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On Some Elastic Instabilities in Biaxial Nematics

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Abstract. — Within the framework of the continuum elastic theory of biaxial nematic liquid crystals, we have addressed ourselves to the structure, stability and energetics of some singular and non–singular topological defects, and certain director configurations. We find that certain non–singular hybrid disclinations could be energetically favourable relative to certain half–strength disclinations. The interaction between singular hybrids depends strongly on the biaxial elastic anisotropy. We suggest possible defect structures that can exist in spherical droplets of biaxial nematics. Further we find structural instabilities, in confined geometries, arising due to the inherent biaxiality of the system.

1. Introduction

In 1970, Freiser [1] theoretically predicted the possibility of a biaxial nematic (BN) phase. Following this, Toulouse [2] used topological methods to show that there are four stable line defects, *viz.* three distinct disclinations of half–integral strength and a disclination of odd–integral strength. He speculated that such a phase with many defects may have a polymer–type structure and "topological rigidity" observable in elastic and flow properties. Immediately thereafter, Yu and Saupe [3] discovered a biaxial nematic liquid crystalline state in a lyotropic system. It is only recently that some of these theoretical predictions about defects in BN have been experimentally verified by De'Neve *et al.* [4]. There has also been theoretical interest in the phase ordering kinetics of BN films [5] and statistical–mechanical properties of defects in this system [6]. Continuum theories to describe the elastic and hydrodynamic behaviour of BN [7–10] have also been developed. Many unusual and interesting elastic instabilities are possible in this system and they can be described effectively within the framework of the continuum theory.

In this paper, we have worked out the structure and energetics of certain singular and non–singular disclinations. In the escaped configuration, the energy of a certain hybrid disclination can become comparable to that of some disclinations of half strength. The nature of the interaction between wedge and hybrid disclinations is found to depend not only on the sign and strength of the defects, but also on the inherent elastic anisotropy due to biaxiality. We have also studied structures of defects associated with a spherical drop with one of the directors normal to the surface. We find that a transformation of a tetrahedral arrangement of four disclination lines of half strength emanating from the centre of the drop to that of a

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boojum is possible as drop size increases. Incidentally, the transformation of certain defects into non–singular structures through an escape into the "third dimension", the interaction of disclinations leading to energetically stable states, and the conversion of line defects associated with droplets into boojums can be all viewed as examples of elastic instabilities. Further we consider instabilities in a director configuration between two parallel plates with different boundary conditions. Some of these instabilities are typical of biaxiality. Lastly we study field induced instabilities in a uniformly aligned state and find that there are structural transitions which are inherently due to the biaxial symmetry.

2. Elasticity of Biaxial Nematics

The most symmetric BN has orthorhombic symmetry. It can be described by a mutually orthonormal triad of directors $(\mathbf{a}, \mathbf{b}, \mathbf{c})$, each of which is a two–fold axis of symmetry, whose orientations vary smoothly and slowly in space. The elasticity of such a BN is described by 15 elastic constants — twelve of these correspond to director distortions in the bulk [7–10]. The elastic free energy density, as given in [7], is

$$\begin{aligned} F \;=\; & F_0 + \sum_{\mathbf{a},\mathbf{b},\mathbf{c}} \frac{1}{2}\left[(K_{aa}(\mathbf{a}\cdot\nabla\mathbf{b}\cdot\mathbf{c})^2 + K_{ab}(\mathbf{a}\cdot\nabla\mathbf{a}\cdot\mathbf{b})^2 + K_{ac}(\mathbf{a}\cdot\nabla\mathbf{a}\cdot\mathbf{c})^2\right] \\ & + C_{ab}(\mathbf{a}\cdot\nabla\mathbf{a})\cdot(\mathbf{b}\cdot\nabla\mathbf{b}) + k_{0,a}\nabla\cdot(\mathbf{a}\cdot\nabla\mathbf{a} - \mathbf{a}\nabla\cdot\mathbf{a}) \end{aligned} \quad (1)$$

where the summation is over a cyclic permutation of the three directors and indices. Here K_{aa}, K_{bb} and K_{cc} are twist elastic constants associated with twist of the orthonormal triad about the directors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ respectively. The elastic constants K_{bc} and K_{cb} are associated with bend and splay deformations in $(\mathbf{b}, \mathbf{c})$ with $\mathbf{a}$ undistorted. Similarly, K_{ab}, K_{ba} [or K_{ca}, K_{ac}] correspond to splay or bend in $(\mathbf{a}, \mathbf{b})$ [or $(\mathbf{c}, \mathbf{a})$] with $\mathbf{c}$ [or $\mathbf{b}$] undistorted. C_{ab}, C_{bc} and C_{ca} are coupling constants. The last three terms involving $k_{0,a}$, $k_{0,b}$ and $k_{0,c}$ are surface terms.

As in the case of uniaxial nematics, in BN, we can have an equivalent "one–constant" approximation whereby elastic anisotropy concerned with twist, bend and splay distortions are neglected. In this approximation, these distortions in $(\mathbf{b}, \mathbf{c})$, $(\mathbf{c}, \mathbf{a})$ and $(\mathbf{a}, \mathbf{b})$ fields involve three constants K_a, K_b and K_c respectively. These three elastic constants are given by

$$\begin{aligned} K_a &= K_{aa} = K_{bc} = K_{cb} \\ K_b &= K_{bb} = K_{ca} = K_{ac} \\ K_c &= K_{cc} = K_{ab} = K_{ba}. \end{aligned}$$

Generally, the twist elastic constants could be expected to be half as small as the curvature constants. In the same spirit as that of the "one–constant" approximation, we do not consider such details in the "three–constants" approximation. In Appendix we have argued in favour of this "three–constants" approximation on the basis of an elasticity theory of BN incorporating Ericksen's [11] idea of variable degree of orientation. This simple formulation gives insight into the elasticity of BN. There we have brought out the dependences of the various constants on the order parameters and, the connection between the coupling constants and elastic anisotropy. This gives a proper extension to continuum theory allowing a more complete description of defects. It also gives a framework within which approximations on the relative magnitudes of the elastic constants can be given a physical basis.

In spite of this "three–constants" approximation, elastic anisotropy due to inherent biaxiality is still preserved. To reduce this simplified theory to that of uniaxial nematics (say, $\mathbf{c}$ goes over to the uniaxial director $\mathbf{n}$) with "one–constant" approximation, we have to take $K_c = 0$ and

$K_a = K_b$. Further, it should be noted that the coupling constants are not really peculiar to BN. It can be shown [7] that the Frank elastic constants of a uniaxial nematic are related to the elastic constants of BN in the following manner, assuming **c** goes over to **n**:

$$K_{11} = K_{ac}, \quad K_{22} = K_{aa}, \quad K_{33} = K_{ca}, \quad K_{24} = 2K_{0,c} + K_{aa} = 2K_{0,c} + K_{ac} - C_{ab},$$
$$K_{aa} = K_{bb}, \quad K_{ca} = K_{cb}, \quad K_{ac} = K_{bc}, \quad K_{0,a} = K_{0,b},$$
$$K_{cc} = C_{ca} = C_{bc} = K_{0,a} = K_{0,b} = 0.$$

Here $K_{11}, K_{22}, K_{33}, K_{24}$ are the splay, twist, bend and saddle–splay Frank elastic constants. From this it can be seen that $C_{ab} = (K_{11} - K_{22})$.

Throughout this study we work in the "three–constants" approximation and also ignore the coupling constants C_{ab}, C_{bc} and C_{ca}. The model considered in Appendix supports these two assumptions. We ignore all surface contributions including the ones similar to that which appears naturally in the standard Frank free energy density for a general non–planar distortion. We consider only the bulk contributions to the energy in all the problems that we have discussed. It should also be pointed out that the equations and solutions will certainly be different when one works in a different approximation or with the complete free energy density but we hope that the "three–constants" approximation is as instructive as the "one–constant" approximation in uniaxial nematics. We emphasize that this theory explores the effects of elastic anisotropy due to inherent biaxiality.

3. Non-Singular Defect Structures

In uniaxial nematics, we know that a non–singular line disclination of integral strength can exist. In BN also, non–singular disclinations are permitted [12]. They are of two types. The first type is a wedge or twist disclination of even integral strength, as in uniaxial nematics and, the second is a hybrid disclination — with both wedge and twist components — of total even integral strength.

The Volterra process for creating a hybrid disclination explicitly incorporates the orthorhombic symmetry of the **a**, **b**, **c** director fields. 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 $\pm\pi$, that is, $\pm 2\pi s_2$. The empty space is filled up with uniform material or overlapping regions are removed and the system is allowed to relax. This Volterra process describes a hybrid disclination 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. We have given an example of a wedge defect of strength s_1 in $(\mathbf{a}, \mathbf{c})$ but with a cyclic permutation of **a**, **b** and **c** we can describe such a defect in (**a**, **b**) and (**b**, **c**) fields, too. It is important to note that s_1 and s_2 can be either 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. It can be shown that the singularity in the case of disclinations of total strength $|s_1 + s_2| = 2$ can be removed by the escape into the third dimension of a director [12]. Here we work out the energetics of the hybrid disclinations, $(2, 0)$ and $(1, 1)$. In the case of (2, 0), we consider a line defect in (**a**, **b**) with **c** undistorted.

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

$$\begin{aligned}
\mathbf{a} &= \sin\psi \sin\theta \mathbf{e}_r + \cos\psi \mathbf{e}_\varphi + \sin\psi \cos\theta \mathbf{e}_z \\
\mathbf{b} &= \cos\psi \sin\theta \mathbf{e}_r - \sin\psi \mathbf{e}_\varphi + \cos\psi \cos\theta \mathbf{e}_z \\
\mathbf{c} &= \cos\theta \mathbf{e}_r - \sin\theta \mathbf{e}_z .
\end{aligned}$$

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), by turning $\mathbf{c}$ through $\frac{\pi}{2}$ and π respectively in the (r, z) plane. For $\psi = \psi(\phi)$ and $\theta = \theta(r)$, the free energy density is given by

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

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 (2) reduces to

$$F = \frac{K_a}{2}\left(\frac{\mathrm{d}\theta}{\mathrm{d}r}\right)^2 + \frac{K_a}{2r^2}\cos^2\theta + \frac{K_c}{2r^2}\left(\frac{\mathrm{d}\psi}{\mathrm{d}\phi} - \sin\theta\right)^2 \tag{3}$$

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

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}\phi^2} = 0 \tag{4}$$

$$\frac{K_a}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}\theta}{\mathrm{d}r}\right) + (K_a - K_c)\frac{\sin\theta\cos\theta}{r^2} + \frac{K_c \cos\theta}{r^2}\frac{\mathrm{d}\psi}{\mathrm{d}\phi} = 0. \tag{5}$$

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

$$r\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}\theta}{\mathrm{d}r}\right) + \left(1 - \frac{K_c}{K_a}\right)\sin\theta\cos\theta + \frac{K_c}{K_a}\cos\theta = 0. \tag{6}$$

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 $r = 0$.

3.1. (2,0) DISCLINATION LINE. — In this case the boundary conditions are $\theta = \frac{\pi}{2}$ at $r = 0$ and $\theta = -\frac{\pi}{2}$ at $r = r_0$, that is, $\mathbf{c}$ 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. The $\mathbf{a}$ and $\mathbf{b}$ directors are in a $s = 2$ disclination configuration. Then it can be shown that

$$\theta = 2\arctan\left[\frac{(\frac{r_0}{r})^2 - 2\sqrt{\frac{K_a}{K_c}}\frac{r_0}{r} - 1}{(\frac{r_0}{r})^2 + 2\sqrt{\frac{K_a}{K_c}}\frac{r_0}{r} - 1}\right]. \tag{7}$$

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

$$E = 4\pi K_a\left[1 + \frac{\frac{K_c}{K_a}}{\sqrt{1 - \frac{K_c}{K_a}}}\ln\left(\frac{1 + \sqrt{1 - \frac{K_c}{K_a}}}{\sqrt{\frac{K_c}{K_a}}}\right)\right]. \tag{8}$$

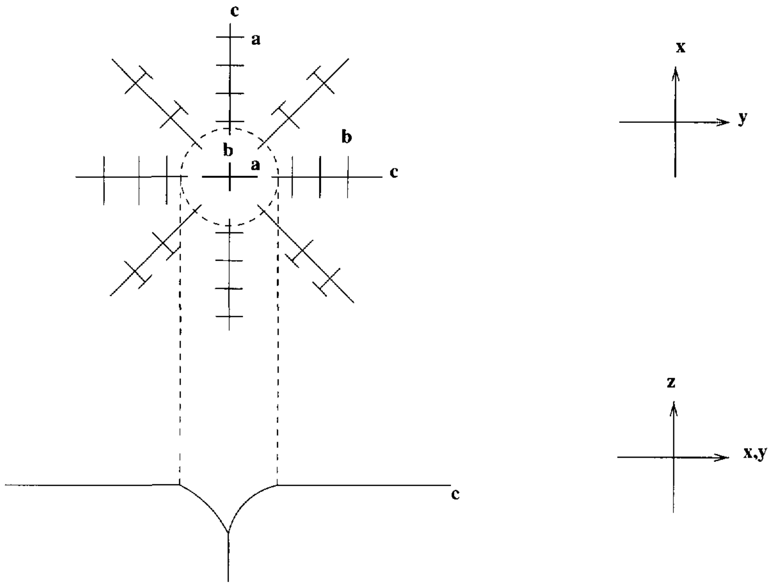


Fig. 1. — Removal of singularity in a hybrid disclination with $s_1 = s_2 = 1$ by an escape of the **c** director through $\pi/2$. The nail representation shows a director going out of the plane of the paper.

3.2. (1,1) HYBRID DISCLINATION LINE. — In this case, the boundary conditions are $\theta = \frac{\pi}{2}$ at $r = 0$ and $\theta = 0$ at $r = r_0$, that is, **c** is homeotropically aligned on the cylinder while **a** and **b** describe a twist about **c** through 2π as we go round the axis. In this case we get

$$\theta = 2\arctan\left[\frac{\sqrt{\frac{K_c}{K_a}}\sinh(\ln(\frac{r_0}{r}) + \sinh^{-1}(\sqrt{\frac{K_a}{K_c}})) - 1}{\sqrt{\frac{K_c}{K_a}}\sinh(\ln(\frac{r_0}{r}) + \sinh^{-1}(\sqrt{\frac{K_a}{K_c}})) + 1}\right]. \tag{9}$$

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

$$E = 4\pi K_a\left[1 - \frac{\sqrt{1+\frac{K_c}{K_a}}}{2} + \frac{\frac{K_c}{K_a}}{\sqrt{1-\frac{K_c}{K_a}}}\ln\left(\frac{\sqrt{2}(1+\sqrt{1-\frac{K_c}{K_a}})}{\sqrt{1-\frac{K_c}{K_a}}+\sqrt{1+\frac{K_c}{K_a}}}\right)\right]. \tag{10}$$

The geometry of the removal of the singularity in the case of (1, 1) hybrid disclination is shown in Figure 1. We get the known result, that is, $E = 2\pi K_a$ [13] for a (1, 0) defect in uniaxial nematics if we set $K_c = 0$. This is exactly 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 of an escaped hybrid disclination (1, 1), $2\pi K_a \leq E_h \leq 2.312\pi K_a$. We know that the energy of a singular wedge disclination of strength $s = \frac{1}{2}$ in $(\mathbf{a}, \mathbf{c})$ or $(\mathbf{b}, \mathbf{c})$ fields is $E_w = \frac{1}{4}\pi K_a \ln\frac{R}{r_c} + E_{core}$. Even without considering E_{core}, relatively, the hybrid is energetically favourable when the ratio of the sample size, R, to the core radius, r_c, that is, $\frac{R}{r_c} \geq 10^4$. This condition is easily realized in usual samples. It should be noted that a half strength disclination in $(\mathbf{a}, \mathbf{b})$ is the most favourable energetically since it does not involve distortion of the corresponding uniaxial director with which one would associate the largest elastic constant. Our analysis implies that a non–singular hybrid disclination would probably be preferred to a half strength disclination in $(\mathbf{a},\mathbf{c})$ or $(\mathbf{b},\mathbf{c})$ fields. It may be noted that even $s=\pm 1$ disclinations in $(\mathbf{a},\mathbf{c})$ or $(\mathbf{b},\mathbf{c})$ can also be favoured relative to the latter since energy can be lowered if $\mathbf{c}$ escapes into the third dimension. However, this will continue to be singular. In the case of $(\mathbf{a},\mathbf{c})$ or $(\mathbf{b},\mathbf{c})$ disclinations cases, the core will be in the isotropic phase for $\pm\frac{1}{2}$, and in the uniaxial phase for ± 1 disclinations.

4. Singular Hybrid Disclinations

In this section we shall study the effect of inherent biaxiality on the structure and energy of singular hybrid disclinations and their mutual interactions. For the quantitative analysis of a single defect or a pair of defects, we describe the orthonormal triad of directors 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 of a Cartesian coordinate system (x,y,z), and $\theta=\theta(x,y)$ and $\phi=\phi(x,y)$. Here ϕ is the angle that $\mathbf{c}$ makes with the x axis and θ describes the twist of $(\mathbf{a},\mathbf{b})$ about $\mathbf{c}$. The director $\mathbf{c}$ lies in the (x,y) plane. This parametrization is convenient to describe the geometry of hybrid disclinations. We shall denote by $[c,b,a]$ a singular hybrid disclination of strength (s_1,s_2) with $\mathbf{c}$ in the $x-y$ plane and the other two directors twisting about $\mathbf{c}$. Similarly, $[b,a,c]$ describes a singular hybrid disclination with $\mathbf{b}$ in the $x-y$ plane and $(\mathbf{a},\mathbf{c})$ twisting about $\mathbf{b}$. The free energy density of $[c,b,a]$ is

$$F=\frac{K_c}{2}[(\nabla_x\theta)^2+(\nabla_y\theta)^2]+\frac{(K_b\sin^2\theta+K_a\cos^2\theta)}{2}[(\nabla_x\phi)^2+(\nabla_y\phi)^2]. \tag{11}$$

The equations of equilibrium (for $[c,b,a]$) are

$$K_c\nabla^2\theta-(K_b-K_a)\sin\theta\cos\theta(\nabla\phi)^2=0 \tag{12}$$

$$(K_b\sin^2\theta+K_a\cos^2\theta)\nabla^2\phi+2(K_b-K_a)\sin\theta\cos\theta(\nabla\theta)\cdot(\nabla\phi)=0. \tag{13}$$

To describe $[b,a,c]$ the following transformations will have to be made: $K_c\to K_b$, $K_b\to K_a$, $K_a\to K_c$. Firstly, we will describe single defects and then consider the interaction of a pair of hybrid disclinations.

4.1. Single Hybrid Disclinations. — For a single defect, we can take $\theta=\theta(\alpha)$ and $\phi=\phi(\alpha)$ where α is the azimuthal angle in cylindrical coordinate system. Then, from (11), the free energy density is

$$F=\frac{K_c}{2r^2}\left(\frac{\mathrm{d}\theta}{\mathrm{d}\alpha}\right)^2+\frac{g(\theta)}{2r^2}\left(\frac{\mathrm{d}\phi}{\mathrm{d}\alpha}\right)^2 \tag{14}$$

where

$$g(\theta)=K_b\sin^2\theta+K_a\cos^2\theta. \tag{15}$$

Table I. — *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	9.953	10.702	10.702

On integrating once the equations of equilibrium, (12) and (13), we get

$$g(\theta)\frac{\mathrm{d}\phi}{\mathrm{d}\alpha} = \text{const.} = k \tag{16}$$

$$K_c\left(\frac{\mathrm{d}\theta}{\mathrm{d}\alpha}\right)^2 + \frac{k^2}{g(\theta)} = \text{const.} = \beta. \tag{17}$$

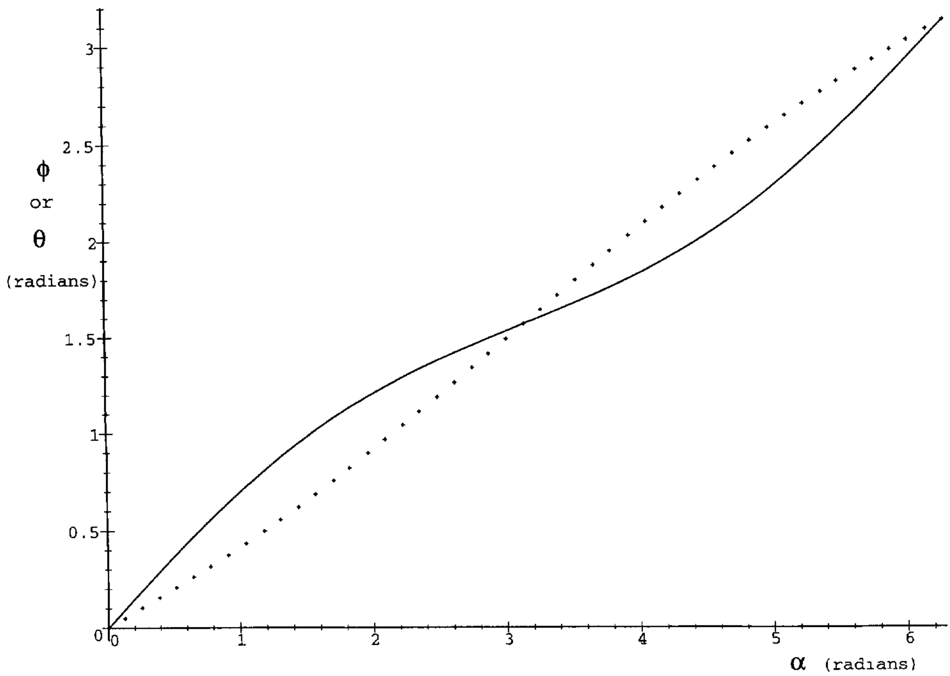
Using this, the free energy density (14) is

$$F = \frac{\beta}{2r^2} \tag{18}$$

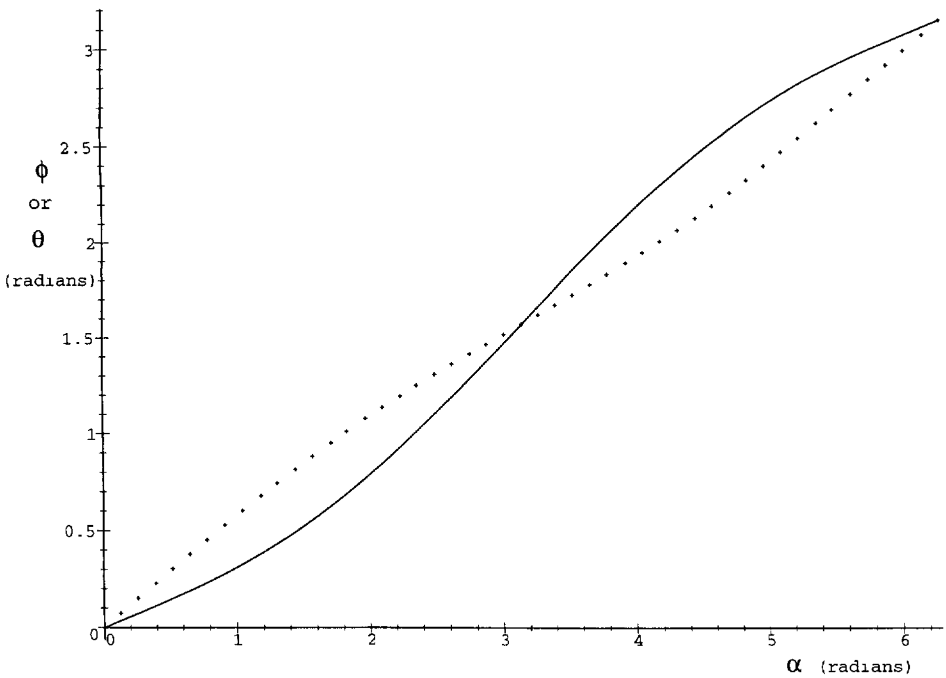
and the energy per unit length excluding that of the core is

$$E = \pi\beta \ln\frac{R}{r_{\mathrm{c}}} \tag{19}$$

where R and r_{c} are respectively the outer and inner limits of integration in the radial direction. We give in Table I 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. We have shown the θ and ϕ profiles in Figures 2a and 2b 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.



a)



b)

Fig. 2. — θ (bold line) and ϕ (dotted line) profiles, as functions of α, for (a) K_a:K_b:K_c = 6:4:1 (b) K_a:K_b:K_c = 4:6:1 — all angles are given in radians.

4.2. INTERACTION BETWEEN HYBRID DISCLINATIONS. — We can use scaling arguments [14] 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 (12) and (13). 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 reduces 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 have the configuration of a (s_1+s_3,s_2+s_4) hybrid disclination.

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

$$F_{\phi',\theta'}=\lambda^{-2}F_{\varphi,\theta}. \tag{20}$$

However a given area in the solution (ϕ',θ') is dilated by a factor λ^2, of course, by taking $\lambda>1$. 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 we can show [14] that the energy per unit length required to separate two defects is

$$E=E_1+E_2-E_{12} \tag{21}$$

where E_1 and E_2 are 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 the (s_1+s_3,s_2+s_4) defect from an outer cutoff R to λR.

In view of (19), the energy to separate two defects is

$$E=\pi(\beta_1+\beta_2-\beta_{12})\ln\lambda \tag{22}$$

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 I, we have come to the following conclusions.

The interaction between pure wedge (or pure twist) disclinations can be deduced from Table I. It is the same as that in uniaxial nematics.

A pure wedge and a pure twist do not interact in the case of $K_a{:}K_b{:}K_c=1{:}1{:}1$. 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 depicts schematically a pure wedge disclination and a pure twist disclination and, the bound state they can form — a hybrid disclination with both wedge and twist components.

In the case of the interaction between a pure wedge disclination and a hybrid disclination, we find 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 I, it can be seen that for the case of $(\frac{1}{2},0)$ and $(\frac{1}{2},\frac{1}{2})$, there is repulsion in all cases except for the state $[b,c,a]$. Whereas in the interaction between $(\frac{1}{2},0)$ and $(\frac{1}{2},1)$, 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 our investigation, 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.

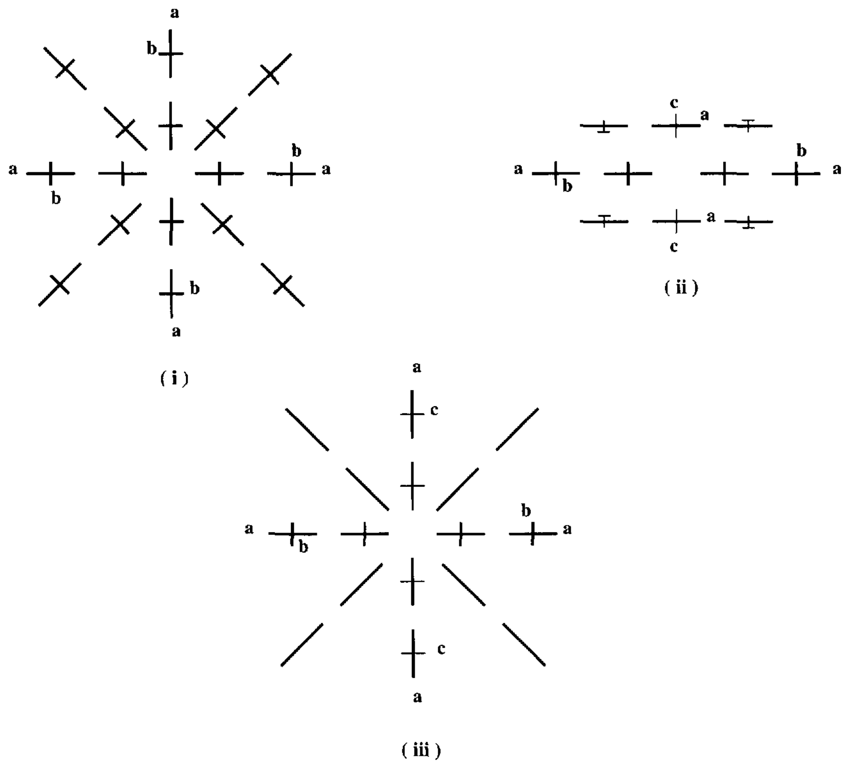


Fig. 3. — (i) A pure wedge disclination which combines with a pure twist disclination shown in (ii) to give the hybrid $s_1 = s_2 = 1$ depicted in (iii). The nail representation shows a director going out of the plane of the paper.

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 what has been said it is clear that the interaction between hybrids are determined not only by the sign and strength of the defects but also by the elastic anisotropy. In view of these results we make the following remarks. The Schlieren texture of hybrid disclinations will be no different from that of disclinations in uniaxial nematics but the 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.

5. Defects in Droplets

We now consider drops of BN with **c** normal to the surface at the boundary of the drop. Topological constraints [15] require the $(\mathbf{a},\mathbf{b})$ configuration to have surface singularities of combined strength, $s = 2$. If **c** is in a radial configuration, then there will be $(\mathbf{a},\mathbf{b})$ disclination lines satisfying the above requirement. An equivalent problem has been discussed by Lubensky and Prost [16]. From their analysis we can conclude that four $(\mathbf{a},\mathbf{b})$ disclination lines of strength $+\frac{1}{2}$ arranged in a tetrahedral configuration is of the least energy. Without considering core energies, the total energy is due to splay in **c** and distortions associated with the four disclinations. In the weak biaxiality limit, $K_a = K_b = K$, $E_{\text{total}} \simeq 4\pi KR + \pi K_c R \ln(\frac{R}{r_c})$. With $K_c = 0$, that is, in the uniaxial limit we get the bulk energy of a radial hedgehog.

For the same boundary condition, there is another possible structure called the boojum [17]. In this case, there are no singular defect lines in the $(\mathbf{a},\mathbf{b})$ 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 we assume $\beta' = \beta'(\theta)$ and $\alpha' = \alpha'(\phi)$. Here, β' describes the angle **c**, makes with the radial direction, and α' is the twist of $(\mathbf{a},\mathbf{b})$ 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

$$F = \frac{K}{2}\left[\frac{1}{r^2}(\frac{\mathrm{d}\beta'}{\mathrm{d}\theta} - 1)^2 + \frac{1}{r^2}(\cot\theta\sin\beta' - \cos\beta')^2\right] + \frac{K}{2r^2\sin^2\theta}\left[\cos(\theta-\beta') + \frac{\mathrm{d}\alpha'}{\mathrm{d}\phi}\right]^2 \quad (23)$$

The equations of equilibrium are

$$\frac{\mathrm{d}^2\alpha'}{\mathrm{d}\phi^2} = 0 \quad (24)$$

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

$$\sin\theta\frac{\mathrm{d}}{\mathrm{d}\theta}(\sin\theta\frac{\mathrm{d}\beta''}{\mathrm{d}\theta}) = -\sin\beta''\frac{\mathrm{d}\alpha'}{\mathrm{d}\phi} \quad (25)$$

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 $(\mathbf{a},\mathbf{b})$ directors are in a singular $s = 2$ disclination configuration with the singularity at the point from where **c** emanates. The structure is depicted in Figures 4a and 4b. The total volume energy of this structure is

$$E = 8\pi KR. \quad (26)$$

It may be noted that we do not have 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. It is then possible that for small droplets, with $\frac{R}{r_c} < 10^5$, the tetrahedral structure of defect lines could be 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

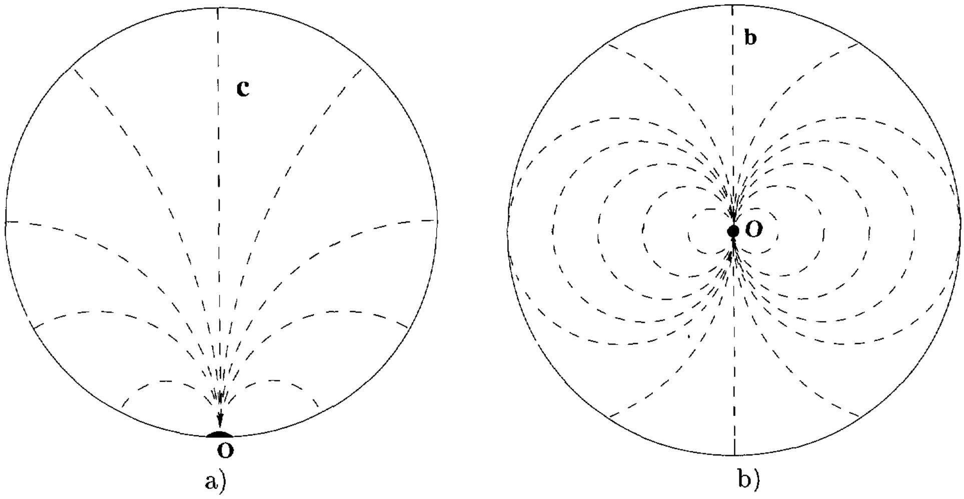


Fig. 4. — Structure of a boojum: (a) the **c** director in the "fountain" configuration within the droplet. The point singularity is at O. (b) The **b** director configuration around the point singularity, at O, on the surface of the droplet. The **a** director configuration will be orthogonal to **b**.

that according to Kurik *et al.* [18] 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 increases ([1]).

6. Director Distortions Due to Rigid Anchoring

When the orthonormal triad of directors spontaneously undergo distortions due to anchoring at the walls, the inherent biaxiality of BN will lead to a coupling between the different field distortions. This is apart from the effects of elastic anisotropy of the splay, bend and twist constants of any pair of the orthonormal triad of directors, and the coupling constants. Here both of them have been neglected.

We consider a particular geometry which imposes twist in **a**. Let **a** be anchored homogeneously on two parallel plates. Let **b** be anchored homeotropically on the lower plate and homogeneously on the upper plate. In the Cartesian coordinate system let

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

Here ϕ describes the angle made by **c** with the x–axis, and θ describes the angle of rotation of $(\mathbf{b}, \mathbf{c})$ about **a**. The free energy density in this case is

$$F = \frac{1}{2}[K_a \left(\frac{\mathrm{d}\theta}{\mathrm{d}z}\right)^2 + f(\theta)\left(\frac{\mathrm{d}\phi}{\mathrm{d}z}\right)^2] \quad (27)$$

where

$$f(\theta) = (K_b \sin^2\theta + K_c \cos^2\theta). \quad (28)$$

([1]) We thank O.D. Lavrentovich for bringing to our notice this aspect.

The equations of equilibrium are

$$\frac{\mathrm{d}}{\mathrm{d}z}[f(\theta)\frac{\mathrm{d}\phi}{\mathrm{d}z}] = 0 \tag{29}$$

$$K_a\frac{\mathrm{d}^2\theta}{\mathrm{d}z^2} = (K_b - K_c)\sin\theta\cos\theta\left(\frac{\mathrm{d}\phi}{\mathrm{d}z}\right)^2 \tag{30}$$

These differential equations can be integrated once to get equations similar to (16) and (17) respectively. Hence, the θ and ϕ profiles will have the two general features shown in Figures 2a and 2b. Firstly, the profiles will be nonlinear. Secondly, while variations in θ are fast, the variations in ϕ are slow and *vice–versa.*

Elastic anisotropy due to inherent biaxiality can also cause instabilities in simpler geometries such as a twisted nematic cell. We consider a pure twist of the $(\mathbf{a}, \mathbf{b})$ pair by proper anchoring. A uniform twist is a solution of the equations of equilibrium. In uniaxial nematics, Leslie [19] has shown that there could be an instability resulting in the director lifting out of the plane of the plates. This happens at a relative twist of nearly π between the plates provided $2K_{22} > K_{33}$. This is unattainable in the laboratory. But, in a BN, we find an instability which occurs at a much lesser relative twist. Let us consider $\phi = (q_0 z + \phi_1)$ and $\theta = \theta_1$ where ϕ_1 and θ_1 are small perturbations. Then to a first approximation

$$\frac{\mathrm{d}^2\theta_1}{\mathrm{d}z^2} = \lambda'\theta_1 \tag{31}$$

where $\lambda' = \frac{q_0^2}{K_a}(K_b - K_c)$. When $\lambda' < 0$ there is an instability which will lift the $\mathbf{b}$ director out of the plane of the plates. This exactly follows Leslie's analysis but what is interesting is that the threshold of relative twist gets lowered. In the general case, without the three–constants approximation, the threshold for relative twist is

$$\phi = \pi\sqrt{\frac{K_{cb}}{2K_{cc} - K_{ca} - K_{ba}}}\ . \tag{32}$$

7. Instabilities in the Presence of a Magnetic Field

Freedericksz transitions in biaxial nematics have been studied by others [20, 21] in geometries with strong anchoring of one of the directors and no anchoring of the other two. We consider a sample with strong anchoring in all the directors and the free energy density includes both elastic deformations and diamagnetic contributions described by

$$F_{\mathrm{mag}} = -\frac{1}{2}\sum_{\mathbf{a},\mathbf{b},\mathbf{c}}\chi_a(\mathbf{H}\cdot\mathbf{a})^2 \tag{33}$$

where χ_a, χ_b and χ_c are the principal diamagnetic susceptibilities along $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ respectively for the orthorhombic symmetry. In the undeformed state, we consider $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ to be along the reference axes x, y and z respectively. Deformations in the orthonormal triad of directors are described by Eulerian angles (θ, ϕ, ψ) [22] which are position dependent. The director representation in terms of (θ, ϕ, ψ) is shown in Figure 5. Let $\mathbf{H}$ be along y axis and director distortions are assumed to vary in the z direction with strong anchoring at $z = 0$ and $z = d$. Just above the threshold field, we assume the deformations to be small and to be of the form

$$f = f_{\mathrm{m}}\sin\frac{\pi z}{d} \tag{34}$$

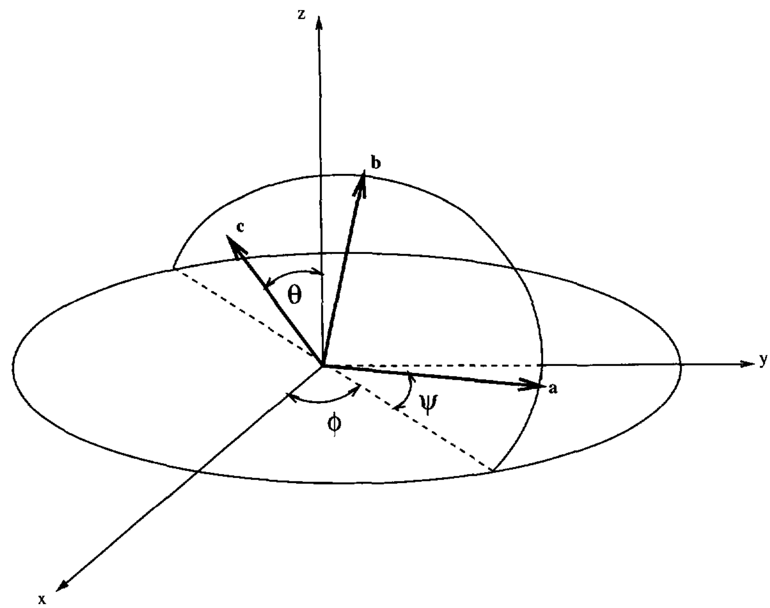


Fig. 5. — The orientations of **a**, **b** and **c** along with the Eulerian angles, θ, ϕ and ψ.

where $f_{\rm m} = \theta_{\rm m}$ (or $\phi_{\rm m}$ or $\psi_{\rm m}$) is the maximum value of the function $f = \theta$ (or ϕ or ψ). After averaging over the sample thickness and collecting terms up to the quartic, the free energy density is

$$F = \frac{K_b\pi^2}{2d^2}\left[\frac{a_1}{2}\zeta^2 + \frac{a_2}{2}\vartheta^2 + \frac{b_1}{4}\zeta^4 + \frac{b_2}{4}\vartheta^4 + \frac{c_1}{2}\zeta^2\vartheta^2 + \frac{c_2}{2}\eta^2\vartheta^2 + c_3\zeta\eta\vartheta^2\right] \quad (35)$$

where $2\zeta = \phi_{\rm m} + \psi_{\rm m}$, $2\eta = \phi_{\rm m} - \psi_{\rm m}$, $\vartheta = \theta_{\rm m}$, $\kappa^2 = \frac{d^2H^2}{\pi^2}$ and

$$\begin{aligned}
a_1 &= \tau_1 - \omega_1\kappa^2\\
a_2 &= \tau_2 - \omega_2\kappa^2\\
b_1 &= \frac{1}{2}\omega_1\kappa^2\\
b_2 &= \frac{1}{2}\omega_2\kappa^2\\
c_1 &= \frac{1}{4}(\tau_2 - 2\tau_1 + 3(\omega_2 + 2\omega_1)\kappa^2)\\
c_2 &= \frac{1}{4}(4 - 3\tau_2 + 3\omega_2\kappa^2)\\
c_3 &= \frac{1}{4}(\tau_2 - \tau_1 + 3(\omega_2 - \omega_1)\kappa^2)
\end{aligned}$$

with $\tau_1 = \frac{K_c}{K_b}$, $\tau_2 = \frac{K_a}{K_b}$, $\omega_1 = \frac{(\chi_a - \chi_b)}{K_b}$ and $\omega_2 = \frac{(\chi_c - \chi_b)}{K_b}$

The equations of equilibrium show that η can be expressed as $\eta = -\frac{c_3}{c_2}\zeta$. Then the free energy density is

$$F = \frac{K_b\pi^2}{2d^2}\left[\frac{a_1}{2}\zeta^2 + \frac{a_2}{2}\vartheta^2 + \frac{b_1}{4}\zeta^4 + \frac{b_2}{4}\vartheta^4 + \frac{\delta}{2}\zeta^2\vartheta^2\right] \quad (36)$$

where $\delta = (c_1 - \frac{c_3^2}{c_2})$. In this form the free energy density is the Lifshitz expression and the possible phase diagrams have been already studied [23]. However, this theory is only valid when $\delta > -\sqrt{b_1 b_2}$. There are four possible states and their stability conditions are:

(a) $\zeta = \vartheta = 0$ or $\theta = \phi = \psi = 0$ is stable when $a_1 > 0$ and $a_2 > 0$.

(b) $\zeta = 0, \vartheta \neq 0$ or $\phi = \psi = 0, \theta \neq 0$ is stable when $a_2 < 0, b_2 > 0, c_2 > 0$, and $(a_1 - \frac{a_2\delta}{b_2}) > 0$. In this state, $\vartheta^2 = -\frac{a_2}{b_2}$.

(c) $\vartheta = 0, \zeta \neq 0$ or $\theta = 0, \phi, \psi \neq 0$ is stable when $a_1 < 0$, $b_1 > 0$ and $(a_2 - \frac{a_1\delta}{b_1}) > 0$. $\zeta^2 = -\frac{a_1}{b_1}$.

(d) $\zeta \neq 0, \vartheta \neq 0$ or $\theta \neq 0$, $\phi \neq 0$, $\psi \neq 0$ is stable when $b_1 > 0$, $b_2 > 0$, $(a_1 b_2 - a_2\delta) < 0$, $(a_2 b_1 - a_1\delta) < 0$, $(b_1 b_2 - \delta^2 > 0$. In this state, the deformations are described by $\zeta^2 = -\frac{(a_1 b_2 - a_2\delta)}{(b_1 b_2 - \delta^2)}$ and $\vartheta^2 = -\frac{(a_2 b_1 - a_1 \delta^2)}{(b_1 b_2 - \delta^2)}$

From what is known of the structural phase transitions allowed by the Lifshitz expression, we can say that there are second order phase transitions from state (a) to either state (b) or state (c). There can be a first order phase transition from (b) to (c). On the other hand, there could be second order transitions from (b) to (d) to (c).

Without loss of generality let us assume that **c** describes the uniaxial director or the direction of the long axis. Then the states described by (c) and (d) are unique to biaxial nematics.

8. Conclusion

Within the framework of a continuum elastic theory of BN, we have studied the effect of biaxiality on the structure, instability and properties of singular and non–singular defects, and instabilities in certain static director configurations. From the energetics of non–singular defect structures, we find that certain non–singular hybrid disclinations could be energetically more favourable relative to some singular half–strength disclinations. We have studied in detail singular hybrid disclinations since they are allowed by BN symmetry and not by that of uniaxial nematics. Elastic anisotropy due to inherent biaxiality is shown to have non–linear effects on the structure of these defects. We have studied the interaction energies between pure wedge, pure twist and hybrid disclinations. The nature of interaction depends not only on the signs of the topological strength of these defects but also strongly on the elastic anisotropy. In droplets of BN, for homeotropic boundary condition at the surface, we find that there can be a transformation, as the drop size increases, from a tetrahedral arrangement of four half–strength disclination lines to a boojum. Elastic anisotropy also produces nonlinear effects on the structure of distortions involving the three directors simultaneously. In a twisted nematic cell, we find that an instability, similar to that found in uniaxial nematics, could occur at a lower twist threshold. New instabilities in a confined system are possible in the presence of a magnetic field. We find that the free energy density reduces to the Lifshitz expression whereby a rich phase diagram for the structural transitions is possible.

Acknowledgments

Our thanks are due to K.A. Suresh for helpful comments.

Appendix

Formulation of a Theory of Elasticity of BN

We follow the procedure of Ericksen developed for uniaxial nematics [11]. It must be remarked that Govers and Vertogen [10] have used similar tensor order representation to formulate their elastic theory of BN but without allowing a variable degree of orientation. We have incorporated this feature since this theory is more suited to describe defects. The orientational order parameter tensor $Q_{\alpha\beta}$ is symmetric and traceless and it is given in terms of the orthonormal triad **a**, **b**, **c**

$$Q_{\alpha\beta} = S(c_\alpha c_\beta - \frac{1}{3}\delta_{\alpha\beta}) + T(a_\alpha a_\beta - b_\alpha b_\beta) \quad (37)$$

where S is the orientational order parameter of uniaxial nematics, T describes the biaxiality and $\delta_{\alpha\beta}$ is the Kronecker delta. When $S = T = 0$, we get the isotropic state. The combined thermal and elastic free energy density in the absence of external fields may be written as

$$F = V(Q) + F_{\text{dist}} \quad (38)$$

where $V(Q)$ describes the homogeneous part of the free energy that describes isotropic–uniaxial–biaxial phase transitions while F_{dist} is the free energy density due to director distortions and order parameter variations in space. $V(Q)$ can be taken in the form [24]

$$V(Q) = \frac{a}{2}\text{Tr}(Q^2) + \frac{b}{3}\text{Tr}(Q^3) + \frac{c}{4}(\text{Tr}(Q^2))^2. \quad (39)$$

On expanding we get

$$V(Q) = \alpha(S) + \frac{\beta(S)}{2}T^2 + \frac{\gamma(S)}{4}T^4 \quad (40)$$

where

$$\begin{aligned} \alpha(S) &= \frac{1}{3}aS^2 + \frac{2}{27}bS^3 + \frac{1}{9}cS^4 \\ \beta(S) &= 2a - \frac{4}{3}bS + \frac{4}{3}cS^2 \\ \gamma(S) &= 4c. \end{aligned}$$

We generalize Ericksen's expression [11] to get F_{dist}, that is,

$$F_{\text{dist}} = \frac{L_1}{2}\partial_\alpha Q_{\beta\gamma}\partial_\alpha Q_{\beta\gamma} + \frac{L_2}{2}\partial_\alpha Q_{\alpha\gamma}\partial_\beta Q_{\beta\gamma} + \frac{L_3}{2}\partial_\alpha Q_{\beta\gamma}\partial_\gamma Q_{\beta\alpha}. \quad (41)$$

We want to compare the elastic constants of a BN with these three constants and the two order parameters S and T. F_{dist} can be written as

$$F_{\text{dist}} = F_{ST} + F_d \quad (42)$$

where F_{ST} is due to order parameter variations and their coupling with the orthonormal triad of directors. F_d contains contributions solely from gradients in the directors. The explicit expressions for F_{ST} and F_d are:

$$\begin{aligned} F_{ST} &= \frac{1}{3}(L_1 + \frac{L_2}{6} + \frac{L_3}{6})(\nabla S)^2 + \frac{1}{6}(L_2 + L_3)(\mathbf{c}\cdot\nabla S)^2 \\ &\quad + L_1(\nabla T)^2 + \frac{1}{2}(L_2 + L_3)[(\mathbf{a}\cdot\nabla T)^2 + (\mathbf{b}\cdot\nabla T)^2] \end{aligned}$$

$$
\begin{aligned}
&+\frac{1}{3}(\nabla S^2)\cdot[(L_2-\frac{L_3}{2})\mathbf{c}\nabla\cdot\mathbf{c}+(L_3-\frac{L_2}{2})\mathbf{c}\cdot\nabla\mathbf{c})]\\
&+\frac{1}{3}(L_2+L_3)[(\mathbf{b}\cdot\nabla S)(\mathbf{b}\cdot\nabla T)-(\mathbf{a}\cdot\nabla S)(\mathbf{a}\cdot\nabla T)]\\
&+T\nabla S\cdot[L_2(\mathbf{c}(\mathbf{a}\cdot\nabla\mathbf{a}\cdot\mathbf{c}-\mathbf{b}\cdot\nabla\mathbf{b}\cdot\mathbf{c}))\\
&+\frac{1}{3}(L_2+L_3)(\mathbf{b}\nabla\cdot\mathbf{b}+\mathbf{b}\cdot\nabla\mathbf{b}-\mathbf{a}\nabla\cdot\mathbf{a}-\mathbf{a}\cdot\nabla\mathbf{a})\\
&+L_3(-\mathbf{a}(\mathbf{c}\cdot\mathbf{c}\cdot\nabla\mathbf{a})+\mathbf{b}(\mathbf{c}\cdot\mathbf{c}\cdot\nabla\mathbf{b}))\\
&+S\nabla T\cdot[L_2(\mathbf{a}(\mathbf{a}\cdot\mathbf{c}\cdot\nabla\mathbf{c})-\mathbf{b}(\mathbf{b}\cdot\mathbf{c}\cdot\nabla\mathbf{c}))\\
&+L_3(\mathbf{c}(\mathbf{b}\cdot\nabla\mathbf{b}\cdot\mathbf{c})-\mathbf{c}(\mathbf{a}\cdot\nabla\mathbf{a}\cdot\mathbf{c}))]\\
&+\frac{1}{2}(\nabla T^2)\cdot[L_2(\mathbf{a}\nabla\cdot\mathbf{a}+\mathbf{b}\nabla\cdot\mathbf{b}-\mathbf{a}(\mathbf{a}\cdot\mathbf{b}\cdot\nabla\mathbf{b})-\mathbf{b}(\mathbf{b}\cdot\mathbf{a}\cdot\nabla\mathbf{a}))\\
&+L_3(\mathbf{a}\cdot\nabla\mathbf{a}+\mathbf{b}\cdot\nabla\mathbf{b}+\mathbf{b}(\mathbf{a}\cdot\mathbf{a}\cdot\nabla\mathbf{b})+\mathbf{a}(\mathbf{b}\cdot\mathbf{b}\cdot\nabla\mathbf{a}))]
\end{aligned}
\tag{43}
$$

$$
\begin{aligned}
F_d = {} & L_1(S+T)^2(\mathbf{a}\cdot\nabla\mathbf{b}\cdot\mathbf{c})^2+L_1(S-T)^2(\mathbf{b}\cdot\nabla\mathbf{c}\cdot\mathbf{a})^2\\
&+4L_1T^2[\mathbf{c}\cdot\nabla\mathbf{a}\cdot\mathbf{b}]^2\\
&+(4L_1+2L_2+2L_3)T^2[(\mathbf{a}\cdot\nabla\mathbf{a}\cdot\mathbf{b})^2+(\mathbf{b}\cdot\nabla\mathbf{b}\cdot\mathbf{a})^2]\\
&+[L_1(S-T)^2+\frac{(L_2+L_3)}{2}(S-T)^2][(\mathbf{a}\cdot\nabla\mathbf{a}\cdot\mathbf{c})^2+(\mathbf{c}\cdot\nabla\mathbf{c}\cdot\mathbf{a})^2]\\
&+[L_1(S+T)^2+\frac{(L_2+L_3)}{2}(S+T)^2][(\mathbf{b}\cdot\nabla\mathbf{b}\cdot\mathbf{c})^2+(\mathbf{c}\cdot\nabla\mathbf{c}\cdot\mathbf{b})^2]\\
&+\frac{(L_2+L_3)}{2}(S^2-2T^2)(\mathbf{a}\cdot\nabla\mathbf{a})\cdot(\mathbf{b}\cdot\nabla\mathbf{b})\\
&-(L_2+L_3)(ST-2T^2)(\mathbf{b}\cdot\nabla\mathbf{b})\cdot(\mathbf{c}\cdot\nabla\mathbf{c})\\
&+(L_2+L_3)(ST+2T^2)(\mathbf{c}\cdot\nabla\mathbf{c})\cdot(\mathbf{a}\cdot\nabla\mathbf{a})\\
&+[(\frac{L_3}{2}-L_1)S^2+L_1T^2]\nabla\cdot(\mathbf{c}\cdot\nabla\mathbf{c}-\mathbf{c}\nabla\cdot\mathbf{c})\\
&+(2L_1ST-2L_1T^2+\frac{L_3}{2}T^2)\nabla\cdot(\mathbf{a}\cdot\nabla\mathbf{a}-\mathbf{a}\nabla\cdot\mathbf{a})\\
&+(-2L_1ST-2L_1T^2+\frac{L_3}{2}T^2)\nabla\cdot(\mathbf{b}\cdot\nabla\mathbf{b}-\mathbf{b}\nabla\cdot\mathbf{b})\\
&+L_3T^2[\nabla\cdot(\mathbf{b}(\mathbf{a}\cdot\nabla\mathbf{a}\cdot\mathbf{b})+\mathbf{a}(\mathbf{b}\cdot\nabla\mathbf{b}\cdot\mathbf{a}))]\\
&+L_3ST[\nabla\cdot(\mathbf{b}(\mathbf{c}\cdot\nabla\mathbf{c}\cdot\mathbf{b})+\mathbf{c}(\mathbf{b}\cdot\nabla\mathbf{b}\cdot\mathbf{c})\\
&-\mathbf{a}(\mathbf{c}\cdot\nabla\mathbf{c}\cdot\mathbf{a})-\mathbf{c}(\mathbf{a}\cdot\nabla\mathbf{a}\cdot\mathbf{c}))].
\end{aligned}
\tag{44}
$$

Hence, comparison of (44) with (1) implies that:

$$
\begin{aligned}
K_{aa} &= 2L_1(S+T)^2\\
K_{bb} &= 2L_1(S-T)^2\\
K_{cc} &= 8L_1T^2\\
K_{ab} &= K_{ba}=2(4L_1+2L_2+2L_3)T^2\\
K_{ac} &= K_{ca}=2(L_1+\frac{(L_2+L_3)}{2})(S-T)^2\\
K_{bc} &= K_{cb}=2(L_1+\frac{(L_2+L_3)}{2})(S+T)^2
\end{aligned}
$$

$$
\begin{aligned}
C_{ab} &= \frac{(L_2+L_3)}{2}(S^2-2T^2)\\
C_{bc} &= -(L_2+L_3)(ST-2T^2)\\
C_{ca} &= (L_2+L_3)(ST+2T^2).
\end{aligned}
$$

It can be seen that the "three–constants" approximation used to describe the elastic distortions of BN is reasonably correct and in the limit of weak biaxiality, our further approximation to work with just two constants is also justified. It should also be noted that the coupling constants do come out to be proportional to the elastic anisotropy between the twist and curvature elastic constants. It should be remembered that such an exercise in uniaxial nematics [25] gave similar results, *viz.* the Frank twist constant, K_{22}, is different from the bend, K_{33}, and splay, K_{11}, constants which are themselves equal in the second–order theory.

As an exercise for this theory, we consider its implications in the structure of a disclination in **a**, **b** director field. In cylindrical coordinate system

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

We take $\alpha = \alpha(\phi)$, $T = T(r)$, $S = S_0$; S_0 being a constant. Then the free energy reduces to

$$
\begin{aligned}
F &= F_0 + \frac{\beta}{2}T^2 + \frac{\gamma}{4}T^4 + K\left(\frac{\mathrm{d}T}{\mathrm{d}r}\right)^2 + 4K\frac{T^2}{r^2}\left(1+\frac{\mathrm{d}\alpha}{\mathrm{d}\phi}\right)^2\\
&\quad +2(L_2-L_3)\frac{T}{r}\frac{\mathrm{d}T}{\mathrm{d}r}\frac{\mathrm{d}\alpha}{\mathrm{d}\phi} + 4L_1ST\frac{\cos 2\alpha}{r^2}\frac{\mathrm{d}\alpha}{\mathrm{d}\phi}
\end{aligned}
\tag{45}
$$

where $K = L_1 + \frac{(L_2+L_3)}{2}$ We have the equations of equilibrium:

$$
\frac{\mathrm{d}^2\alpha}{\mathrm{d}\phi^2} = 0 \tag{46}
$$

$$
-\beta T - \gamma T^3 = \frac{8KT}{r^2}\left(1+\frac{\mathrm{d}\alpha}{\mathrm{d}\phi}\right)^2 + 4L_1S\frac{\cos 2\alpha}{r^2}\frac{\mathrm{d}\alpha}{\mathrm{d}\phi} - \frac{2K}{r}\frac{\mathrm{d}}{\mathrm{d}r}(r\frac{\mathrm{d}T}{\mathrm{d}r}). \tag{47}
$$

It can be seen that this reduces to the Ginzburg–Pitaevskii equation [26] for the $s=1$ disclination where $\alpha =$ const. The solution has the features: $S = S_0$, $\alpha =$ const., and $(r = 0, T = 0)$, $(r = \infty, T = T_0 = \sqrt{\frac{-\beta}{\gamma}})$.

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