PHYSICAL PROPERTIES OF

Liquid Crystals: Nematics

Edited by

DAVID DUNMUR
University of Southampton, UK

ATSUO FUKUDA
Shinshu University, Japan

and

GEOFFREY LUCKHURST
University of Southampton, UK

IEE

INSPEC

Published by: INSPEC, The Institution of Electrical Engineers,
London, United Kingdom

The Institution of Electrical Engineers,
Michael Faraday House,
Six Hills Way, Stevenage,
Herts. SG1 2AY, United Kingdom

British Library Cataloguing in Publication Data

Physical properties of liquid crystals: nematics.–(EMIS Datareviews series; no.25)
1. Liquid crystals
I. Dunmar, D.A. II. Fukuda, A. III. Luckhurst, G. R.
530.4'29

ISBN 0 85296 784 5

Printed in England by Short Run Press Ltd., Exeter

5.4 Quantitative aspects of defects in nematics

T. Ishikawa and O.D. Lavrentovich

August 1998

A INTRODUCTION

Defects in nematic liquid crystals are reviewed at three levels: (1) topological classification; (2) elastic features; (3) experimental observations.

B TOPOLOGICAL CLASSIFICATION

Defects in uniaxial nematics are described in terms of the spatial distribution of the director $\mathbf{n}(\mathbf{r})$. There are two types of functions $\mathbf{n}(\mathbf{r})$: those containing singularities (at which $\mathbf{n}$ is not defined) and those without singularities. For three-dimensional nematics, the singular regions may be either zero-dimensional (points), one-dimensional (lines), or two-dimensional (walls). These are the defects. Whenever a non-homogeneous state cannot be eliminated by continuous variations of $\mathbf{n}(\mathbf{r})$ (i.e. the homogeneous state $\mathbf{n}(\mathbf{r})$ = const cannot be generated), it is called a topologically stable, or simply a topological defect. If the inhomogeneous state does not contain singularities, but nevertheless is not deformable continuously into a homogeneous state, the system is said to contain a topological configuration (or soliton).

Wall defects as singular defects are not topologically stable [1]. The energy per unit area of a singular wall $\sim U/a^2$ is defined by the energy U of molecular interactions and the molecular length scale a. If such a singularity is replaced by a smooth director reorientation over a macroscopic length $l \gg a$, its energy reduces to $U/al \sim K/l$; here $K \sim U/a$ is an average value of the Frank elastic constants. Thus the singular walls are unstable and tend to smear out. The term 'wall' is often used to describe continuous reorientation of the director field by an angle π or 2π. When the macroscopic width l of the wall is fixed by some external factor, such as electromagnetic field or surface anchoring, the wall is a topological soliton.

Line defects can be topologically stable. Topological stability of defects is controlled by the order parameter space of the medium [2,3]. This space is the manifold of all possible values of the order parameter that do not alter the thermodynamical potentials of the system. In uniaxial nematics, the order parameter space is a sphere with pairs of diametrically opposite points being identical. Such a sphere is denoted as S^2/Z_2; every point of S^2/Z_2 represents a particular orientation of $\mathbf{n}$. Any reorientation of the nematic as a whole leaves the thermodynamical potentials unchanged. In addition, since the nematics are non-polar, $\mathbf{n} \equiv -\mathbf{n}$, any two diametrically opposite points describe the same state.

Imagine now a singular line in a bulk nematic (FIGURE 1); the goal is to verify its topological stability. Let us surround the line by a loop γ; the only requirement is that γ does not approach the singular region too closely (the 'safe' distance is usually a few molecular lengths), so that the direction of $\mathbf{n}$ is well-defined at every point along γ. The function $\mathbf{n(r)}$ maps the points of a real space along γ into the order parameter space. When one goes around γ, $\mathbf{n(r)}$ draws some closed contour Γ on S^2/Z_2 that might be of two types: (a) a contour that starts and terminates at the very same point (for example, a circle); (b) a contour that connects two diametrically opposite points of S^2/Z_2. Contours (a) can be continuously contracted into a single point. When Γ shrinks smoothly into a point, the corresponding director field in real space becomes uniform, $\mathbf{n(r)}$ = const, and the singularity disappears. Contours (b) cannot be contracted: under any continuous deformations, their ends remain the ends of a diameter of S^2/Z_2. The corresponding defect lines are topologically stable since they cannot be transformed into a uniform state (although they can be transformed one into another).

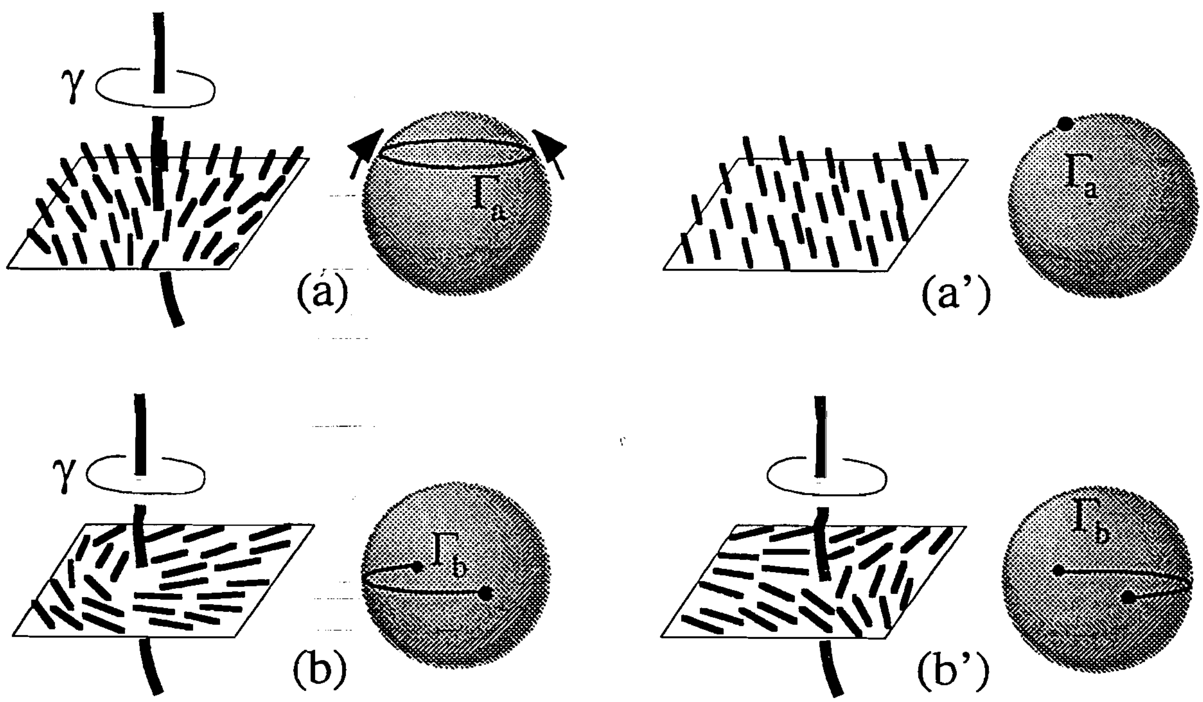

FIGURE 1 Topologically unstable (a) and stable (b) defect lines - disclinations in a uniaxial nematic.

We conclude that there are two classes of nematic line defects, called also disclinations: topologically stable and unstable. Transformation between these classes is possible only when the nematic order is destroyed at the whole half-plane ending at the line. The energy of such a singular wall is much larger than the energy of a singular line, which gives a physical interpretation of the topological stability of disclinations.

Point defects-hedgehogs are another type of topological defect in the bulk nematic [3]. The simplest is a radial hedgehog $\mathbf{n(r)} = \pm\mathbf{r}/|\mathbf{r}|$: a point with a radial director field around it, as shown in FIGURE 2. Generally, to elucidate the stability of a point defect, it is enclosed by a closed surface (e.g. a sphere) σ. The function $\mathbf{n(r)}$ produces a mapping of σ onto some surface Σ in the order parameter space. If Σ can be contracted to a single point, the point defect is topologically unstable. If Σ is wrapped $N \neq 0$ times around the sphere S^2/Z_2, the point singularity is a stable defect with a topological charge $N \neq 0$ (see FIGURE 2). Analytically,

$$N = \frac{1}{4\pi}\oiint\left(\frac{\partial\theta}{\partial u}\frac{\partial\varphi}{\partial v} - \frac{\partial\theta}{\partial v}\frac{\partial\varphi}{\partial u}\right)\sin\theta\,du\,dv = 0, \pm 1, \pm 2, \ldots.. \qquad (1)$$

for the director parametrised as $\mathbf{n} = \{\sin\theta\cos\varphi; \sin\theta\sin\varphi; \cos\theta\}$, with the polar angle θ and the azimuthal angle φ being functions of the coordinates u and v on σ.

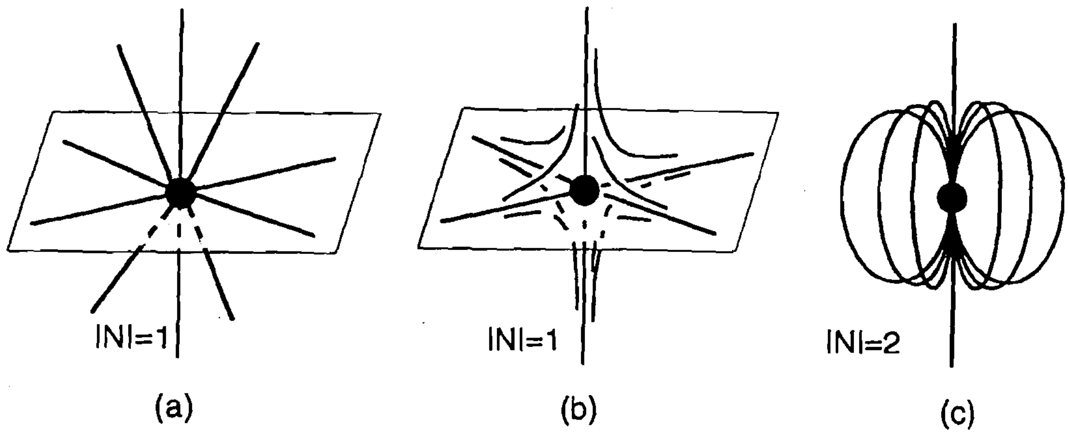

FIGURE 2 Topological point defects in a uniaxial nematic.

Since $\mathbf{n} \equiv -\mathbf{n}$, each point defect can be equally labelled by N and -N. The coalescence of two points N_1 and N_2 can result in a defect with a charge $|N_1 + N_2|$ or $|N_1 - N_2|$, depending on the presence of disclinations in the system and the path of coalescence [3].

Point defects-boojums (see FIGURE 3) are special point defects that, in contrast to hedgehogs, exist only at the boundary [4]. Any attempt to move a boojum from the surface into the bulk is accompanied by energetically costly additional deformations. In addition to the integer N, boojums are characterised by a two-dimensional topological charge k of the unit vector field **t** projected by the director onto the surface:

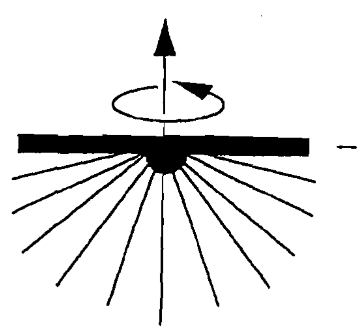

FIGURE 3 An axisymmetric boojum at a surface with tangential anchoring.

$$k = \frac{1}{2\pi}\oint\left(t_x\frac{dt_y}{dl} - t_y\frac{dt_x}{dl}\right)ds = 0, \pm 1, \pm 2, \ldots.. \qquad (2)$$

Here s is the natural parameter defined along the loop at the surface enclosing the defect core; k shows how many times **t** rotates by the angle 2π when we move once around the defect.

Bounded nematic volumes. Usually, defects are considered as perturbations of the uniform state, caused, for example, by some mechanical admixtures. There are, however, many situations when topological defects correspond to the equilibrium state of a system. Nematic droplets suspended in an isotropic matrix (a fluid such as water or a polymer such as polyvinylalcohol) and inverted systems (water droplets in a nematic matrix) provide the most evident examples.

The balance of the elastic energy of director distortions and surface energy defines the equilibrium of a bounded nematic such as a droplet. Representative estimates are $\sigma_0 R^2$ for the isotropic part of the surface energy, $W_a R^2$ for the anisotropic surface energy, and, finally, KR for the elastic energy. Here R is the radius of the droplet, σ_0 is the surface tension coefficient and W_a is the surface anchoring coefficient, which measures the energy penalty for director deviations from some preferred surface orientation (e.g. molecular interactions might favour perpendicular orientation of **n** at the boundary). Usually, $\sigma_0 >> W_a$, so that the droplets are practically spherical with the interior director field defined by the balance of KR and $W_a R^2$.

Small droplets with $R << K/W_a$ avoid spatial variations of **n** at the expense of violated boundary conditions. In contrast, large droplets, $R >> K/W_a$, satisfy boundary conditions by aligning **n** along the preferred direction(s) at the surface. Since the boundary of the droplet is curved, this anchoring effect leads to a distorted director distribution in the bulk, for example a radial hedgehog in the case where the surface director orientation is normal. With typical values of $W_a \approx 10^{-5}$ J/m^2 and $K \approx 10^{-11}$ N, the characteristic radius R is of the order of 1 μm. Generally, bounded nematic volumes at scales $R >> K/W_a$ contain defects with total topological charges satisfying the following two relationships that have their roots in the Poincaré and Gauss theorems of differential geometry:

$$\sum_i k_i = E \text{ and } \sum_j N_j = E/2 \qquad (3)$$

Here E is the topological invariant of the bounding surface, called the Euler characteristic; for a sphere E = 2 and for a torus E = 0. FIGURE 4 shows nematic droplets freely suspended in a glycerin matrix; each droplet contains a pair of boojums at the poles, $k_1 = k_2 = 1$, in agreement with the first expression of EQN (3).

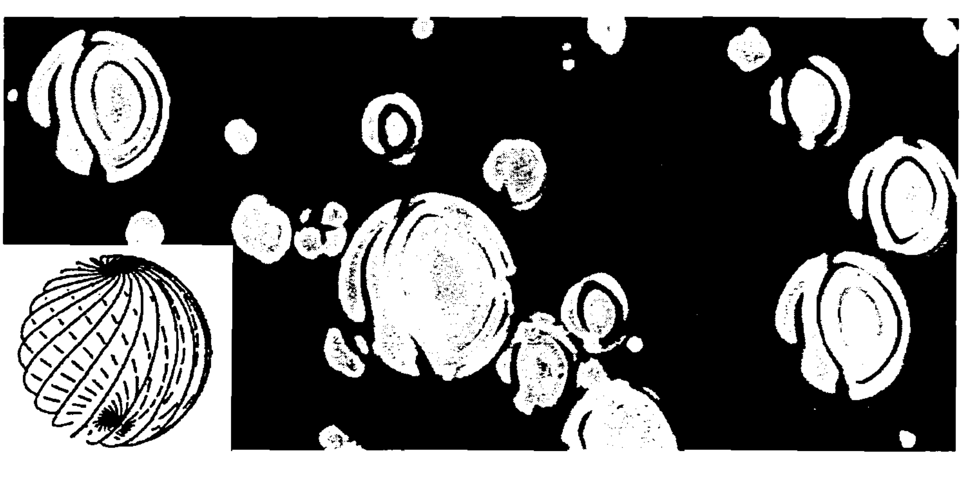

FIGURE 4 Bipolar nematic droplets with point defects-boojums at the poles. The droplets are suspended in a glycerol matrix and illuminated by polarised light. The inset shows the director configuration at the surface of the droplet.

C ENERGETICS OF THE DEFECTS

Disclinations within the same topological class but of different configurations can be continuously transformed into one another. Their relative stability depends on the Frank elastic constants of splay (K_1), twist (K_2), bend (K_3) and saddle-splay (K_{24}) in the elastic free energy density functional:

$$F = \frac{1}{2}K_1(\mathrm{div}\mathbf{n})^2 + \frac{1}{2}K_2(\mathbf{n}.\mathrm{curl}\mathbf{n})^2 + \frac{1}{2}K_3(\mathbf{n}\times\mathrm{curl}\mathbf{n})^2 - K_{24}\mathrm{div}(\mathbf{n}.\mathrm{div}\mathbf{n} + \mathbf{n}\times\mathrm{curl}\mathbf{n}) \qquad (4)$$

Here we assume the so-called K_{13} constant to be zero.

Frank [5] considered planar disclinations in which **n** is perpendicular to the line. For such disclinations, the K_{24}-term in EQN (4) is always zero. In the one-constant approximation $K_1 = K_2 = K_3 = K$, the equilibrium director field around the planar disclination reads

$$\mathbf{n} = \{\cos[k\varphi + c], \sin[k\varphi + c], 0\} \qquad (5)$$

where $\varphi = \arctan(y/x)$, x and y are Cartesian coordinates in the plane normal to the line, and c and k are constants; k is called the strength of the disclination that shows the number of 2π-rotations of the director around the line; it can be integer or half-integer. For the line in FIGURE 1(b), $k = 1/2$, while for the line in FIGURE 1(b'), $k = -1/2$.

The energy per unit length (line tension) of a planar disclination is

$$F_{ll} = \pi K k^2 \ln\frac{R}{r_c} + F_c \qquad (6)$$

where R is the characteristic size of the system, and r_c and F_c are respectively the radius and the energy of the disclination's core, a region in which the distortions are too strong to be described by a phenomenological theory.

The Frank theory does not distinguish lines of integer and half-integer strength, except for the fact that the lines with $|k| = 1$ tend to split into pairs of lines with $|k| = 1/2$, which reduces the energy, according to EQN (6). However, the lines of integer strength are unstable in a more fundamental topological sense: they can be continuously transformed into a non-singular uniform state, as already discussed. Imagine a circular cylinder with normal orientation of molecules at the boundaries, as shown in FIGURE 5(a). The planar disclination would have a radial-like director field normal to the axis of the cylinder. However, the director can be reoriented along the axis, as indicated in FIGURE 5(b). The process, called 'escape in the third dimension', is energetically favourable, since the energy of the escaped configuration is $3\pi K$ [6,7].

Detailed calculations of the disclination energies have been performed by Anisimov and Dzyaloshinskii [8]. They showed that, in addition to planar lines, 'bulk' disclinations can exist, in which the director does not lie in a single plane. Planar lines are stable when $2K_2 > K_1 + K_3$; bulk lines are preferable when $2K_2 < K_1 + K_3$.

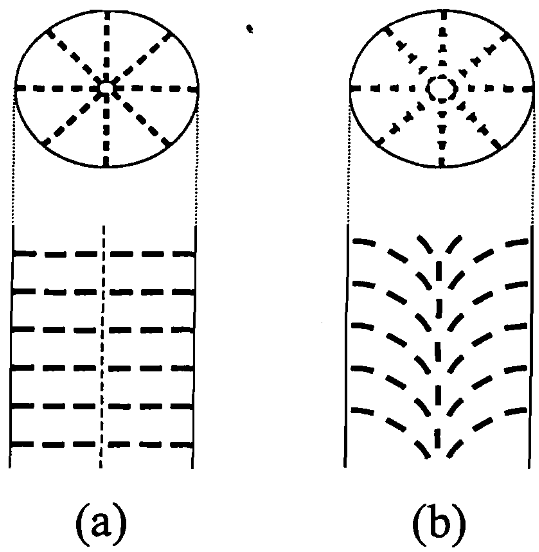

FIGURE 5 A cylinder with a disclination k = 1 (a) and an escaped configuration (b).

Point defects. Unlike point defects such as vacancies in solids, the topological point defects in nematics cause disturbances over the whole nematic volume. The energy of the point defect is proportional to the size R of the system. For example,

$$F_{rh} = 8\pi R(K_1 - K_{24}) + F_{cr} \tag{7}$$

$$F_{hh} = 8\pi R\left(\frac{K_1}{5} + \frac{2K_3}{15} + \frac{K_{24}}{3}\right) + F_{ch} \tag{8}$$

for the radial hedgehog (see FIGURE 2(a)) with

$$\mathbf{n} = (x, y, z)/\sqrt{x^2 + y^2 + z^2}$$

and the hyperbolic hedgehog (FIGURE 2(b)) with

$$\mathbf{n} = (-x, -y, z)/\sqrt{x^2 + y^2 + z^2}$$

respectively [9].

Interaction between defects. The interaction energy between two planar disclinations with strength k_1 and k_2 separated by a distance d is [10]

$$F = \pi K(k_1 + k_2)^2 \ln(R/r_c) - 2\pi K k_1 k_2 \ln(d/r_c) \tag{9}$$

The lines with opposite signs of k attract each other. Note that if $k_1 = -k_2$ the energy of the pair does not depend on the size R of the system.

D EXPERIMENTAL OBSERVATIONS

When viewed under a polarising microscope, a nematic slab between two glass plates shows distinctive textures. The simplest one is the homeotropic texture that occurs when the director is oriented strictly perpendicular to the bounding plates. Between crossed polarisers, the entire area of the texture appears dark, since the optical axis of the nematic is oriented along the optical axis of the microscope. If the surface orientation of **n** is tangential (**n** is in the plane of the plates) or tilted conical, then a so-called Schlieren texture can form. The main feature of Schlieren textures (see FIGURE 6) is the presence of two types of centres from which two or four extinction bands emerge. The extinction bands (also called brushes) occur in areas where **n** is parallel to either polariser or analyser of the microscope. The centres with two bands have a sharp (singular) core, insofar as can be seen, of submicron dimensions and correspond to the ends of disclinations. The two ends of the disclinations can be located on the opposite plates or on the same plate. The centres with four brushes correspond to boojums, or, on rare occasions, to hedgehogs. On some occasions, points with higher numbers of brushes are encountered [11,12]. There is a simple relationship between the number of brushes B emerging from the point and the defect strength k: $|k| = B/4$. Note, however, that this relationship has limited validity: when the director field is distorted non-uniformly around the defect, the number of brushes fails to provide the information about k [12].

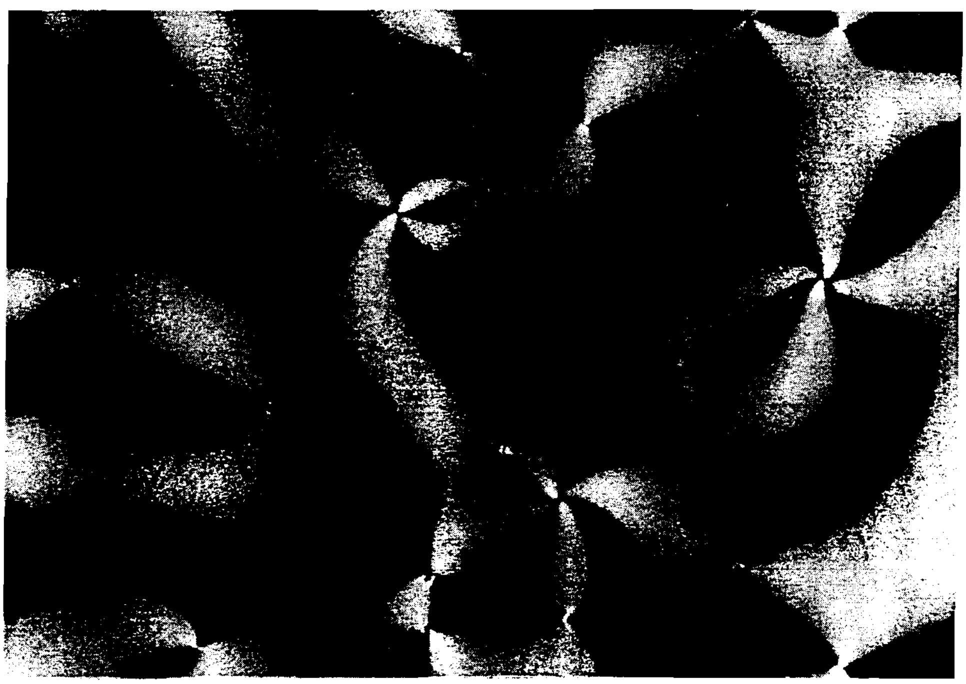

FIGURE 6 A typical Schlieren texture in a film of 4-pentyl-4′-cyanobiphenyl (thickness 23 μm) between two glass plates coated with thin layers of glycerol.

E ENTANGLEMENT OF DISCLINATIONS

Disclinations can pass through each other. Experiments [13,14] show the process of reconnection: two initial lines exchange ends as they cross so that each of the two ensuing lines has segments of the two original disclinations (see FIGURE 7). The result of crossing depends on the local director field in the region of crossing. In the cells that favour a planar distribution of the director around the disclinations, the result of crossing depends on the total strength of the pair [14,15]: $k_1 + k_2 = 0$ favours scheme (a) and $k_1 + k_2 = 1$ favours scheme (b) shown in FIGURE 7.

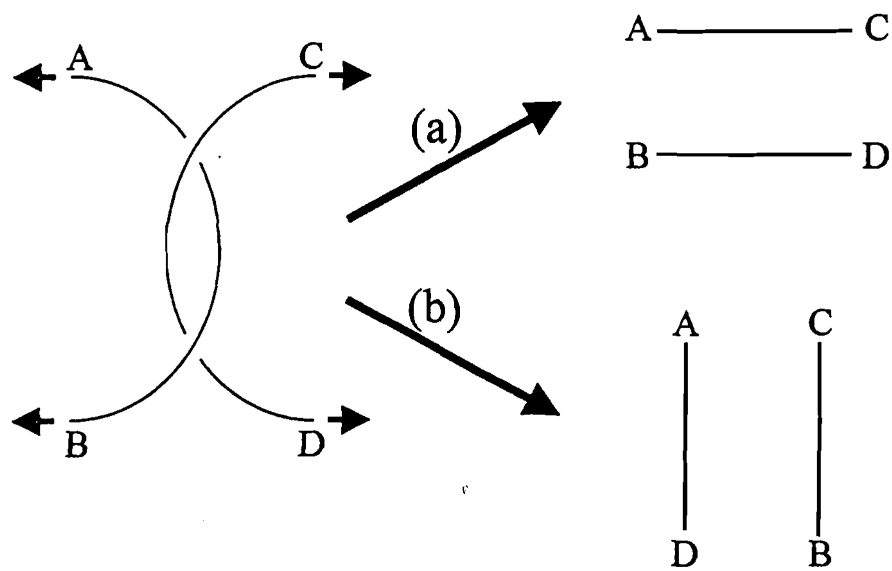

FIGURE 7 Two possible results of reconnection of line defects.

F CONCLUSION

Although the topological classification of defects in nematics has been firmly established, there are still many open questions concerning the behaviour of defects in external fields, their dynamics and interaction. Note that the classification of defects in biaxial nematics is drastically different from that in the uniaxial nematics considered here: in biaxial nematics, there are no hedgehogs (although boojums are allowed), and there are five topological classes of disclinations. Some pairs of these disclinations cannot cross each other without a creation of a third disclination that joins the original pair [16]. A detailed discussion of defects in liquid crystals can be found in the book by Kléman [17].

REFERENCES

[1] P.G. de Gennes, J. Prost [*The Physics of Liquid Crystals* 2nd edition (Oxford Science Publishers, Oxford, 1993) p.166-8]

[2] G. Toulouse, M. Kléman [*J. Phys. Lett. (France)* vol.37 (1976) p.L-149]

[3] G.E. Volovik, V.P. Mineyev [*Zh. Eksp. Teor. Fiz. (USSR)* vol.72 (1977) p.2256; *Sov. Phys.-JETP Lett. (USA)* vol.45 (1977) p.1186]

[4] G.E. Volovik [*Pis'ma Zh. Eksp. Teor. Fiz. (USSR)* vol.28 (1978) p.65; *JETP Lett. (USA)* vol.28 (1978) p.59]

[5] F.C. Frank [*Trans. Faraday Soc. (UK)* vol.25 (1958) p.19]

[6] P.E. Cladis, M. Kléman [*J. Phys. (France)* vol.33 (1970) p.1443]

[7] R.B. Meyer [*Philos. Mag. (UK)* vol.27 (1973) p.405]

[8] S.I. Anisimov, I.E. Dzyaloshinskii [*Zh. Eksp. Teor. Fiz. (USSR)* vol.63 (1972) p.1460; *Sov. Phys.-JETP (USA)* vol.36 (1973) p.774]

[9] M.V. Kurik, O.D. Lavrentovich [*Usp. Fiz. Nauk (USSR)* vol.154 (1988) p.381; *Sov.Phys.-JETP (USA)* vol.31 (1988) p.196]

[10] C.M. Dafermos [*Quart. J. Mech. Appl. Math. (UK)* vol.23 (1970) p.S49]

[11] N.V. Madhusudana, R. Pratibha [*Mol. Cryst. Liq. Cryst. (UK)* vol.103 (1983) p.31]

[12] O.D. Lavrentovich, Yu.A. Nastishin [*Europhys. Lett. (France)* vol.12 (1990) p.135]

[13] I. Chuang, R. Durrer, N. Turok, B. Yurke [*Science (USA)* vol.251 (1991) p.1336]

[14] T. Ishikawa, O.D. Lavrentovich [*Europhys. Lett. (France)* vol.41 (1998) p.171]

[15] K. Janich, H.-R. Trebin [in *Physique de Defauts/Physics of Defects* Ed. R. Balian (North Holland Publishers, Amsterdam, 1981) p.421-9]

[16] G. Toulouse [*J. Phys. Lett. (France)* vol.38 (1977) p.L-67]

[17] M. Kléman [*Points, Lines, and Walls* (John Wiley and Sons, New York, 1983)]