Vol 11 No 5, May 2002
1009-1963/2002/11(05)/0415-04
Chinese Physics
© 2002 Chin. Phys. Soc.
and IOP Publishing Ltd

Topological quantization of disclination points in three-dimensional liquid crystals*

Yang Guo-Hong(杨国宏)[a)†], Zhang Hui(张 慧)[b)], and Duan Yi-Shi(段一士)[c)]

[a)] *Department of Physics, Shanghai University, Shanghai* 200436, *China*
[b)] *Department of Chemistry, Shanghai University, Shanghai* 200436, *China*
[c)] *Institute of Theoretical Physics, Lanzhou University, Lanzhou* 730000, *China*

(Received 17 October 2001; revised manuscript received 25 November 2001)

Using the ϕ-mapping method and topological current theory, we study the inner structure of disclination points in three-dimensional liquid crystals. By introducing the strength density and the topological current of many disclination points, it is pointed out that the disclination points are determined by the singularities of the general director field and they are topologically quantized by the Hopf indices and Brouwer degrees.

Keywords: topological current, wrapping number, director field, disclination point
PACC: 0240

1. Introduction

A disclination is one of a class of topological defects.[1−3] It is defined by means of the well-known Volterra process for the case of rotations[4,5] in which the two lips of the cut surface are rotated with respect to each other. The disclinations have the property that no continuous distortion can make them disappear (i.e. to restore the system to its undistorted aligned 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.[6] In liquid crystals, due to the equivalence of the general director fields $\boldsymbol{n}$ and $-\boldsymbol{n}$ in physics, a disclination is labelled by the disclination strength which is an integer or half-integer.

Disclinations play a large part in liquid crystal physics and play important roles in the static structures and dynamic behaviours of liquid crystals.[7−9] Because of their 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.[3] Work in this field was originated by the papers of Finkelstein,[10] Rogula,[11] Toulouse and Kléman,[12] Volovik and Mineev,[13] Shankar[14] and Kléman *et al.*,[15] and was summarized by Mermin,[3] Anderson[16] and Bray.[17]

In 1976, Blaha[18] proposed a quantization rule for point singularities in superfluid ^{3}He and liquid crystals, which was expressed in terms of the local symmetry axis of the order parameter. In this paper, we discuss the topological quantization of disclination points in three-dimensional liquid crystals directly in terms of the general director field. This work is based on the so-called ϕ-mapping method and topological current theory.[19−21]

This paper is organized as follows. In section 2, the topological current of disclination points in three dimensions is introduced through the Volterra process. The topological quantization of disclination points is introduced in section 3. The conclusions of this paper are summarized in section 4.

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 the system. For the stable states, the rotation Ω must satisfy[22]

$$\Omega = 2\pi m, \tag{1}$$

*Project supported by the Science Foundation from the Education Commission of Shanghai, China (Grant Nos 2000QN64 and 2000A15).
†Author to whom correspondence should be addressed. E-mail: yguohong@yahoo.com

where m is called the disclination strength. In liquid crystals, due to the equivalence of the director fields $\boldsymbol{n}(x)$ and $-\boldsymbol{n}(x)$ in physics, m can be integers and half-integers, i.e. $m = \pm\frac{1}{2}, \pm 1, \pm\frac{3}{2}, \cdots$. A more general definition of the disclination strength is the winding number[14] in two dimensions or the wrapping number[18] in three dimensions of the general director field $\boldsymbol{n}(x)$ around the disclination line or disclination point, respectively. In the three-dimensional case, suppose there are N isolated disclination points in system, then the lth disclination strength is

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

where σ_l is a closed surface around the lth disclination point and "$\wedge$" represents for the wedge product. Using the Gauss formula, equation (2) is changed into

$$\begin{aligned} m_l =& \frac{1}{4\pi}\frac{1}{2}\int_{V_l} \epsilon_{ijk}\mathrm{d}n^i \wedge \mathrm{d}n^j \wedge \mathrm{d}n^k \\ =& \frac{1}{8\pi}\int_{V_l} \epsilon^{\alpha\beta\gamma}\epsilon_{ijk}\partial_\alpha n^i \partial_\beta n^j \partial_\gamma n^k \mathrm{d}x\mathrm{d}y\mathrm{d}z, \\ & \alpha,\beta,\gamma = 1,2,3, \end{aligned} \tag{3}$$

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

$$m = \sum_l m_l = \int_V \rho \mathrm{d}x\mathrm{d}y\mathrm{d}z, \tag{4}$$

where

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

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

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

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

$$j^\alpha = \frac{1}{8\pi}\epsilon^{\alpha\beta\gamma\delta}\epsilon_{ijk}\partial_\beta n^i \partial_\gamma n^j \partial_\delta n^k,$$

$$\alpha,\beta,\gamma,\delta = 0,1,2,3, \quad i,j,k = 1,2,3. \tag{7}$$

It is obvious that

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

i.e. the topological current is identically conserved and its zero-component is the strength density of the disclination points. In the following, we 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

Let us consider the ϕ-mapping ϕ^i: $x \longrightarrow \phi^i(x)$ $(i = 1,2,3)$, which is called the order parameter of the disclination point. In liquid crystals, the order parameter can be taken as the molecular field $\phi^i(x) = \nabla^2 n^i(x)$ or the gradient field $\phi(x) = \nabla\theta(x)$, where $\theta(x)$ is the angle between $\boldsymbol{n}(x)$ and the x^1 axes. Since the order parameter $\phi^i(x)$ is parallel to the director field $\boldsymbol{n}(x)$,[22] which is a unit vector field

$$n^i(x)n^i(x) = 1, \qquad i = 1,2,3, \tag{9}$$

the director field can be expressed as the direction field of the order parameter at the places $\phi^i(x) \neq 0$, i.e.

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

At the zeros of $\phi^i(x)$, the director field is indefinite, which is called the singular point of $\boldsymbol{n}(x)$. In liquid crystals, it is well known that the disclination points locate at the singularities of the director field. This property should be reflected mathematically, which is what we do in this paper. Using equation (10) and

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

j^α in equation (7) can be rewritten as

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

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

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

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

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

From equations (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 $\boldsymbol{\phi}(x)$, i.e. at the singularities of the general director field $\boldsymbol{n}(x)$. So, let us concentrate on the zeros of $\boldsymbol{\phi}(x)$.

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 parameter x^0 as

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

with the generalized velocity

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

Then, as we have proven in Ref.[23], the δ-function $\delta^3(\boldsymbol{\phi})$ can be expanded by these zeros as

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

where the positive β_l is called the Hopf index of $\phi^i(x)$ at $\boldsymbol{z}_l$. This means that, when the point $\boldsymbol{x}$ wraps the zero $\boldsymbol{z}_l$ 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 fields $\boldsymbol{n}$ and $-\boldsymbol{n}$, β_l can be integers and half-integers. Substituting equations (18) and (19) into (15), the inner structure of the topological current is formulated by

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

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 $\boldsymbol{z}_l$

$$\eta_l = \frac{J(\phi/x)}{|J(\phi/x)|}|\boldsymbol{z}_l = \pm 1 \tag{21}$$

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

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

and

$$m = \sum_{l=1}^{N}\beta_l\eta_l. \tag{23}$$

Here, we stress that the total strength of disclinations in liquid crystals is not arbitrary, it is a topological invariant. From the Gauss–Bonnet–Chern theorem and the Hopf index theorem,[24,25] the total disclination strength equals the Euler characteristic of the material body. Meanwhile, in liquid crystals, since the free energy is proportional to the square of the disclination strength, there exist in general the disclination lines of strength $\frac{1}{2}$ in two dimensions and the disclination points of strength 1 in three dimensions. In the two-dimensional case, the general director $\boldsymbol{n}$ 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 $\theta\left(0 \leq \theta < \frac{\pi}{2}\right)$ and $\frac{\pi}{2} + \theta$, in which one can see two brushes when observed between the orthogonal Nicol prisms. While for a disclination point of strength 1 in the three-dimensional case, the director $\boldsymbol{n}$ 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.

4. Conclusion

In summary, we conclude that the disclination points are determined by the singularities of the general director field and they are topologically quantized by the Hopf indices and Brouwer degrees (i.e. the wrapping numbers). Due to the equivalence of the director fields $\boldsymbol{n}(x)$ and $-\boldsymbol{n}(x)$ in physics, the Hopf indices can be integers and half-integers, which represent a great generalization of our previous theory of integer Hopf indices.

References

[1] Kléman M 1983 Points, Lines and Walls *Liquid Crystals, Magnetic Systems and Various Disordered Media* (New York: Wiley)

[2] Kurik M V and Lavrentovich O D 1988 *Usp. fiz. Nauk* **154** 381
Kurik M V and Lavrentovich O D 1988 *Sov. Phys. Usp.* **31** 196

[3] Mermin N D 1979 *Rev. Mod. Phys.* **51** 591

[4] Friedel J 1964 *Dislocations* (Oxford: Pergamon)

[5] Nabarro F R N 1967 *Theory of Crystal Dislocations* (London: Oxford University Press)

[6] Lubensky T C 1997 *Solid State Commun.* **102** 187

[7] De Gennes P G 1970 *Lecture Notes* (Orsay)

[8] Kléman M 1972 *Liquid Crystalline Systems* ed by G W Gray and P Windsor (New York: Academic)
Kléman M 1973 *Phil. Mag.* **27** 1057

[9] Holz A 1992 *Physica* A **182** 240

[10] Finkelstein D 1966 *J. Math. Phys.* **7** 1218

[11] Rogula D 1976 *Trends in Applications of Pure Mathematics to Mechanics* ed G Fichera (New York: Pitman)

[12] Toulouse G and Kléman M 1976 *J. Physique Lett.* **37** L149

[13] Volovik G E and Mineev V P 1977 *Sov. Phys. JETP* **45** 1186
Volovik G E *et al* 1977 *Sov. Phys. JETP* **46** 401
Volovik G E 1976 *Sov. Phys. JETP Lett.* **48** 561

[14] Shankar R 1977 *J. Physique* **38** 1405

[15] Kléman M, Michel L and Toulouse G 1977 *J. Physique Lett.* **38** L195

[16] Anderson P W 1984 *Basic Notions of Condensed Matter Physics* (London: Benjamin)

[17] Bray A J 1994 *Adv. Phys.* **43** 375

[18] Blaha S 1976 *Phys. Rev. Lett.* **36** 874

[19] Yang G H and Duan Y S 1998 *Int. J. Theor. Phys.* **37** 2371

[20] Yang G H and Duan Y S 1999 *Int. J. Eng. Sci.* **37** 1037

[21] Duan Y S, Yang G H and Jiang Y 1997 *Gen. Relativ. Grav.* **29** 715

[22] De Gennes P G 1974 *The Physics of Liquid Crystals* (London: Oxford University Press)

[23] Duan Y S, Yang G H and Jiang Y 1997 *Helv. Phys. Acta* **70** 565

[24] Yang G H 1998 *Mod. Phys. Lett.* A **13** 2123

[25] Duan Y S, Li S and Yang G H 1998 *Nucl. Phys.* B **514** 705