

CHAPTER 2

ELASTIC INSTABILITIES IN BIAXIAL NEMATICS

2.1 Introduction

In 1970, Freiser [1] theoretically predicted the possibility of a biaxial nematic (BN) phase. Nearly a decade later, Yu and Saupe [2] discovered a biaxial nematic liquid crystalline state in a lyotropic system. This led to the development of continuum theories of the elastic and the hydrodynamic behaviour of BN [3-6]. Most of the theoretical studies to date have been largely aimed at suggesting experimental situations for extracting the elastic and viscosity coefficients. Not much attention has been paid to structural instabilities. Many unusual and interesting elastic instabilities are possible in this system and they can be described effectively within the framework of a continuum theory. Here, instabilities in a director configuration confined between two parallel plates with different boundary conditions have been considered. Some of these instabilities are typical of biaxiality. Field induced instabilities in a uniformly aligned state have also been studied and it is found that there

are structural transitions which are inherently due to the biaxial symmetry. Most of the results described in this chapter have been published [7].

2.2 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 was first described by Saupe [3] and later refined by others [4-6]. The elastic distortions are described by 15 elastic constants - twelve of these correspond to director distortions in the bulk. The elastic free energy density is given by [3]

$$\begin{aligned}
 F = F_0 + \sum_{\mathbf{a}, \mathbf{b}, \mathbf{c}} \frac{1}{2} \left[K_{aa} (\mathbf{a} \cdot \nabla \mathbf{b} \cdot \mathbf{c})^2 + K_{ab} (\mathbf{a} \cdot \nabla \mathbf{a} \cdot \mathbf{b})^2 \right. \\
 \left. + K_{ac} (\mathbf{a} \cdot \nabla \mathbf{a} \cdot \mathbf{c})^2 \right] + C_{ab} (\mathbf{a} \cdot \nabla \mathbf{a}) \cdot (\mathbf{b} \cdot \nabla \mathbf{b}) \\
 + k_{0,a} \nabla \cdot (\mathbf{a} \cdot \nabla \mathbf{a} - \mathbf{a} \nabla \cdot \mathbf{a})
 \end{aligned} \tag{2.1}$$

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 which distinguishes between twist, bend and splay elastic constants are neglected. In this approximation, the 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

$$K_a = K_{aa} = K_{bc} = K_{cb}$$

$$K_b = K_{bb} = K_{ca} = K_{ac}$$

$$K_c = K_{cc} = K_{ab} = K_{ba}$$

As in uniaxial nematics, even in BN, the twist elastic constants can be expected to be half as small as the bend and splay constants. But, the important point to be stressed is that 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, c goes over to the uniaxial director n) with "one-constant" approximation, we have to make $K_c = 0$ and $K_a = K_b$. Further, it should be noted that the coupling constants are not really peculiar to BN. Saupe [3], who developed the first continuum theory of BN, showed that the Frank elastic constants of a uniaxial nematic are related to the elastic constants of BN. Assuming that c goes over to n , then it is found that:

$$K_{11} = K_{ac}, K_{22} = K_{aa}, K_{33} = K_{ca}, K_{24} = 2K_{0,c} + K_{aa} = 2K_{0,c} + K_{ac} - C_{ab},$$

$$K_{aa} = K_{bb}, K_{ca} = K_{cb}, K_{ac} = K_{bc}, K_{0,a} = K_{0,b},$$

$$K_{cc} = C_{ca} = C_{bc} = K_{0,a} = K_{0,b} = 0.$$

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

Throughout this chapter and the next, the "three-constants" approximation is assumed and also, the coupling constants C_{ab}, C_{bc} and C_{ca} , and the surface terms of F are ignored. Only the bulk contributions to the energy are considered in all the problems. 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 it is found that the "three-constants" approximation is as instructive as the "one-constant" approximation in uniaxial nematics. It is to be emphasized that this theory explores the effects of elastic anisotropy due to inherent biaxiality.

2.3 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 BS will lead to a coupling between the different director field distortions even when elastic anisotropy that distinguishes between twist, bend and splay, and coupling constants are ignored. We consider a particular geometry which imposes twist in c . Let c be anchored homogeneously (*i.e.* parallel to the surface) on two parallel plates but with a relative twist of $\delta\phi$. Let a be anchored homeotropically (*i.e.* normal to the surface) on the lower plate and homogeneously on the upper plate. The geometry is schematically represented in Figure 2.1.

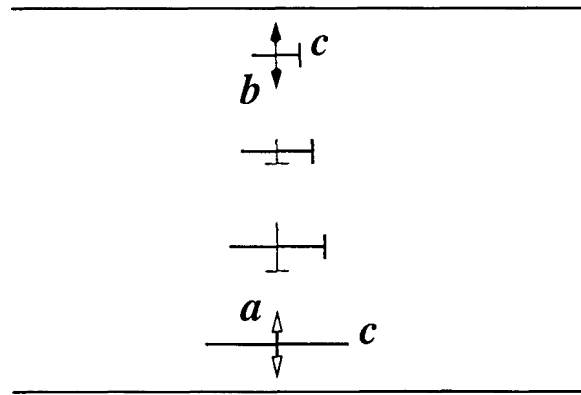


Figure 2.1: The c director is homogeneously aligned on the two plates but with a relative twist of $\delta\phi$. The nail heads indicate the end of the directors that is coming out of the plane. The a and b directors are anchored homeotropically on the lower and upper plates respectively. The twist of the (a,b) pair about c is also indicated.

In the cartesian coordinate system let

$$\mathbf{a} = -\cos \theta \sin \phi \mathbf{e}_x + \cos \theta \cos \phi \mathbf{e}_y + \sin \theta \mathbf{e}_z$$

$$\mathbf{b} = \sin \theta \sin \phi \mathbf{e}_x - \sin \theta \cos \phi \mathbf{e}_y + \cos \theta \mathbf{e}_z$$

$$\mathbf{c} = \cos \phi \mathbf{e}_x + \sin \phi \mathbf{e}_y$$

Here ϕ describes the angle made by $\mathbf{c}$ with the x-axis, and θ describes the angle of rotation of $(\mathbf{a}, \mathbf{b})$ about $\mathbf{c}$.

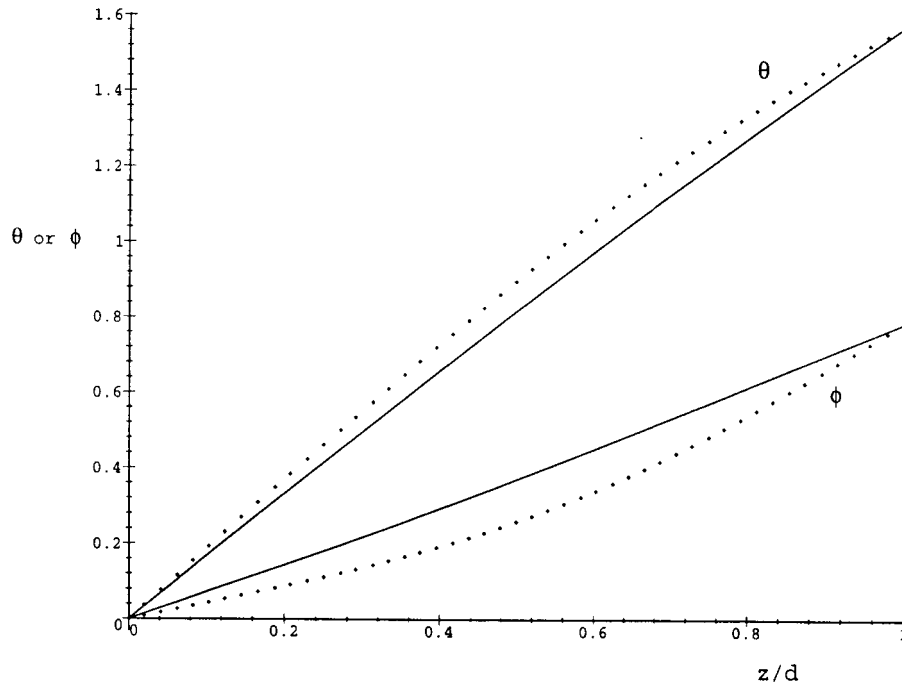


Figure 2.2: The profiles of θ and ϕ . Here, d is the separation between the plates. The plots with continuous line is for $K_a = 5, K_b = 6, K_c = 1$ dynes, and dots are for $K_a = 2, K_b = 6, K_c = 1$ dynes. The angles are shown in radians.

Within the "three-constants" approximation, the free energy density in this case is

$$F = \frac{1}{2} \left[K_c \left(\frac{d\theta}{dz} \right)^2 + f(\theta) \left(\frac{d\phi}{dz} \right)^2 \right] \quad (2.2)$$

where

$$f(\theta) = (K_a \sin^2 \theta + K_b \cos^2 \theta) \quad (2.3)$$

The equations of equilibrium are

$$\frac{d}{dz} \left[f(\theta) \frac{d\phi}{dz} \right] = 0 \quad (2.4)$$

$$K_c \frac{d^2\theta}{dz^2} = (K_a - K_b) \sin \theta \cos \theta \left(\frac{d\phi}{dz} \right)^2 \quad (2.5)$$

Equations (2.4) and (2.5) can be solved numerically with the appropriate boundary conditions. The calculations have been done for $\phi(0) = 0$, $\phi(d) = \pi/4$. $\theta(0) = 0$, $\theta(d) = \pi/2$. Here, d is the separation between the plates. The θ and ϕ variations with z are shown in Figure 2.2. Firstly, it should be noted that the profiles are nonlinear and the departure from linearity increases with greater difference between the elastic constants K_a and K_b . Elastic anisotropy, *i.e.*, $K_a \neq K_b \neq K_c$ is due to inherent biaxiality. Secondly, while variations in θ are fast, the variations in ϕ are slow and vice-versa.

Elastic anisotropy also results in instabilities even in simpler geometries such as a pure twisted director field. We consider a pure twist of the (c.a) pair by proper anchoring at the walls. It is easy to show that a uniform twist is a solution of the equations of equilibrium. In uniaxial nematics, Leslie [8] has shown that there could be an instability in this situation resulting in the director lifting out of the plane of the plates. This happens at a relative twist of nearly 180° or π between the plates provided $2K_{22} > K_{33}$. But, the way a nematic is, any twist above 90° is unattainable in the laboratory. In a BN, we find a similar instability occurring at a much lesser

relative twist. A schematic representation of this instability is shown in Figure 2.3. Here, the nail-head representation indicates that the b and the c directors are lifting out of the plane of the figure.

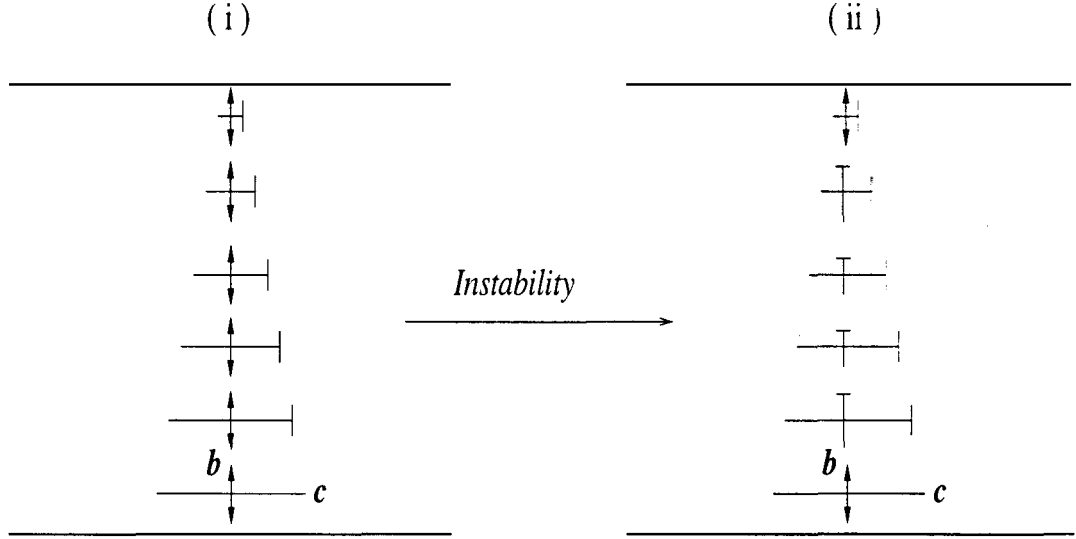


Figure 2.3: A schematic representation of an instability when the uniform twist in (a,c) as shown in (i) exceeds a threshold relative twist. The director b is shown twisting about (a,c) due to the instability depicted in (ii).

The triad of directors are parametrized as in the previous case. Let us consider $\phi = (q_0 z + \phi_1)$ and $\theta = \theta_1$ where ϕ_1 and θ_1 are small perturbations. Here, $q_0 = \delta\phi/d$ and 64 is the relative twist of the director c by proper anchoring at the walls. Then to a first approximation, the free energy density can be written as

$$F = F_0 + \frac{1}{2}K_b \left(\frac{d\phi_1}{dz} \right)^2 + \frac{1}{2} \left[K_c \left(\frac{d\theta_1}{dz} \right)^2 + (K_a - K_b) q_0^2 \theta_1^2 \right] \quad (2.6)$$

From this, it can be seen that there will not be any instability in ϕ_1 whereas there will be an instability which will lift the a director out of the plane of the plates. This occurs when the coefficient of the θ_1^2 term becomes negative. For this to happen, the condition $K_a < K_b$ has to be satisfied. This exactly follows Leslie's analysis but what is interesting is that the threshold relative twist, $\delta\phi_c$, for this instability to

occur is attainable experimentally. The threshold relative twist is given by

$$\frac{\delta\phi_c}{\pi} = \sqrt{\frac{K_c}{K_b - K_a}} \quad (2.7)$$

Depending upon the biaxial anisotropy, $\delta\phi_c$ can be less than $\pi/2$. For example, when $K_a = 3 \times 10^{-6}$ dynes, $K_b = 12 \times 10^{-6}$ dynes and $K_c = 1 \times 10^{-6}$ dynes, the threshold relative twist is $\delta\phi_c = \pi/3$. In the general case, without the three-constants approximation, the threshold relative twist is

$$\frac{\delta\phi_c}{\pi} = \sqrt{\frac{K_{ba}}{2K_{bb} - K_{bc} - K_{ac}}}$$

2.4 Instabilities in the presence of a magnetic field

When an external electric or magnetic field is applied to a uniformly aligned sample of nematic confined between parallel plates, there can arise an instability to a deformed director configuration. The geometry has to be so chosen that the orienting effect of the field conflicts with the orientation imposed by the surfaces with which the liquid crystal is in contact. A typical example of such an instability, called Freedericksz transition, is shown in Figure 2.4.

Freedericksz transitions in biaxial nematics have been studied by earlier workers [9, 10] in geometries with strong anchoring of one of the directors and no anchoring of the other two. We consider the case with strong anchoring in all the directors, **a**, **b** and **c**. The free energy density due to diamagnetic contributions is given by

$$F_{mag} = -\frac{1}{2} \sum_{\mathbf{a}, \mathbf{b}, \mathbf{c}} \chi_a (\mathbf{a} \cdot \mathbf{H})^2 \quad (2.8)$$

where χ_a , χ_b and χ_c are the principal diamagnetic susceptibilities along **a**, **b** and **c** respectively for the orthorhombic symmetry. In the undeformed state, we consider **a**, **b** and **c** to be along the reference axes *x*, *y* and *z* respectively. Deformations

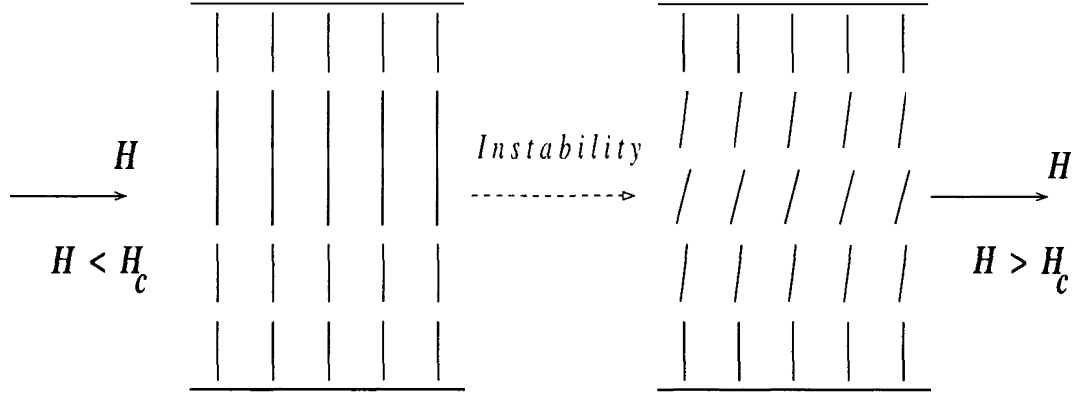


Figure 2.4: An example of Freedericksz transition. Here, the director is aligned homeotropically. The external magnetic is applied normal to the imposed alignment. Below a critical magnetic field, H_c , the uniform state is stable. Above H_c , an instability sets in and the distorted state is the stable state provided $(\chi_{||} - \chi_{\perp}) > 0$.

in the orthonormal triad of directors are described by Eulerian angles (θ, ϕ, ψ) [11] which are position dependent. The director representation in terms of (θ, ϕ, ψ) is shown in Figure 2.5.

Let $\mathbf{H}$ be along y -axis and director distortions are assumed to vary in the z direction with strong anchoring at the walls of the sample! $z = 0$ and $z = d$. Just above the threshold field, we assume the deformations to be small and to be of the form

$$f = f_m \sin \frac{\pi z}{d} \quad (2.9)$$

where $f_m = \theta_m$ (or ϕ_m or ψ_m) is the maximum value of the function $f = \theta$ (or ϕ or ψ). After averaging over the sample thickness and collecting terms upto the quartic, the free energy density is

$$F = \frac{K_b \pi^2}{2d^2} \left[\frac{a_1}{2} \zeta^2 + \frac{a_2}{2} \vartheta^2 + \frac{b_1}{4} \zeta^4 + \frac{b_2}{4} \vartheta^4 + \frac{c_1}{2} \zeta^2 \vartheta^2 + \frac{c_2}{2} \eta^2 \vartheta^2 + c_3 \zeta \eta \vartheta^2 \right] \quad (2.10)$$

where $2\zeta = \phi_m + \psi_m$, $2\eta = \phi_m - \psi_m$, $\vartheta = \theta_m$, $\kappa^2 = (d^2 H^2)/n^2$ and $a_1 = \tau_1 - \omega_1 \kappa^2$,

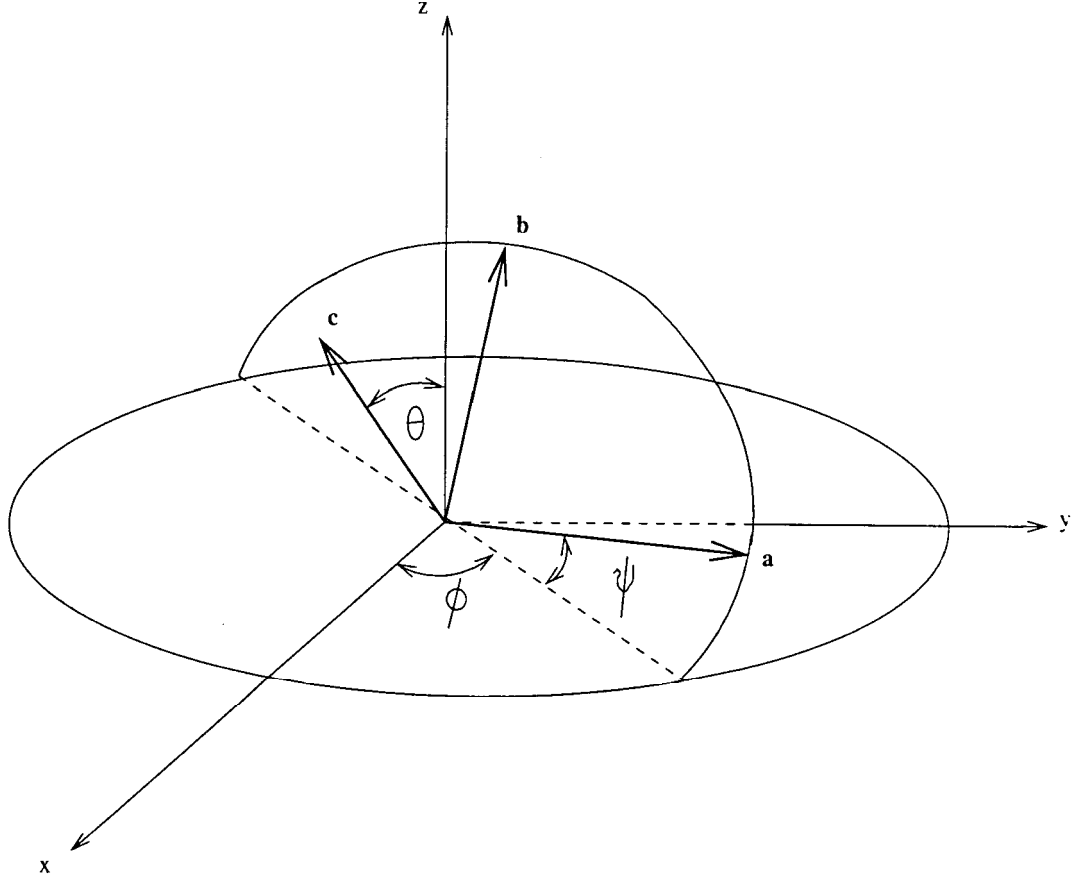


Figure 2.5: The orientations of $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ along with the Eulerian angles, θ , ϕ and ψ .

$$a_2 = \tau_2 - \omega_2 \kappa^2, b_1 = \frac{1}{2} \omega_1 \kappa^2, b_2 = \frac{1}{2} \omega_2 \kappa^2, c_1 = \frac{1}{4} (\tau_2 - 2\tau_1 + 3(\omega_2 + 2\omega_1) \kappa^2),$$

$$c_2 = \frac{1}{4} (4 - 3\tau_2 + 3\omega_2 \kappa^2), c_3 = \frac{1}{4} (\tau_2 - \tau_1 + 3(\omega_2 - \omega_1) \kappa^2) \text{ with } \tau_1 = \frac{K_c}{K_b}, \tau_2 = \frac{K_{c'}}{K_b},$$

$$\omega_1 = \frac{(\chi_a - \chi_b)}{K_b} \text{ and } \omega_2 = \frac{(\chi_c - \chi_b)}{K_b}.$$

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

$$F = \frac{K_b \pi^2}{2d^2} \left[\frac{a_1}{2} \zeta^2 + \frac{a_2}{2} \vartheta^2 + \frac{b_1}{4} \zeta^4 + \frac{b_2}{4} \vartheta^4 + \frac{\delta}{2} \zeta^2 \vartheta^2 \right] \quad (2.11)$$

where $\delta = (c_1 - \frac{c_3^2}{c_2})$. However, this theory is valid only when $\delta > -\sqrt{b_1 b_2}$ since F must be positive definite at high values of ζ and ϑ . There are four possible director

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

(d) $\zeta \neq 0, \delta \neq 0$ or $\theta \neq 0, \phi \neq 0, \psi \neq 0$ is stable when $b_1 > 0, b_2 > 0, (a_1b_2 - a_2\delta) < 0, (a_2b_1 - a_1\delta) < 0, (b_1b_2 - \delta^2) > 0$. In this state, the deformations are described by $\zeta^2 = -\frac{(a_1b_2 - a_2\delta)}{(b_1b_2 - \delta^2)}$ and $\delta^2 = -\frac{(a_2b_1 - a_1\delta^2)}{(b_1b_2 - \delta^2)}$.

It is found 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). Possible phase diagrams are schematically represented in Figure 2.6.

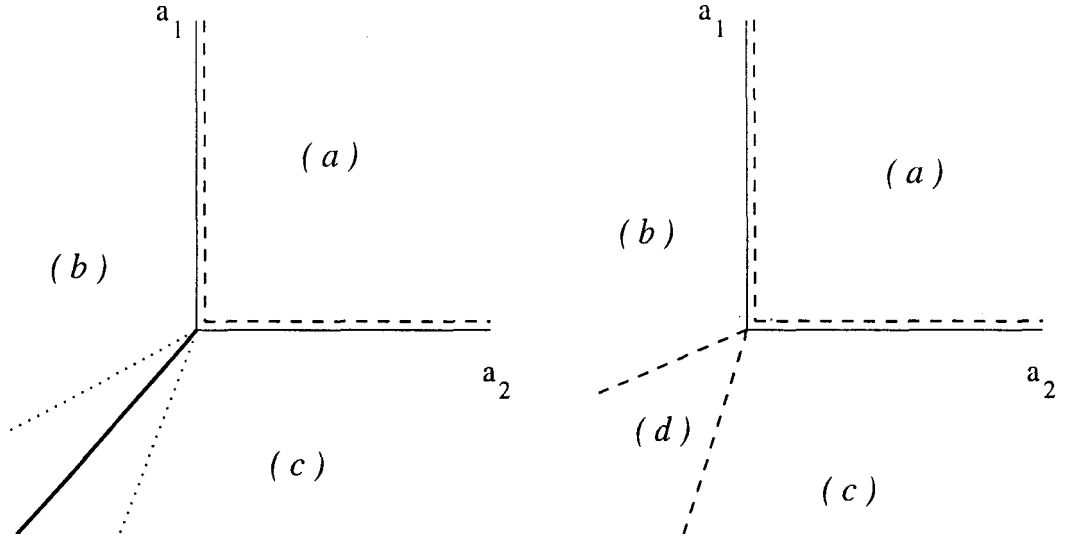


Figure 2.6: Schematic representation of possible phase diagrams. The bold and dashed lines indicate first-order and second-order phase boundaries. The dotted line corresponds to the stability of the metastable states.

Without any loss of generality, we can assume that $\mathbf{c}$ describes the uniaxial director

or the direction of the long axis. Then the states described by (c) and (d) are unique to biaxial nematics. It should also be noted that this theory does not allow the simultaneous onset of ζ and ϑ ($\zeta \neq 0, \vartheta \neq 0$) at a first-order transition line. It is known [12] that such a transition can be described if a sixth-order term in ϑ is added.

2.5 Formulation of a theory of elasticity of biaxial nematics

In this section, we argue in favour of the "three-constants" approximation on the basis of an elasticity theory of BN incorporating Ericksen's [13] idea of variable degree of orientation. This simple formulation gives insight into the elasticity of BS. We have brought out the dependences of the various constants on the orientational order parameters and, the connection between the coupling constants and elastic anisotropy. This gives a proper extension to the continuum theory allowing for a more complete description of topological defects. It also provides a framework within which approximations on the relative magnitudes of the elastic constants can be given a physical basis.

We follow the procedure developed for uniaxial nematics by Ericksen [13]. It must be remarked that Govers and Vertogen [6] have used similar tensor order representation to formulate their elastic theory of BN but without allowing for a variable degree of orientation. Here, this feature has been incorporated since this theory can also describe defects. The orientational order parameter tensor $Q_{\alpha\beta}$ is symmetric and traceless and it is given in terms of the orthonormal triad $\mathbf{a}, \mathbf{b}, \mathbf{c}$

$$Q_{\alpha\beta} = S \left(c_{\alpha}c_{\beta} - \frac{1}{3}\delta_{\alpha\beta} \right) + T \left(a_{\alpha}a_{\beta} - b_{\alpha}b_{\beta} \right) \quad (2.12)$$

where S is the orientational order parameter of uniaxial nematics, T describes the biaxiality and $\delta_{\alpha\beta}$ is the Kronecker delta. Here, $a_i, b_i, c_i, i = 1, 2, 3$ are the components

of $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$. 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

$$F = V(Q) + F_{dist} \quad (2.13)$$

where $V(Q)$ describes the homogeneous part of the free energy that describes phase transitions between the isotropic, uniaxial nematic and biaxial nematic phases, and F_{dist} is the free energy density due to director distortions and order parameter (S and T) variations in space. $V(Q)$ can be taken in the form [14]

$$V(Q) = \frac{a}{2} \text{Tr}(Q^2) + \frac{b}{3} \text{Tr}(Q^3) + \frac{c}{4} (\text{Tr}(Q^2))^2 \quad (2.14)$$

where Tr is the trace of the matrix Q . The coefficients a , b and c are coefficients suitable to describe the phase transitions. Usually, the coefficient a is assumed to be a function of temperature, and the coefficients b and c are taken to be constants. On expanding it is found that

$$V(Q) = \alpha(S) + \frac{\beta(S)}{2} T^2 + \frac{\gamma(S)}{4} T^4 \quad (2.15)$$

where

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

We generalize Ericksen's expression [13] for uniaxial nematics to BN to get the free energy density

$$F_{dist} = \frac{L_1}{2} \partial_\alpha Q_{\beta\gamma} \partial_\alpha Q_{\beta\gamma} + \frac{L_2}{2} \partial_\alpha Q_{\alpha\gamma} \partial_\beta Q_{\beta\gamma} + \frac{L_3}{2} \partial_\alpha Q_{\beta\gamma} \partial_\gamma Q_{\beta\alpha} \quad (2.16)$$

We want to compare the elastic constants of a BN with these three constants L_1, L_2 and L_3 , and the two order parameters S and T . F_{dist} can be written as

$$F_{dist} = F_{ST} + F_d \quad (2.17)$$

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:

$$\begin{aligned} F_{ST} = & \frac{1}{3}(L_1 + \frac{L_2}{6} + \frac{L_3}{6}) (\nabla S)^2 + \frac{1}{6}(L_2 + L_3) (\mathbf{c} \cdot \nabla S)^2 \\ & + L_1 (\nabla T)^2 + \frac{1}{2}(L_2 + L_3) \left[(\mathbf{a} \cdot \nabla T)^2 + (\mathbf{b} \cdot \nabla T)^2 \right] \\ & + \frac{1}{3}(\nabla S^2) \cdot \left[(L_2 - \frac{L_3}{2}) \mathbf{c} \nabla \cdot \mathbf{c} + (L_3 - \frac{L_2}{2}) \mathbf{c} \cdot \nabla \mathbf{c} \right] \\ & + \frac{1}{3}(L_2 + L_3) \left[(\mathbf{b} \cdot \nabla S)(\mathbf{b} \cdot \nabla T) - (\mathbf{a} \cdot \nabla S)(\mathbf{a} \cdot \nabla T) \right] \\ & + T \nabla S \cdot \left[L_2 (\mathbf{c} (\mathbf{a} \cdot \nabla \mathbf{a} \cdot \mathbf{c} - \mathbf{b} \cdot \nabla \mathbf{b} \cdot \mathbf{c})) \right. \\ & + \frac{1}{3}(L_2 + L_3) (\mathbf{b} \nabla \cdot \mathbf{b} + \mathbf{b} \cdot \nabla \mathbf{b} - \mathbf{a} \nabla \cdot \mathbf{a} - \mathbf{a} \cdot \nabla \mathbf{a}) \\ & + L_3 (\mathbf{b} (\mathbf{c} \cdot \nabla \mathbf{b} \cdot \mathbf{c}) - \mathbf{a} (\mathbf{c} \cdot \nabla \mathbf{a} \cdot \mathbf{c})) \left. \right] \\ & + S \nabla T \cdot \left[L_2 (\mathbf{a} (\mathbf{c} \cdot \nabla \mathbf{c} \cdot \mathbf{a}) - \mathbf{b} (\mathbf{c} \cdot \nabla \mathbf{c} \cdot \mathbf{b})) \right. \\ & + L_3 (\mathbf{c} (\mathbf{b} \cdot \nabla \mathbf{b} \cdot \mathbf{c}) - \mathbf{c} (\mathbf{a} \cdot \nabla \mathbf{a} \cdot \mathbf{c})) \left. \right] \\ & + \frac{1}{2}(\nabla T^2) \cdot \left[L_2 (\mathbf{a} \nabla \cdot \mathbf{a} + \mathbf{b} \nabla \cdot \mathbf{b} - \mathbf{a} (\mathbf{b} \cdot \nabla \mathbf{b} \cdot \mathbf{a}) - \mathbf{b} (\mathbf{a} \cdot \nabla \mathbf{a} \cdot \mathbf{b})) \right. \\ & + L_3 (\mathbf{a} \cdot \nabla \mathbf{a} + \mathbf{b} \cdot \nabla \mathbf{b} + \mathbf{b} (\mathbf{a} \cdot \nabla \mathbf{b} \cdot \mathbf{a}) + \mathbf{a} (\mathbf{b} \cdot \nabla \mathbf{a} \cdot \mathbf{b})) \left. \right] \end{aligned} \quad (2.18)$$

$$\begin{aligned} F_d = & L_1 (S + T)^2 (\mathbf{a} \cdot \nabla \mathbf{b} \cdot \mathbf{c})^2 + L_1 (S - T)^2 (\mathbf{b} \cdot \nabla \mathbf{c} \cdot \mathbf{a})^2 \\ & + 4L_1 T^2 (\mathbf{c} \cdot \nabla \mathbf{a} \cdot \mathbf{b})^2 \\ & + (4L_1 + 2L_2 + 2L_3) T^2 \left[(\mathbf{a} \cdot \nabla \mathbf{a} \cdot \mathbf{b})^2 + (\mathbf{b} \cdot \nabla \mathbf{b} \cdot \mathbf{a})^2 \right] \end{aligned}$$

$$\begin{aligned}
& + \left[L_1(S-T)^2 + \frac{(L_2+L_3)}{2}(S-T)^2 \right] \left[(a \cdot \nabla a \cdot c)^2 + (c \cdot \nabla c \cdot a)^2 \right] \\
& + \left[L_1(S+T)^2 + \frac{(L_2+L_3)}{2}(S+T)^2 \right] \left[(b \cdot \nabla b \cdot c)^2 + (c \cdot \nabla c \cdot b)^2 \right] \\
& - \frac{(L_2+L_3)}{2} (S^2 - 2T^2) (a \cdot \nabla a) \cdot (b \cdot \nabla b) \\
& - (L_2+L_3) (ST - 2T^2) (b \cdot \nabla b) \cdot (c \cdot \nabla c) \\
& + (L_2+L_3) (ST + 2T^2) (c \cdot \nabla c) \cdot (a \cdot \nabla a) \\
& + \left[\left(\frac{L_3}{2} - L_1 \right) S^2 + L_1 T^2 \right] \nabla \cdot (c \cdot \nabla c - c \nabla \cdot c) \\
& + \left[2L_1 ST - 2L_1 T^2 + \frac{L_3}{2} T^2 \right] \nabla \cdot (a \cdot \nabla a - a \nabla \cdot a) \\
& + \left[-2L_1 ST - 2L_1 T^2 + \frac{L_3}{2} T^2 \right] \nabla \cdot (b \cdot \nabla b - b \nabla \cdot b) \\
& + L_3 T^2 \left[\nabla \cdot (b (a \cdot \nabla a \cdot b) + a (b \cdot \nabla b \cdot a)) \right] \\
& + L_3 ST \left[\nabla \cdot (b (c \cdot \nabla c \cdot b) + c (b \cdot \nabla b \cdot c) \right. \\
& \left. - a (c \cdot \nabla c \cdot a) - c (a \cdot \nabla a \cdot c)) \right] \tag{2.19}
\end{aligned}$$

Hence, a comparison of (2.19) with the elastic free energy density (2.1) obtained by Saupe yields

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

The elastic anisotropy between the twist and splay or bend elastic constants is proportional to $(L_2 + L_3)$. When this anisotropy is assumed to be negligible, it can be seen that the "three-constants" approximation used to describe the elastic distortions of BN is correct. In the limit of weak biaxiality, a 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 [15] 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 the application of this theory, we consider its implications in the structure of a disclination in a, b director field. In Figure 2.7, an example of a $s = 1$ disclination is shown.

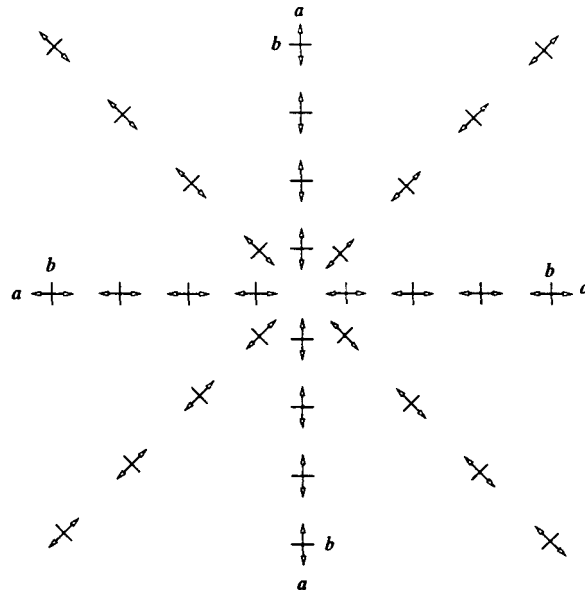


Figure 2.7: A $s = 1$ disclination in (a, b). At $r = \infty$, $S = S_0$, $T = T_0$, and at $r = 0$, $S = S_0$, $T = 0$.

In cylindrical coordinate system,

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

where $\mathbf{e}_r$, $\mathbf{e}_\phi$ and $\mathbf{e}_z$ are unit vectors in cylindrical polar coordinate system. We take $\alpha = \alpha(\phi)$, $T = T(r)$, $S = S_0$ where S_0 is a constant. Then the free energy reduces to

$$\begin{aligned}F &= F_0 + \frac{\beta}{2} T^2 + \frac{\gamma}{4} T^4 + K \left(\frac{dT}{dr} \right)^2 \\ &+ 4K \frac{T^2}{r^2} \left(1 + \frac{d\alpha}{d\phi} \right)^2 + 2(L_2 - L_3) \frac{T}{r} \frac{dT}{dr} \frac{d\alpha}{d\phi} \\ &+ 4L_1 S T \frac{\cos 2\alpha}{r^2} \frac{d\alpha}{d\phi}\end{aligned}\quad (2.20)$$

where $K = L_1 + \frac{1}{2}(L_2 + L_3)$. The minimization of the total free energy leads to the following equations of equilibrium:

$$\begin{aligned}\frac{d^2\alpha}{d\phi^2} &= 0 \\ -\beta T - \gamma T^3 &= \frac{8KT}{r^2} \left(1 + \frac{d\alpha}{d\phi} \right)^2 + 4L_1 S \frac{\cos 2\alpha}{r^2} \frac{d\alpha}{d\phi} - \\ &\frac{2K}{r} \frac{d}{dr} \left(r \frac{dT}{dr} \right)\end{aligned}\quad (2.21)$$

It can be seen that for $s = 1$ disclination in (a, b) with $\alpha = \text{constant}$, this reduces to the Ginzburg-Pitaevskii equation for a quantum vortex in type II superconductors [16]. The solution has the features : $S = S_0$, $T = 0$, $\alpha = \text{constant}$, at $r = 0$; and at $r = \infty$, $S = S_0$, $T = T_0 = \sqrt{-\beta/\gamma}$, $\alpha = \text{constant}$.

References

- [1] M. J. Freiser, Phys. Rev. Lett. 24, 1041 (1970)
- [2] L. J. Yu and A. Saupe, Phys. Rev. Lett. 45, 1000 (1980)
- [3] A. Saupe, J. Chem. Phys. 75, 5118 (1981)
- [4] H. Brand And H. Pleiner, Phys. Rev. A 24, 2777 (1981)
- [5] U. D. Kini, Mol. Cryst. Liq. Cryst. 108, 71 (1984)
- [6] E. Govers and G. Vertogen, Phys. Rev. A 30, 1998 (1984)
- [7] Sreejith Sukumaran and G. S. Ranganath, Journal de Physique II **7**, 583 (1997)
- [8] F. M. Leslie, Pramana Suppl. **1**, 41 (1975)
- [9] U. D. Kini and S. Chandrasekhar, Physica A **156**, 364 (1989)
- [10] T. Carlsson and F. M. Leslie, Liquid Crystals 10, 325 (1991)
- [11] H. Goldstein, *Classical Mechanics* (Addison Wesley,1988)
- [12] J. C. Toledano and P. Toledano, *The Landau Theory of Phase Transitions* (World Scientific,1987)
- [13] J. L. Ericksen, Arch. Rational. Mech. Anal. 113, 97 (1991)
- [14] E. Gransbergen, L. Longa and W. de Jeu, Phys. Rep. 135, 196 (1986)
- [15] D. W. Berreman and S. Meiboom, Phys. Rev. A 30, 1955 (1984)
- [16] V. L. Ginzburg and L. P. Pitaevskii, Sov. Phys. JETP 34, 858 (1958)