quad (70)$$

As shown in the above section, for the first-order partial derivatives of the functions $F_1(x^0, x^1, x^2)$ and $F_2(x^0, x^1, x^2)$, one can prove the following six formulas similar to (54)

$$\frac{\partial F_k}{\partial x^0} \Big|_{x^*} = 0, \quad \frac{\partial F_k}{\partial x^1} \Big|_{x^*} = 0, \quad \frac{\partial F_k}{\partial x^2} \Big|_{x^*} = 0, \quad k = 1, 2. \quad (71)$$

So the Taylor expansions of $F_1(x^0, x^1, x^2)$ and $F_2(x^0, x^1, x^2)$ can be read in the neighborhood of x^* as

$$\begin{aligned} F_k(x^0, x^1, x^2) &\approx A_{k1}(x^0 - x^{0*})^2 + A_{k2}(x^0 - x^{0*})(x^1 - x^{1*}) \\ &\quad + A_{k3}(x^0 - x^{0*})(x^2 - x^{2*}) + A_{k4}(x^1 - x^{1*})^2 \\ &\quad + A_{k5}(x^1 - x^{1*})(x^2 - x^{2*}) + A_{k6}(x^2 - x^{2*})^2 \\ &= 0, \end{aligned} \quad (72)$$

where $k = 1, 2$ and

$$A_{k1} = \frac{1}{2} \frac{\partial^2 F_k}{(\partial x^0)^2} \Big|_{x^*}, \quad A_{k2} = \frac{\partial^2 F_k}{\partial x^0 \partial x^1} \Big|_{x^*}, \quad A_{k3} = \frac{\partial^2 F_k}{\partial x^0 \partial x^2} \Big|_{x^*}, \quad (73)$$

$$A_{k4} = \frac{1}{2} \frac{\partial^2 F_k}{(\partial x^1)^2} \Big|_{x^*}, \quad A_{k5} = \frac{\partial^2 F_k}{\partial x^1 \partial x^2} \Big|_{x^*}, \quad A_{k6} = \frac{1}{2} \frac{\partial^2 F_k}{(\partial x^2)^2} \Big|_{x^*}. \quad (74)$$

Dividing (72) by $(x^0 - x^{0*})^2$ and taking the limit $x^0 \rightarrow x^{0*}$, one obtains the two quadratic equations of dx^1/dx^0 and dx^2/dx^0

$$A_{k1} + A_{k2} \frac{dx^1}{dx^0} + A_{k3} \frac{dx^2}{dx^0} + A_{k4} \left(\frac{dx^1}{dx^0} \right)^2 + A_{k5} \frac{dx^1}{dx^0} \frac{dx^2}{dx^0} + A_{k6} \left(\frac{dx^2}{dx^0} \right)^2 = 0 \quad (75)$$

and further, eliminating the variable dx^1/dx^0 , has the equation of dx^2/dx^0 in the form of a determinant

$$\begin{vmatrix} A_{14} & A_{15}v + A_{12} & A_{16}v^2 + A_{13}v + A_{11} & 0 \\ 0 & A_{14} & A_{15}v + A_{12} & A_{16}v^2 + A_{13}v + A_{11} \\ A_{24} & A_{25}v + A_{22} & A_{26}v^2 + A_{23}v + A_{21} & 0 \\ 0 & A_{24} & A_{25}v + A_{22} & A_{26}v^2 + A_{23}v + A_{21} \end{vmatrix} = 0 \quad (76)$$

with the variable $v = dx^2/dx^0$, which is a fourth-order equation of dx^2/dx^0

$$a_1 \left(\frac{dx^2}{dx^0} \right)^4 + a_2 \left(\frac{dx^2}{dx^0} \right)^3 + a_3 \left(\frac{dx^2}{dx^0} \right)^2 + a_4 \left(\frac{dx^2}{dx^0} \right) + a_5 = 0. \quad (77)$$

Therefore we get the different directions of the branch curves at the second-order degenerated point x^* . The largest number of the different branch curves is four, which means an original disclination point with the strength $\beta\eta$ can split into four disclination points with the strengths $\beta_1\eta_l$ ($l = 1, 2, 3, 4$) satisfying

$$\beta_1\eta_1 + \beta_2\eta_2 + \beta_3\eta_3 + \beta_4\eta_4 = \beta\eta \quad (78)$$

at one time at most.

7. CONCLUSIONS

In this paper, using the ϕ -mapping method and topological current theory, the properties and behaviors of disclination points in three-dimensional liquid crystals are studied. By introducing the strength density and the topological current of disclination points, we obtain the inner structure and the topological quantization of the disclination points when the Jacobian determinant of the general director field does not vanish. It is pointed out that the disclination points are topologically quantized by the Hopf indices and Brouwer degrees (i.e., the wrapping numbers) at the singularities of the general director field, and the total disclination strength of liquid crystal is not arbitrary but a topological invariant, the Euler characteristic. Because of the equivalence of the director fields \mathbf{n} and $-\mathbf{n}$ in physics, the Hopf indices can be integers and half-integers, which represent a great generalization to our previous theory of integer Hopf indices. When the liquid crystals are distorted by some external factors from outside such that the Jacobian determinant of the general director field vanishes, the origin, annihilation, and bifurcation of disclination points are detailed in the neighborhoods of the limit points and bifurcation points, respectively. The branch solutions at the limit points and the different directions of all branch curves at the first- and second-order degenerated points are calculated. The largest number of the different branch curves is four, i.e., an original disclination point can split into four disclination points at one time at most. For the topological current of disclination points is identically conserved, the strengths of the two generated disclination points must be opposite at the limit point and, at the first- and second-order degenerated points, the sum of the strengths of the split disclination points must be equal to that of the original disclination point. Since the free energy is proportional to the square of the disclination strength, it is pointed out that a disclination point with a higher value of strength is unstable and it will evolve to the lower value of strength through the bifurcation process. Furthermore, we see that either the origin and annihilation of disclination points at the limit point or the branch process at the bifurcation point are not gradual

changes, but start at a critical value of external parameters, i.e., sudden changes with the varying of external factors.

ACKNOWLEDGMENTS

This work was supported by the Science Foundation of Shanghai Municipal Commission of Education under Grant Nos. 2000QN64 and 2000A15.

REFERENCES

- Anderson, P. W. (1984). *Basic Notions of Condensed Matter Physics*, Benjamin, London.
- Blaha, S. (1976). *Physical Review Letters* **36**, 874.
- Bray, A. J. (1994). *Advances in Physics* **43**, 375.
- de Gennes, P. G. (1970). *Lecture Notes*, Orsay.
- de Gennes, P. G. (1974). *The Physics of Liquid Crystals*, Oxford University Press, London.
- Duan, Y. S., Li, S., and Yang, G. H. (1998). *Nuclear Physics B* **514**, 705.
- Duan, Y. S., Yang, G. H., and Jiang, Y. (1997a). *General Relativity and Gravitation* **29**, 715.
- Duan, Y. S., Yang, G. H., and Jiang, Y. (1997b). *Helvetica Physica Acta* **70**, 565.
- Finkelstein, D. (1966). *Journal of Mathematical Physics* **7**, 1218.
- Friedel, J. (1964). *Dislocations*, Pergamon, Oxford.
- Holz, A. (1992). *Physica A* **182**, 240.
- Jiang, Y. and Duan, Y. S. (2000). *Journal of Mathematical Physics* **41**, 2616.
- Kléman, M. (1972). *Liquid Crystalline Systems*, G. W. Gray and P. Windsor, eds., Academic Press, New York.
- Kléman, M. (1973). *Philosophical Magazine* **27**, 1057.
- Kléman, M. (1983). *Points, Lines and Walls: In Liquid Crystals, Magnetic Systems and Various Disordered Media*, Wiley, New York.
- Kléman, M., Michel, L., and Toulouse, G. (1977). *Journal of Physical Letters (Paris)* **38**, L195.
- Kurik, M. V. and Lavrentovich, O. D. (1988a). *Uspekhi Fizicheskikh Nauk*, **154**, 381.
- Kurik, M. V. and Lavrentovich, O. D. (1988b). *Soviet Physics-Uspekhi* **31**, 196.
- Lubensky, T. C. (1997). *Solid State Communications* **102**, 187.
- Mermin, N. D. (1979). *Reviews of Modern Physics* **51**, 591.
- Nabarro, F. R. N. (1967). *Theory of Crystal Dislocations*, Oxford University Press, London.
- Rogula, D. (1976). *Trends in Applications of Pure Mathematics to Mechanics*, G. Fichera, eds., Pitman, New York.
- Shankar, R. (1977). *Le Journal de Physique* **38**, 1405.
- Toulouse G. and Kléman, M. (1976). *Journal of Physical Letters (Paris)* **37**, L149.
- Trebin, H.-R. (1982). *Advances in Physics* **31**, 195.
- Volovik, G. E. and Mineev, V. P. (1976). *Soviet Physics JETP Letters* **48**, 561.
- Volovik, G. E. and Mineev, V. P. (1977a). *Soviet Physics JETP* **45**, 1186.
- Volovik, G. E. and Mineev, V. P. (1977b). *Soviet Physics JETP* **46**, 401.
- Yang, G. H. (1998). *Modern Physics Letters A* **13**, 2123.
- Yang, G. H. and Duan, Y. S. (1998). *International Journal of Theoretical Physics* **37**, 2371.
- Yang, G. H. and Duan, Y. S. (1999). *International Journal of Engineering Science* **37**, 1037.