

CHAPTER 3

TOPOLOGICAL DEFECTS IN BIAXIAL NEMATICS

3.1 Introduction

In the previous chapter, a continuum theory of elasticity of biaxial nematics (BN) was presented. It was emphasized that elastic anisotropy due to inherent biaxiality can lead to elastic instabilities. Here, the effects of inherent biaxiality on topological defects such as disclinations and boojums will be explored.

It was mentioned in the introductory chapter that in BN, four stable singular line defects are possible [1]. They are three distinct disclinations of half-integral strength in a-b, **b-c** and c-a director fields, and a disclination of odd-integral strength in any two of the director fields. Incidentally, even-integral strength line defects exist but they can be made nonsingular through a 180° director distortion of one of the directors. In Figure 3.1, this is shown for a $s = 2$ disclination. This does not exhaust all possible topological defects in these systems. It is only recently that some of these theoretical predictions about defects in BS have been experimentally

verified by De'Neve *et al.* [2]. There has also been theoretical interest in the phase ordering kinetics of BN films [3] and statistical-mechanical properties of defects in this system [4]. In this context, it is important to know the structure, energetics and interaction of the various kinds of defects in biaxial nematics. In this chapter, the structure and energetics of certain other singular and non-singular disclinations are considered [5].

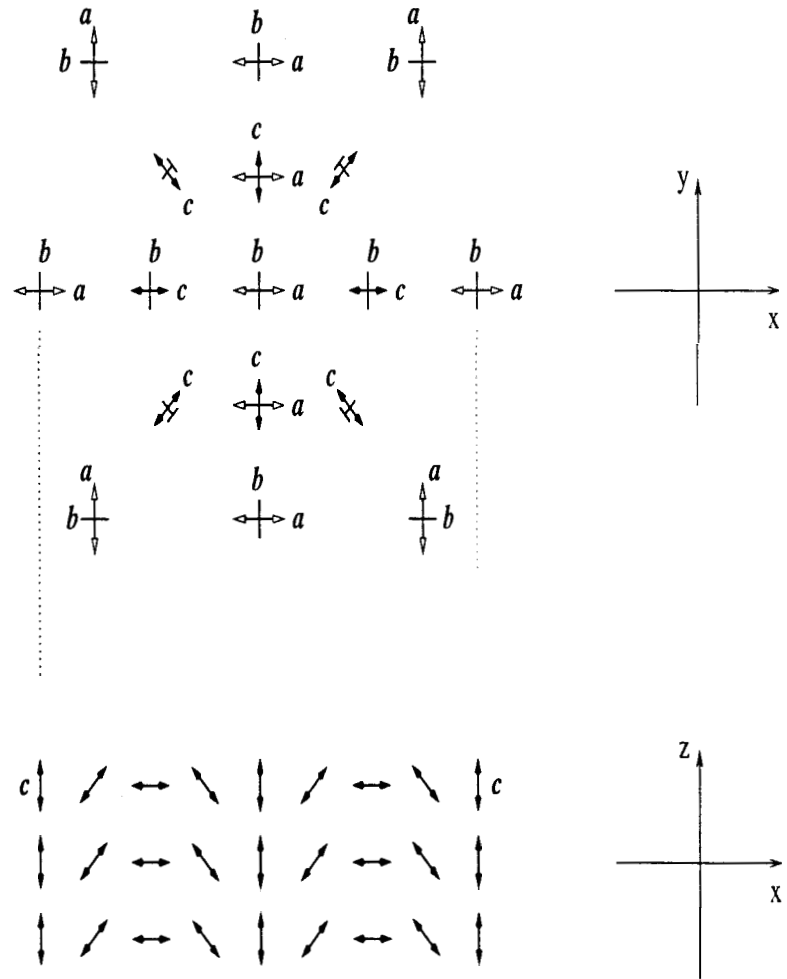


Figure 3.1: The singularity in a $s = 2$ disclination in (a,b) is removed by the "escape into the third dimension" through 180° of the c director. The nail representation shows a director going out of the plane of the paper.

3.2 Nonsingular defect structures

In uniaxial nematics, we know that a nonsingular line disclination of integral strength can exist. Nonsingular disclinations are also permitted in BN [6]. They are of two types. It has been already mentioned that a $s = 2$ or an even-integral strength disclination is nonsingular. Apart from wedge and twist disclinations, the symmetry of BN permits another type of disclination called a hybrid disclination which can also be nonsingular depending upon the strength of the defect. Before describing nonsingular hybrid disclinations, the process for creating such defects will be discussed.

The process for creating a hybrid disclination explicitly incorporates the orthorhombic symmetry of the **a**, **b**, **c** director fields. The process is schematically shown in Figure 3.2.

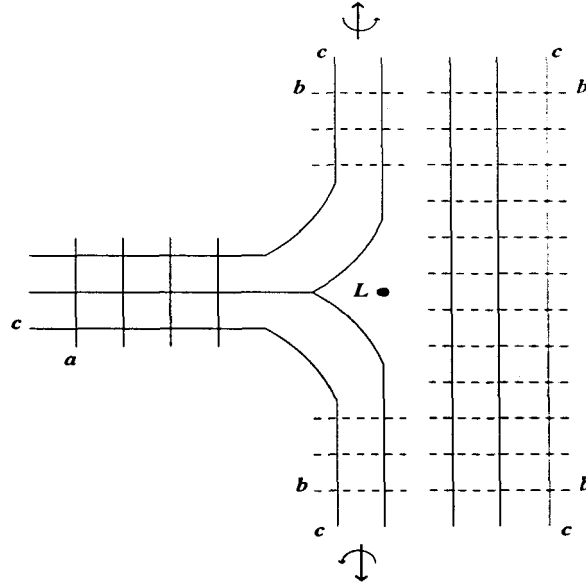


Figure 3.2: The Volterra process for creating a hybrid disclination composed of a wedge disclination in (**a**, **c**) and a twist disclination in (**a**, **b**).

Here, the plane of cut is limited by a line *L* parallel to any one of the directors, say *b*, and perpendicular to the other two, viz. *c* and *a*. The two faces of the cut are

relatively rotated through an integral multiple of $\pm\pi$, say, $\pm 2\pi s_1$ about L. These faces are further rotated about a or c, through an integral multiple of $\pm\pi$, *i.e.*, $\pm 2\pi s_2$. The empty space is filled up with uniform material or overlapping regions are removed and the system is allowed to relax. This process, also called a Volterra process, leads to a hybrid disclination which can be designated by a pair of numbers (s_1, s_2) where s_1 represents the strength of the wedge component and s_2 represents the strength of the twist component. This construction describes a wedge defect of strength s_1 in (a,c). But with a cyclic permutation of a, b and c similar defects in (a, b) and (b, c) fields can be described, too. It is important to note that s_1 and s_2 can be positive or negative integral or half-integral numbers. When $s_2 = 0$, we get a pure wedge disclination and when $s_1 = 0$, we get a pure twist disclination which was described in the introductory chapter. Thus, any line disclination can be looked upon as a hybrid disclination.

It can be shown that the singularity in the case of hybrid disclinations of total strength $|s_1| + |s_2| = 2$ can be removed by the "escape into the third dimension" through 90° of a director [6]. It is not enough to point out the mechanism of removing the singularity. We must also verify whether the equations of equilibrium permit such solutions. Here, the structure and energetics of the hybrid disclinations, (2,0) and (1,1), are worked out. In the case of (2,0), a line defect in (a,b) with c undistorted, as shown in Figure 3.1, has been considered.

Using $(\mathbf{e}_r, \mathbf{e}_\phi, \mathbf{e}_z)$ as the unit basis vectors of a cylindrical coordinate system (r, ϕ, z) , we can define the orthonormal triad of directors **(a,b,c)**:

$$\mathbf{a} = \sin \psi \sin \theta \mathbf{e}_r + \cos \psi \mathbf{e}_\phi + \sin \psi \cos \theta \mathbf{e}_z$$

$$\mathbf{b} = \cos \psi \sin \theta \mathbf{e}_r - \sin \psi \mathbf{e}_\phi + \cos \psi \cos \theta \mathbf{e}_z$$

$$\mathbf{c} = \cos \theta \mathbf{e}_r - \sin \theta \mathbf{e}_z$$

Here θ is the angle that $\mathbf{c}$ makes with the radial direction and ψ describes the angle of rotation of $(\mathbf{a}, \mathbf{b})$ about $\mathbf{c}$. With this parametrization, $\mathbf{c}$ is always in the (r, z) plane which suits the description of the removal of singularity in (1,1) and (2,0). For $\psi = \psi(\phi)$ and $\theta = \theta(r)$, the free energy density is given by

$$F = \frac{(K_a \cos^2 \psi + K_b \sin^2 \psi)}{2} \left(\frac{d\theta}{dr} \right)^2 + \frac{(K_a \sin^2 \psi + K_b \cos^2 \psi)}{2r^2} \cos^2 \theta + \frac{K_c}{2r^2} \left(\frac{d\psi}{d\phi} - \sin \theta \right)^2 \quad (3.1)$$

Without any loss of generality, we consider a particular situation where the director described by $\mathbf{c}$ goes over to the uniaxial nematic director $\mathbf{n}$ in the absence of biaxiality. In the weak-biaxiality limit, $K_a \simeq K_b$, the free energy density (3.1) reduces

$$F = \frac{K_a}{2} \left(\frac{d\theta}{dr} \right)^2 + \frac{K_a}{2r^2} \cos^2 \theta + \frac{K_c}{2r^2} \left(\frac{d\psi}{d\phi} - \sin \theta \right)^2 \quad (3.2)$$

The equations of equilibrium obtained by the minimization of the total energy are

$$\frac{d^2 \psi}{d\phi^2} = 0 \quad (3.3)$$

$$\frac{K_a}{r} \frac{d}{dr} \left(r \frac{d\theta}{dr} \right) + (K_a - K_c) \frac{\sin \theta \cos \theta}{r^2} + \frac{K_c \cos \theta}{r^2} \frac{d\psi}{d\phi} = 0 \quad (3.4)$$

It may be noted that $(\psi = \phi, \theta = -\pi/2)$ which describes a singular wedge disclination of strength (2,0) is a permitted solution while $(\psi = \phi, \theta = 0)$ which describes a singular hybrid disclination (1,1) with $\mathbf{c}$ in an all radial configuration and a uniform twist of $(\mathbf{a}, \mathbf{b})$ about $\mathbf{c}$ does not satisfy the equations of equilibrium. However, singularities in both these disclinations can be removed with a three dimensional escape of $\mathbf{c}$, described by $\psi = \phi$ and $\theta = \theta(r)$, provided

$$r \frac{d}{dr} \left(r \frac{d\theta}{dr} \right) + \left(1 - \frac{K_c}{K_a} \right) \sin \theta \cos \theta + \frac{K_c}{K_a} \cos \theta = 0 \quad (3.5)$$

To solve this equation, we consider the sample to be confined in a tube of radius r_0 with $\mathbf{c}$ aligned along the tube axis at $r = 0$.

(a) (2,0) disclination line : In this case the boundary conditions are $\theta = \frac{\pi}{2}$ at $r = 0$ and $\theta = -\frac{\pi}{2}$ at $r = r_0$, *i.e.*, $\mathbf{c}$ is parallel to the tube axis both at $r = 0$ and $r = r_0$ and these two states get connected by a smooth bend of $\mathbf{c}$ through π (see Figure 3.1). The $\mathbf{a}$ and $\mathbf{b}$ directors are in a $s = 2$ disclination configuration at $r = r_0$. Then it can be shown that

$$\delta = 2 \arctan \left[\frac{\left(\frac{r_0}{r}\right)^2 - 2\sqrt{\frac{K_a}{K_c}} \frac{r_0}{r} - 1}{\left(\frac{r_0}{r}\right)^2 + 2\sqrt{\frac{K_a}{K_c}} \frac{r_0}{r} - 1} \right] \quad (3.6)$$

If $\mathbf{c}$ is identified as the uniaxial director $\mathbf{n}$, $K_c < K_a$. Then the energy per unit length is

$$E = 4\pi K_a \left[1 + \frac{\frac{K_c}{K_a}}{\sqrt{1 - \frac{K_c}{K_a}}} \ln \left(\frac{1 + \sqrt{1 - \frac{K_c}{K_a}}}{\sqrt{\frac{K_c}{K_a}}} \right) \right] \quad (3.7)$$

(b) (1,1) hybrid disclination line : In this case, the boundary conditions are $\theta = \frac{\pi}{2}$ at $r = 0$ and $\theta = 0$ at $r = r_0$, *i.e.*, $\mathbf{c}$ is homeotropically aligned on the cylinder at $r = r_0$ and $\mathbf{c}$ is parallel to the tube axis at $r = 0$, and these two states are connected by a smooth bend of $\mathbf{c}$ through $\pi/2$ (see Figure 3.3). At $r = r_0$, $\mathbf{a}$ and $\mathbf{b}$ describe a twist about $\mathbf{c}$ through 2π as we go round the tube axis. In this case we get

$$\delta = 2 \arctan \left[\frac{\sqrt{\frac{K_c}{K_a}} \sinh(\ln(\frac{r_0}{r}) + \sinh^{-1}(\sqrt{\frac{K_a}{K_c}})) - 1}{\sqrt{\frac{K_c}{K_a}} \sinh(\ln(\frac{r_0}{r}) + \sinh^{-1}(\sqrt{\frac{K_a}{K_c}})) + 1} \right] \quad (3.8)$$

The energy per unit length - again with $K_c < K_a$ - is

$$E = 4\pi K_a \left[1 - \frac{\sqrt{1 + \frac{K_c}{K_a}}}{2} + \frac{\frac{K_c}{K_a}}{\sqrt{1 - \frac{K_c}{K_a}}} \ln \left(\frac{\sqrt{2}(1 + \sqrt{1 - \frac{K_c}{K_a}})}{\sqrt{1 - \frac{K_c}{K_a}} + \sqrt{1 + \frac{K_c}{K_a}}} \right) \right] \quad (3.9)$$

In Figure 3.3, a schematic representation of the removal of singularity of this hybrid

disclination is shown.

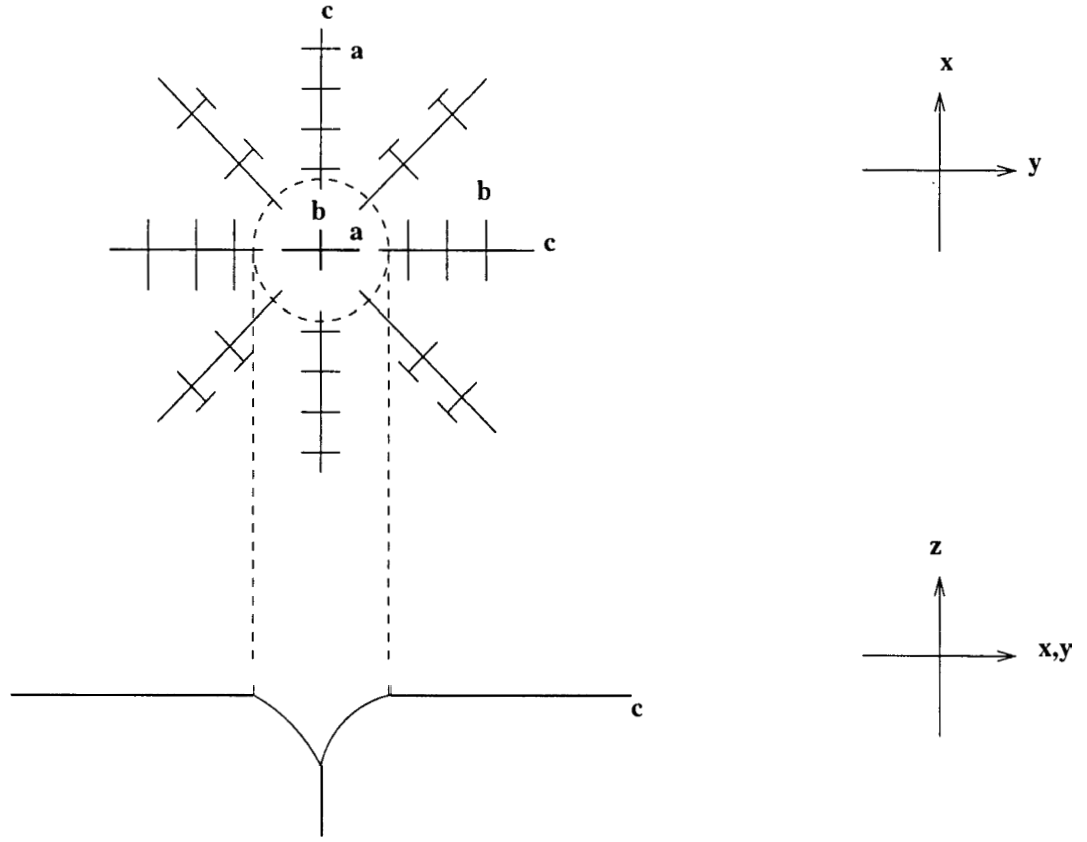


Figure 3.3: Removal of singularity in a hybrid disclination with $s_1 = s_2 = 1$ by an escape of the c director through $\pi/2$. The nail representation shows a director going out of the plane of the paper.

We get the known result, *i.e.*, $E = 2\pi K_a$ [7] for a $(1,0)$ defect in uniaxial limit if we set $K_c = 0$. This is the volume contribution to the energy per unit length. In this context, we point out that for $0 \leq \frac{K_c}{K_a} \leq 0.9$, the energy per unit length, E_h , of an escaped hybrid disclination $(1,1)$ is such that $2\pi K_a \leq E_h \leq 2.312\pi K_a$. We know that the energy of a singular wedge disclination of strength $s = \frac{1}{2}$ in (a,c) or (b,c) fields is $E_w = \frac{1}{4}\pi K_a \ln \frac{R}{r_c} + E_{core}$. Even without considering the core energy, E_{core} , relatively the hybrid is energetically favourable when the ratio of the sample size: R , to the core radius, r_c , *i.e.*, $\frac{R}{r_c} \geq 10^4$. This condition is easily realized in usual

samples.

It should be noted that a half strength disclination in **(a,b)** is the most favourable energetically since it does not involve distortion in the **c** director with which one would associate the largest elastic constant. The above analysis implies that a non-singular hybrid disclination would be preferred to a half strength disclination in **(a,c)** or **(b,c)** fields which involve the energetically expensive **c** director distortions. It may be noted that even $s = \pm 1$ disclinations in **(a,c)** or **(b,c)** may be favoured relative to the latter since energy can be lowered if **c** escapes into the third dimension. However, as made clear in the introduction, this will continue to be singular but in a different pair of directors **(a,b)**. A further splitting of the core of this into a pair of $s = \pm \frac{1}{2}$ can also be envisaged. Finally, in the case of planar **(a,c)** or **(b,c)** disclinations, the core will be in the isotropic phase for $\pm \frac{1}{2}$, while for $s = \pm 1$ planar disclinations, the core will be in the isotropic phase or the uniaxial phase depending upon whether **c** director is planar or in escaped state.

3.3 Singular hybrid disclinations

In this section we consider the effect of inherent biaxiality on the structure and energy of singular hybrid disclinations and their mutual interactions. We describe the orthonormal triad of directors in cartesian coordinates by

$$\begin{aligned}\mathbf{a} &= \sin \theta \sin \phi \mathbf{e}_x - \sin \theta \cos \phi \mathbf{e}_y + \cos \theta \mathbf{e}_z \\ \mathbf{b} &= -\cos \theta \sin \phi \mathbf{e}_x + \cos \theta \cos \phi \mathbf{e}_y + \sin \theta \mathbf{e}_z \\ \mathbf{c} &= \cos \phi \mathbf{e}_x + \sin \phi \mathbf{e}_y\end{aligned}$$

where $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$ are the orthonormal basis vectors. Here, ϕ is the angle **c** makes with the x -axis and θ describes the twist of **(a,b)** about **c**. The director **c** lies in the xy -plane. This parametrization is convenient to describe the geometry of hybrid

disclinations. A singular hybrid disclination of strength (s_1, s_2) with $\mathbf{c}$ in the xy -plane and the other two directors twisting about $\mathbf{c}$ is denoted by $[\mathbf{c}, \mathbf{b}, \mathbf{a}]$. Similarly, $[\mathbf{b}, \mathbf{a}, \mathbf{c}]$ describes a singular hybrid disclination with $\mathbf{b}$ in the xy -plane and $(\mathbf{a}, \mathbf{c})$ twisting about $\mathbf{b}$. With $\theta = \theta(x, y)$ and $\phi = \phi(x, y)$, the free energy density of $[\mathbf{c}, \mathbf{b}, \mathbf{a}]$ is

$$F = \frac{K_c}{2} \left[\left(\frac{\partial \theta}{\partial x} \right)^2 + \left(\frac{\partial \theta}{\partial y} \right)^2 \right] + \frac{(K_b \sin^2 \theta + K_a \cos^2 \theta)}{2} \left[\left(\frac{\partial \phi}{\partial x} \right)^2 + \left(\frac{\partial \phi}{\partial y} \right)^2 \right] \quad (3.10)$$

The equations of equilibrium - for $[\mathbf{c}, \mathbf{b}, \mathbf{a}]$ - are

$$K_c \nabla^2 \theta - (K_b - K_a) \sin \theta \cos \theta (\nabla \phi)^2 = 0 \quad (3.11)$$

$$(K_b \sin^2 \theta + K_a \cos^2 \theta) \nabla^2 \phi + 2(K_b - K_a) \sin \theta \cos \theta (\nabla \theta) \cdot (\nabla \phi) = 0 \quad (3.12)$$

It may be mentioned in passing that to describe $[\mathbf{b}, \mathbf{a}, \mathbf{c}]$ the following transformations will have to be made : $K_c \rightarrow K_b$, $K_b \rightarrow K_a$, $K_a \rightarrow K_c$. Firstly, we deal with single defects and then consider the interaction between a pair of hybrid disclinations.

(a) Single hybrid disclinations: For a single defect, we can take $\theta = \theta(\alpha)$ and $\phi = \phi(\alpha)$ where $\alpha (= \tan^{-1} y/x)$ is the azimuthal angle in cylindrical coordinate system. Then, from (3.10), the free energy density is

$$F = \frac{K_c}{2r^2} \left(\frac{d\theta}{d\alpha} \right)^2 + \frac{g(\theta)}{2r^2} \left(\frac{d\phi}{d\alpha} \right)^2 \quad (3.13)$$

where

$$g(\theta) = K_b \sin^2 \theta + K_a \cos^2 \theta \quad (3.14)$$

On integrating once the equations of equilibrium, (3.11) and (3.12), we get

$$g(\theta) \frac{d\phi}{d\alpha} = \text{constant} = k \quad (3.15)$$

$$K_c \left(\frac{d\theta}{d\alpha} \right)^2 + \frac{k^2}{g(\theta)} = \text{constant} = 3 \quad (3.16)$$

Table 3.1: The values of β (in units of 10^{-6} dynes) for the various defect states.

(s_1, s_2)	$K_a : K_b : K_c$						
	1 : 1 : 1	6 : 5 : 1					
	Defect State						
	All	[c,b,a]	[c,a,b]	[b,c,a]	[b,a,c]	[a,c,b]	[a,b,c]
(0.5 , 0)	0.25	1.5	1.25	1.5	0.25	1.25	0.25
(0 , 0.5)	0.25	0.25	0.25	1.25	1.25	1.5	1.5
(1 , 0)	1.0	6.0	5.0	6.0	1.0	5.0	1.0
(0 , 1)	1.0	1.0	1.0	5.0	5.0	6.0	6.0
(0.5 , 0.5)	0.5	1.612	1.612	1.832	1.832	2.042	2.042
(0.5 , 1)	1.25	2.367	2.367	5.604	5.604	6.555	6.555
(1 , 1)	2.0	6.447	6.447	7.328	7.328	8.167	8.167
(1 , 0.5)	1.25	5.621	5.621	3.315	3.315	3.497	3.497
(1 , 1.5)	3.25	7.713	7.713	13.644	13.644	15.705	15.705
(1 5 1)	3.25	13.176	13.176	9.953	9.933	10.702	10.702

Using this, the free energy density (3.13) becomes

$$F = \frac{\beta}{2r^2} \quad (3.17)$$

Then, the energy per unit length of the defect is

$$E = \pi\beta \ln \frac{R}{r_c} + E_{core} \quad (3.18)$$

where R and r_c are respectively the outer and inner limits of integration in the radial direction. Without explicitly considering E_{core} , we undertake an analysis which can be easily done. We give in Table 3.1 the values of β (in units of 10^{-6} dynes) calculated numerically for various structures for certain elastic anisotropies. Incidentally, values of β are not dependent on the sign of s_1 and s_2 . We have also

considered for pedagogic reasons, the case $K_a = K_b = K_c$ where we get analytical solutions. The differential equations with the appropriate boundary conditions i.e. at $\alpha = 0, \phi = 0, \theta = 0$, and at $\alpha = 2\pi, \phi = 2\pi s_1, \theta = 2\pi s_2$, have been solved using the shooting method incorporating Runge-Kutta-Fehlberg method.

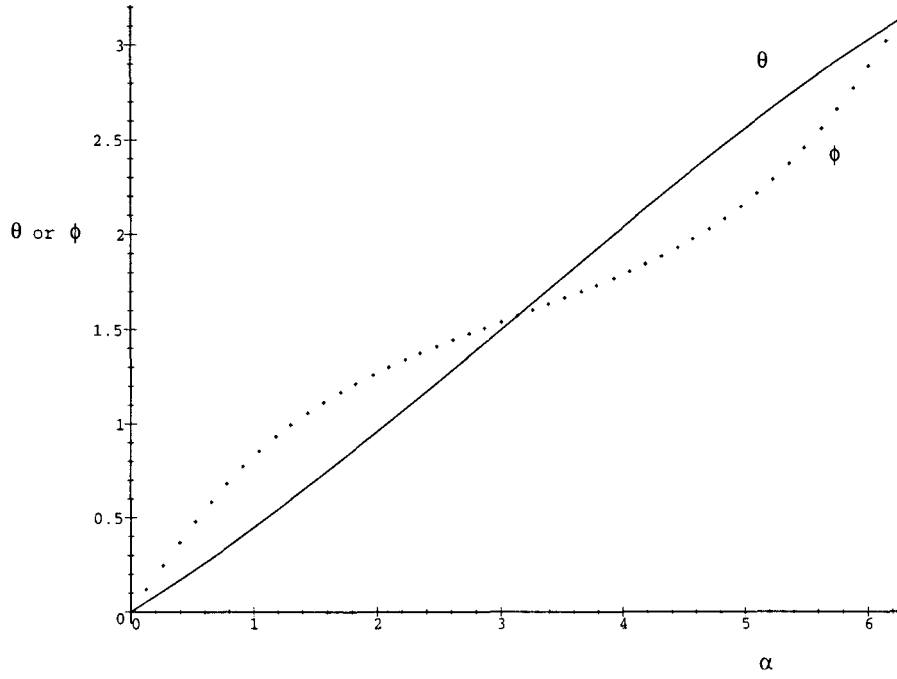


Figure 3.4: θ (bold line) and ϕ (dotted line) profiles, as functions of α , for $K_a : K_b : K_c = 6 : 4 : 1$ - all angles are given in radians.

The θ and ϕ profiles are shown in Figure 3.4 and it is apparent that the nonlinear profiles are distinct from the linear profiles usually expected for pure wedge and twist disclinations in uniaxial nematics in the "one-constant" approximation.

(b) Interaction between hybrid disclinations: Scaling arguments [8] can be used to find the energy of interaction between singular hybrids. We note that if

$\phi(x, y)$ and $\theta(x, y)$ are solutions, then $\phi(\frac{x}{\lambda}, \frac{y}{\lambda})$ and $\theta(\frac{x}{\lambda}, \frac{y}{\lambda})$ are also solutions of (3.11) and (3.12). Consider two hybrid disclinations (s_1, s_2) and (s_3, s_4) located at $(\frac{d}{2}, 0)$ and $(-\frac{d}{2}, 0)$ respectively. Near $(\frac{d}{2}, 0)$ the director pattern is a very good approximation to that of the hybrid (s_1, s_2) and near $(-\frac{d}{2}, 0)$ to that of (s_3, s_4) . At distances large compared to d we can assume the configuration of a $(s_1 + s_3, s_2 + s_4)$ hybrid disclination. Figure 3.5 shows the two operations that are employed in calculating the energy of interaction between disclinations.

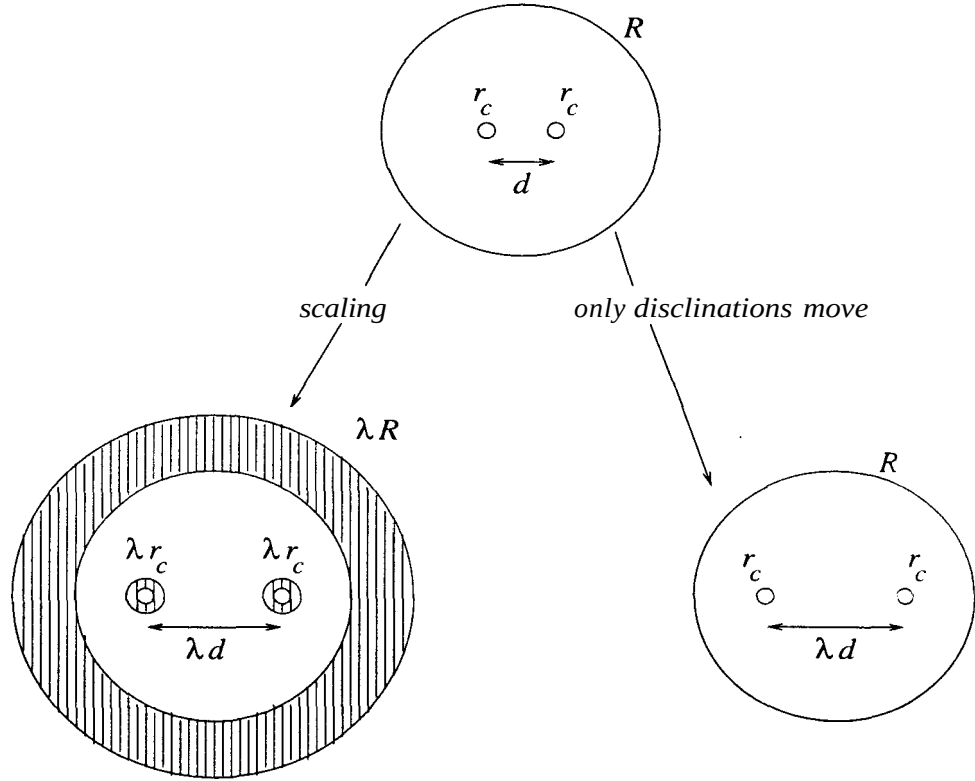


Figure 3.5: A schematic representation of the operations of scaling and disclination movement. (a) The scaling process does not change the energy but increases the size of the cores and moves the boundary. (b) The defects move apart as in (a) but the cores and the boundary remain unaltered in size.

To compute the force between the two defects, we consider the change in energy when the disclinations which are originally at a separation d are moved to a separation λd . The functions $\phi'(x, y) = \phi(\frac{x}{\lambda}, \frac{y}{\lambda})$ and $\theta'(x, y) = \theta(\frac{x}{\lambda}, \frac{y}{\lambda})$ describe the same two

defects separated by a distance λd . The elastic energy density associated with (ϕ', θ') is given by

$$F_{\phi', \theta'} = \lambda^{-2} F_{\phi, \theta} \quad (3.19)$$

However a given area in the solution (ϕ', θ') is dilated by a factor λ^2 , if $\lambda > 1$. Hence the total energy is the same as that of (ϕ, θ) solution. The scaling process does not change the energy per unit length but increases the size of the cores and pushes out the boundary. But we want the energy of the configuration where the defects move apart but the cores and boundary remain unaltered in size. Then the energy per unit length required to separate two defects, *i.e.*, the energy of interaction per unit length is

$$E = E_1 + E_2 - E_{12} \quad (3.20)$$

where E_1 and E_2 are respectively the elastic energies per unit length of the individual (s_1, s_2) and (s_3, s_4) defects obtained for the volume between the boundary of its core radius. ϵ . to $\lambda\epsilon$. E_{12} is the energy per unit length of a $(s_1 + s_3, s_2 + s_4)$ defect from an outer cutoff R to λR .

In view of (3.20). the energy of interaction between two defects is

$$E = \pi(\beta_1 + \beta_2 - \beta_{12}) \ln \lambda \quad (3.21)$$

where β_1 and β_2 are values of β for the individual (s_1, s_2) and (s_3, s_4) defects while β_{12} is that of the $(s_1 + s_3, s_2 + s_4)$ defect. If $E > 0$, we can say that the defects attract while for $E < 0$ they will repel and when $E = 0$. they do not interact. From the values of β given in Table 3.1, we can come to the following important conclusions.

- It is found that the interaction between pure wedge (or pure twist) disclinations is the same as that in uniaxial nematics.
- For $K_a : K_b : K_c = 1 : 1 : 1$, a pure wedge and a pure twist do not interact.

However, for $K_a : K_b : K_c = 6 : 5 : 1$, such a pair of defects attract if they are in the state $[c, b, a]$, $[b, c, a]$ or $[a, c, b]$ and repel if they are in $[c, a, b]$, $[b, a, c]$ or $[a, b, c]$ state. These results are independent of the sign of the defects. Figure 3.6 depicts schematically a pure wedge disclination and a pure twist disclination and, the bound hybrid disclination state with both wedge and twist components. In the case of the interaction between a pure wedge disclination and a hybrid disclination, it is found that there can be attraction if the wedge components are of the opposite sign. But if these components are of the same sign, the answer is not so straightforward. From Table 3.1, it can be seen that for the case of $(\frac{1}{2}, 0)$ and $(\frac{1}{2}, f)$, there is repulsion in all cases except for the state $[b, c, a]$. Whereas in the interaction between $(\frac{1}{2}, 0)$ and $(f, 1)$, it is always repulsion. But in the case of the defects $(1, 0)$ and $(\frac{1}{2}, 1)$, they repel in all states except $[b, c, a]$ and $[a, c, b]$.

- Within the range of parameters considered, the interaction between pure twist and hybrid disclinations seem to depend entirely on the sign of the twist components - with opposite signs they attract and with the same sign they repel.
- Finally, hybrids which have the same sign for both wedge and twist components repel. If the respective components are of opposite sign, then they attract. When only one of the components are of opposite sign, then they may attract or repel. For example, in the case of $(\frac{1}{2}, \frac{1}{2})$ and $(-\frac{1}{2}, \frac{1}{2})$, for $K_a : K_b : K_c = 1 : 1 : 1$ there is no interaction. But with $K_a : K_b : K_c = 6 : 5 : 1$, the defects attract each other when they are in the state $[c, b, a]$ or $[c, a, b]$; and in the other states they repel. For $(\frac{1}{2}, \frac{1}{2})$ and $(\frac{1}{2}, -\frac{1}{2})$, there is no interaction for $K_a : K_b : K_c = 1 : 1 : 1$; while for $K_a : K_b : K_c = 6 : 5 : 1$ there is attraction in the states $[b, a, c]$ and $[a, b, c]$, and repulsion in the other states.

From these results, it is clear that the interaction between hybrids is determined

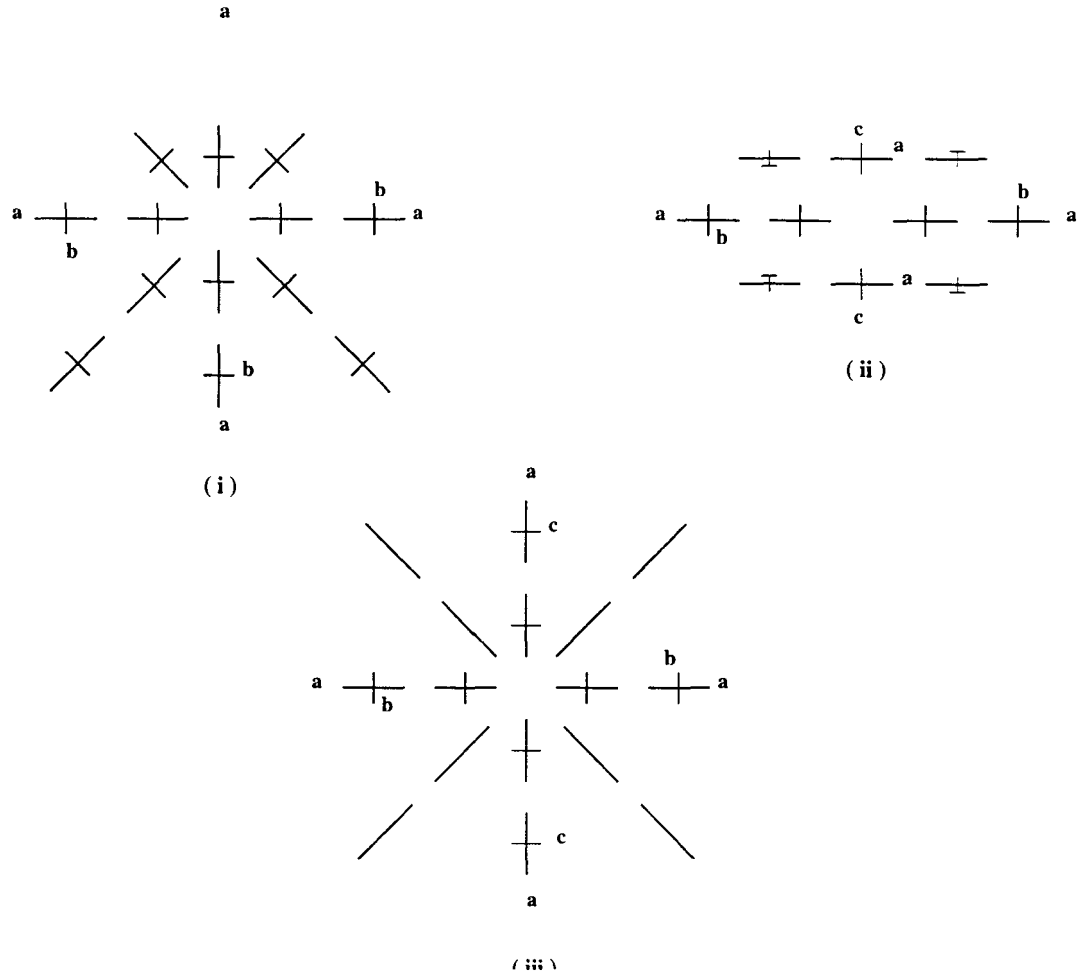


Figure 3.6: (i) A pure wedge disclination which combines with a pure mist disclination shown in (ii) to give the hybrid $s_1 = s_2 = 1$ depicted in (iii). The nail representation shows a director going out of the plane of the paper.

not only by the sign and the strength of the defects but also by the biaxial elastic anisotropy.

In view of this conclusion, we can make the following remarks. When an anisotropic media is viewed optically through crossed polarizers, the image will be dark if the principal axes of the dielectric tensor is either parallel or perpendicular to the polarizer. Knowing the structure of disclinations, it is easy to see that $s = \frac{1}{2}$ and $s = 1$ disclinations will have two and four regions of darkness respectively. These

appear as brushes, and they are called Schlieren textures. The Schlieren texture of hybrid disclinations of BN will be no different from that of usual disclinations of uniaxial nematics. But, its underlying structure can manifest itself in peculiar ways. For example, two two-brush defects of the same strength in the wedge component may even attract since they could be hybrids with opposite strengths in the twist component. Under crossed polarizers, a pure twist disclination as described above would be invisible when the polarization of light is either parallel or perpendicular to the uniform director. But at an angle, a contrast would show up.

3.4 Defects in droplets

We now consider drops of BN with $\mathbf{c}$ normal to the surface at the boundary of the drop. Topological constraints [9] require the $(\mathbf{a}, \mathbf{b})$ configuration to have surface singularities of combined strength, $s = 2$. If $\mathbf{c}$ is in a radial configuration, then there will be $(\mathbf{a}, \mathbf{b})$ disclination lines satisfying the above requirement. For example, if $\mathbf{a}$ is along longitudes and $\mathbf{b}$ along latitudes, then there will be $s = 1$ defects in $(\mathbf{a}, \mathbf{b})$ at the north and south poles. But, we know that a $s = 1$ strength line can split into two $s = \frac{1}{2}$ lines. Hence, this is also equivalent to four $s = \frac{1}{2}$ lines. How are these four $s = \frac{1}{2}$ lines oriented in space? A mathematically equivalent problem has been discussed by Lubensky and Prost [10]. They considered a spherical vesicle whose constituent molecules have biaxial orientational ordering. The orientational order due to biaxiality will have singularities of total strength $s = 2$. They show that the structure which minimizes the elastic energy is that which has four singularities of strength $s = \frac{1}{2}$ arranged in a tetrahedral configuration. An extension of their analysis implies that four $(\mathbf{a}, \mathbf{b})$ disclination lines of strength $s = \frac{1}{2}$ arranged in a tetrahedral configuration is of the least elastic energy. In the present case, the total elastic energy has not only splay energy in $\mathbf{c}$ but also energy due to distortions in $(\mathbf{a}, \mathbf{b})$ associated with the four $s = \frac{1}{2}$ disclinations. In the weak biaxiality limit,

$$K_a = K_b = K,$$

$$E_{tetrahedral} \simeq 4\pi KR + \pi K_c R \ln\left(\frac{R}{r_c}\right) + E_{core}$$

With $K_c = 0$, *i.e.*, in the uniaxial limit we get the bulk energy of a radial hedgehog.

For the same boundary condition, there is another possible structure called a boojum [11]. In this case, the four $s = \frac{1}{2}$ lines are collected at one point and the singularity at the centre is also drawn to this point on the surface so that there is no line singularity. Thus, there are no singular defect lines in the **(a,b)** field but there is a singularity in the director fields at a point on the surface of the drop. We describe the orthonormal triad in spherical polar coordinates:

$$\begin{aligned} \mathbf{a} &= \sin \beta' \cos \alpha' \mathbf{e}_r + \cos \beta' \cos \alpha' \mathbf{e}_\theta + \sin \alpha' \mathbf{e}_\phi \\ \mathbf{b} &= -\sin \beta' \sin \alpha' \mathbf{e}_r - \cos \beta' \sin \alpha' \mathbf{e}_\theta + \cos \alpha' \mathbf{e}_\phi \\ \mathbf{c} &= \cos \beta' \mathbf{e}_r - \sin \beta' \mathbf{e}_\theta \end{aligned}$$

where it is assumed that $\beta' = \beta'(\theta)$ and $\alpha' = \alpha'(\phi)$. Here, β' describes the angle the **c** director makes with the radial direction, and α' is the twist in **(a,b)** about **c**. The origin of the coordinate system is at the point singularity of the boojum. This problem cannot be solved exactly even in the weak biaxiality limit. However, in the one-constant limit, *viz.* $K_a = K_b = K_c = K$, it is solvable. The free energy density is

$$\begin{aligned} F &= \frac{K}{2} \left[\frac{1}{r^2} \left(\frac{d\beta'}{d\theta} - 1 \right)^2 + \frac{1}{r^2} (\cot \theta \sin \beta' - \cos \beta')^2 \right] \\ &\quad + \frac{K}{2r^2 \sin^2 \theta} \left[\cos(\theta - \beta') + \frac{d\alpha'}{d\phi} \right]^2 \end{aligned} \quad (3.22)$$

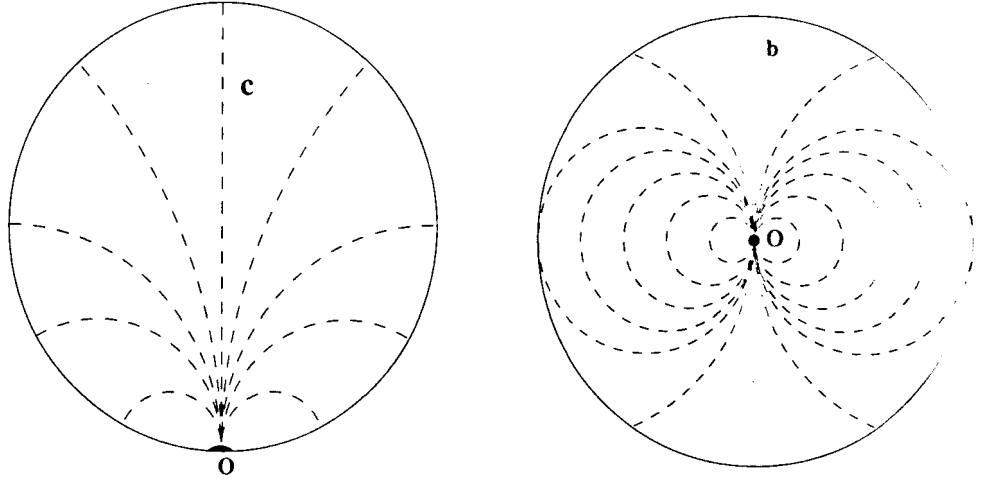


Figure 3.7: Structure of a boojum. The c director in the "fountain" configuration within the droplet. The point singularity is at O . The b director configuration around the point singularity, at O , on the surface of the droplet. The a director configuration will be orthogonal to b .

Then, the equations of equilibrium are

$$\frac{d^2 \alpha'}{d\phi^2} = 0 \quad (3.23)$$

and with $\beta'' = \theta - \beta'$,

$$\sin \theta \frac{d}{d\theta} \left(\sin \frac{d\beta''}{d\theta} \right) = -\sin \beta'' \frac{d\alpha'}{d\phi} \quad (3.24)$$

This has a simple analytical solution : $\beta'' = 2\theta$ and $\alpha' = -\phi$. This describes the standard boojum configuration with c radiating out like a "fountain" from a point on the surface of the drop. The (a,b) directors are in a singular $s = 2$ disclination configuration with the singularity at the point from where c emanates. The director configuration in a boojum is depicted in Figure 3.7. The total volume energy of this

structure is

$$E_{\text{boojum}} = 8\pi KR \quad (3.25)$$

It may be noted that it has not been possible to get an analytical solution for the boojum in the case of uniaxial nematics even in the "one-constant" approximation. With weak biaxial elastic anisotropy, we can expect the energy of the boojum to be a few times πKR . Thus, there are two possible structures for the drop, *viz.* tetrahedral configuration of four $s = \frac{1}{2}$ lines and the boojum. It is found that for $\frac{R}{r_c} < 10^5$, the tetrahedral structure is the lower energy state. But for larger drops the boojum would be of lower energy for the same boundary conditions. However, proper estimate of the radius at which such an instability occurs would have to include the core energies and the elastic anisotropy. In this context it may be noted that according to Kurik et al. [12], a boojum can exist with any kind of boundary condition. Since surface anchoring is proportional to R^2 , anchoring could be weak for smaller drops and the tetrahedral structure would develop only as the drop size increases¹.

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