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## Liquid Crystals

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## A new configurational transition in inhomogeneous nematics

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At the wall in a hybrid cell with strong anchoring, the nematic director is parallel to one wall and perpendicular to the other. Usually, the free energy is minimized by a configuration where the director orientation changes continuously with position across the cell. The boundary conditions can also be satisfied, however, by a biaxial configuration without such rotation. Under certain conditions, such as under increased curvature strains, a transition can take place between these configurations. The transition typically occurs when the wavelength of the deformation becomes comparable to the coherence length of the material. The hybrid cell considered is a simple illustrative example; in real systems, such a transition may be expected in highly strained thermotropics, or in strained lyotropics which are easily made biaxial.

### 1. Introduction

Nematic liquid crystals undergoing long wavelength elastic deformations are usually described using the Frank free energy density [1]

$$\mathcal{F} = \frac{1}{2}K_1(\nabla \cdot \hat{\mathbf{n}})^2 + \frac{1}{2}K_2(\hat{\mathbf{n}} \cdot \nabla \times \hat{\mathbf{n}})^2 + \frac{1}{2}K_3(\hat{\mathbf{n}} \times \nabla \times \hat{\mathbf{n}})^2, \quad (1)$$

where  $\hat{\mathbf{n}}$  is the nematic director, and  $K_1$ ,  $K_2$  and  $K_3$  are the splay, twist and bend elastic constants. This model assumes that there exists only one distinguished direction  $\hat{\mathbf{n}}$ ; that is, that the material is uniaxial, and that the degree of orientational order on which the elastic constants depend does not vary with position.

In nematic liquid crystals, under the influence of strong fields or severe confinement, curvature strains can be large. In such highly strained nematics, the above assumptions do not hold, and an alternative description is required. One such description is the Landau-de Gennes formalism [2], which makes use of the order parameter tensor  $Q_{\alpha\beta}$ . The free energy density is formed from scalar invariants of  $Q_{\alpha\beta}$  and its derivatives. This description allows for the possibility of biaxiality, and for the spatial variation of the order parameters.

Physically realized configurations are those which minimize the free energy and satisfy boundary conditions. In a broad class of problems, the unit vector  $\hat{\mathbf{n}}$  or, alternatively, the tensor  $Q_{\alpha\beta}$  is specified on the boundaries. The Frank free energy is usually minimized by a configuration where the director varies with position, that is, where it rotates from its orientation at one boundary surface to that at the other. In the Landau-de Gennes formalism, there are two distinct simple configurations which can satisfy such boundary conditions. One configuration consists of a rotation of eigenvectors of  $Q_{\alpha\beta}$  with position, corresponding to rotation of the director. The other is

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a configuration where there is little or no net rotation of the eigenvectors, but the eigenvalues vary with position [3], and the dominant eigenvalue is associated with different eigenvectors at the different boundaries. We call the first scenario director rotation, and the second eigenvalue exchange.

The purpose of this paper is twofold. First, it is to point out that boundary conditions which usually result in simple curvature strains, as exemplified by the hybrid cell, can also be satisfied by a competing biaxial configuration. Second, it is to study the configurations corresponding to director rotation and to eigenvalue exchange, and to examine the possibility of a transition [4] between them. The hybrid cell, because of its simplicity, is an ideal system to study such a transition, and to illustrate its salient features. We discuss possible realizations of such transitions, and make a connection with recent experimental results of surface melting.

## 2. The free energy of a hybrid cell

A simple system which exhibits the configurational states discussed above is the hybrid cell. The Landau–de Gennes free energy [5] is

$$F = \int (\frac{1}{2}A \operatorname{tr} Q^2 - \frac{1}{3}B \operatorname{tr} Q^3 + \frac{1}{4}C(\operatorname{tr} Q^2)^2 + \frac{1}{2}L(\nabla Q)^2) d^3r, \quad (2)$$

where  $\operatorname{tr} Q^2 = Q_{\alpha\beta}Q_{\beta\alpha}$ ,  $\operatorname{tr} Q^3 = Q_{\alpha\beta}Q_{\beta\gamma}Q_{\gamma\alpha}$  and  $\nabla Q = \partial Q_{\alpha\beta}/\partial x_\gamma$ . For simplicity, we keep only terms up to fourth order, and only one derivative term. The latter is equivalent to the one elastic constant approximation.

We consider a hybrid cell with parallel plane walls in the  $v$ – $\zeta$  plane, where  $\xi$ ,  $v$  and  $\zeta$  are cartesian coordinates in a lab-fixed frame. For simplicity, we assume that the nematic is uniaxial at the cell walls, with the director in the  $\xi$  direction at  $\xi=0$  and in the  $v$  direction at  $\xi=d$ . We assume that one eigenvector of the order parameter  $Q_{\alpha\beta}$  is always parallel to the  $\zeta$  axis, and that  $Q_{\alpha\beta}$  is the function of only the coordinate  $\xi$ . The boundary conditions in the lab frame are assumed to be

$$Q(0) = \begin{bmatrix} S_0 & 0 & 0 \\ 0 & -\frac{1}{2}S_0 & 0 \\ 0 & 0 & -\frac{1}{2}S_0 \end{bmatrix} \quad (3)$$

and

$$Q(d) = \begin{bmatrix} -\frac{1}{2}S_0 & 0 & 0 \\ 0 & S_0 & 0 \\ 0 & 0 & -\frac{1}{2}S_0 \end{bmatrix}, \quad (4)$$

where  $S_0$  is the order parameter in the homogenous bulk. One parameterization of the order parameter is given below:

$$Q(\xi) = \frac{1}{4} \begin{bmatrix} (S+P) + (3S-P)\cos^2\theta & (3S-P)\sin 2\theta & 0 \\ (3S-P)\sin 2\theta & (S+P) - (3S-P)\cos 2\theta & 0 \\ 0 & 0 & -2(S+P) \end{bmatrix}. \quad (5)$$

Here  $S$  and  $P$  are the usual orientational order parameters; that is,  $S = \langle \frac{1}{2}(3(\hat{n} \cdot \hat{n})^2 - 1) \rangle$  and  $P = \langle \frac{3}{2}((\hat{u} \cdot \hat{m})^2 - (\hat{u} \cdot \hat{l})^2) \rangle$  where  $\hat{u}$  is a unit vector along the symmetry axis of a molecule,  $\hat{n}$ ,  $\hat{m}$  and  $\hat{l}$  are the eigenvectors of  $Q_{\alpha\beta}$ , and  $\langle \rangle$  denotes the ensemble average.

In this representation,  $\hat{n}$  and  $\hat{m}$  are parallel to the  $\xi$  and  $v$  axes respectively at  $\xi=0$ , and they both rotate through an angle  $\theta$  as the cell is traversed.  $\hat{l}$  is assumed to remain parallel to the  $\zeta$  axis throughout.

A schematic of the cell illustrating the two configurations is shown in figure 1. It is useful to consider another representation, given below.

$$Q(\xi) = \frac{1}{\sqrt{6}} \begin{bmatrix} z + \sqrt{3}x & \sqrt{3}y & 0 \\ \sqrt{3}y & z - \sqrt{3}x & 0 \\ 0 & 0 & -2z \end{bmatrix}. \tag{6}$$

With this representation, the dimensionless free energy  $\mathcal{F} = F/(\mathcal{A}dC)$  where  $\mathcal{A}$  is the area of the cell, becomes

$$\mathcal{F} = \int_0^1 \left\{ \frac{1}{2}a(x^2 + y^2 + z^2) - bz \left( x^2 + y^2 - \frac{z^2}{3} \right) + \frac{1}{4}(x^2 + y^2 + z^2)^2 + \frac{l}{2} \left( \left( \frac{\partial x}{\partial \eta} \right)^2 + \left( \frac{\partial y}{\partial \eta} \right)^2 + \left( \frac{\partial z}{\partial \eta} \right)^2 \right) \right\} d\eta, \tag{7}$$

where  $\eta = \xi/d$ ,  $a = A/C$ ,  $b = (B/\sqrt{6}C)$  and  $l = (L/d^2C)$ . One advantage of using the coordinates  $x, y$  and  $z$  is the simple form of the derivative terms in the free energy; a connection can be made with the representation introduced by Freiser [6] by letting  $x = \rho \sin \psi \cos \phi$ ,  $y = \rho \sin \psi \sin \phi$  and  $z = \rho \cos \psi$ , then  $x^2 + y^2 + z^2 = \rho^2$  and  $z(x^2 + y^2 - (z^2/3)) = -(\rho^3/3) \cos 3\psi$ . Since in a uniaxial material  $\psi = 0$ ,  $B$  provides a measure of the energy cost of a biaxial phase.

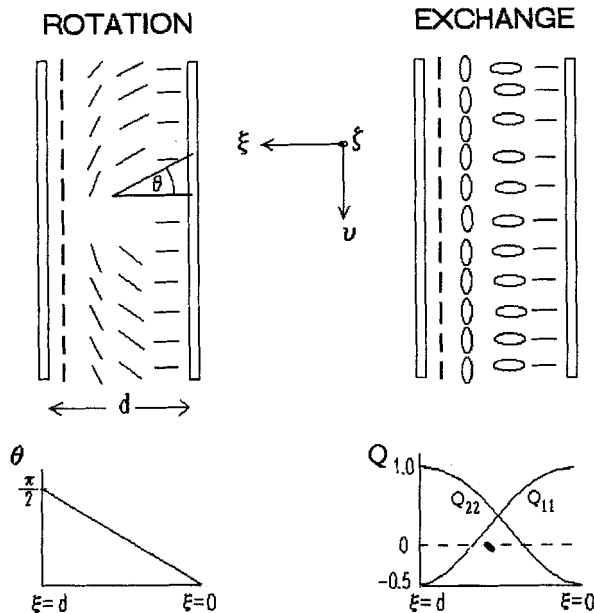


Figure 1. Schematic of the hybrid cell showing director rotation and eigenvalue exchange. In the case of rotation,  $\theta$  varies with position; but for every eigenvector, the associated eigenvalue has the same value at both cell walls. In the case of exchange,  $\theta=0$  everywhere, but the eigenvalue associated with  $\hat{n}$  at one wall will be associated with  $\hat{m}$  at the other, and vice versa.

**3. Minimization of the free energy**

Configurations which minimize the free energy  $\mathcal{F} = \int f d\eta$  of equation 7 correspond to solutions of the Euler-Lagrange equations  $\delta f/\delta x = \delta f/\delta y = \delta f/\delta z = 0$ . These coupled non-linear, second order, ordinary differential equations are solved numerically using a relaxation scheme. In a non-equilibrium state, the x-component of the thermodynamic force acting on the system is  $-(\delta f/\delta x)$ , and, if the system response to this force is predominantly viscous, then  $\gamma(\partial x/\partial t) = (\delta f/\delta x)$  where  $t$  is time and  $\gamma$  is a viscosity coefficient. Explicitly, the approach of the system to an equilibrium state is described by

$$\gamma_1 \frac{\partial x}{\partial t} = -ax + 2bzx - x(x^2 + y^2 + z^2) + l \frac{\partial^2 x}{\partial \eta^2}, \tag{8 a}$$

$$\gamma_2 \frac{\partial y}{\partial t} = -ay + 2bzy - y(x^2 + y^2 + z^2) + l \frac{\partial^2 y}{\partial \eta^2}, \tag{8 b}$$

$$\gamma_3 \frac{\partial z}{\partial t} = -az + b(x^2 + y^2 - z^2) - z(x^2 + y^2 + z^2) + l \frac{\partial^2 z}{\partial \eta^2}. \tag{8 c}$$

The above equations were discretized, and the method of finite differences was used to allow the system, starting from different initial conditions, to relax to equilibrium.

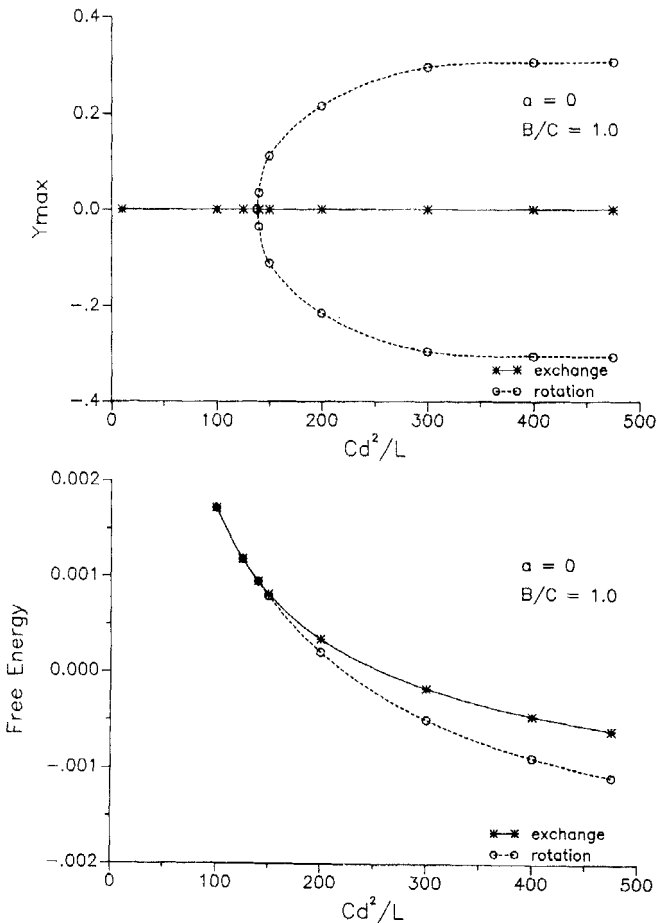


Figure 2. Order parameter  $y_{max}$ , which gives a measure of director rotation, and free energy  $\mathcal{F}$  as function of  $1/l = (d^2 C/L)$ .

#### 4. Results and discussions

We have calculated equilibrium configurations for the hybrid cell using equations 8 for a range of values of the parameters. Once the configurations are determined, the corresponding free energy can be calculated from equation 7. A suitable order parameter which allows the configurations to be distinguished is  $y_{\max} = y(0.5)$ ; that is, the value of  $y(3/2\sqrt{2})(3S - P) \sin 2\theta$  at the centre of the cell. For eigenvalue exchange,  $y_{\max} = 0$ , while for director rotation  $y_{\max} \neq 0$ . For the range of parameters studied, we have found that the exchange configuration is always a solution, while the configuration corresponding to director rotation is a solution only if the parameter  $1/l = (d^2C/L)$  is greater than some critical value. Typical results for  $y_{\max}$  and the free energy  $\mathcal{F}$  are shown in figure 2.

A second order transition occurs between the exchange and director rotation configurations at a critical value of the parameter  $1/l = (d^2C/L)$ . For thermotropic nematics,  $B$  and  $C$  are of the order [5, 7] of  $k_{\beta\rho}$ , where  $k_{\beta}$  is Boltzmann's constant and  $\rho$  is the number density, and  $L \simeq K/S^2$ , where  $K$  is a Frank elastic constant [5]. As the temperature is increased, the critical value of  $1/l$  increases. If the value of the coefficient  $B$  of the cubic term in equation 2 is decreased, the critical value of  $1/l$  increases. The free energy  $\mathcal{F}$ , in equation 7, may be regarded as the action of a particle with position  $\mathbf{r} = (x, y, z)$  and velocity  $\partial\mathbf{r}/\partial\eta$ . If  $B = 0$ , the particle feels only a central force, and hence  $y = 0$  for all  $\eta$ . Thus the critical value of  $1/l + \infty$  as  $B \rightarrow 0$ .

#### 5. Conclusions

Highly strained nematics with curvature comparable to  $(L/B)$  can undergo a configurational transition from a state characterized by director rotation to a predominantly biaxial state. This configurational transition is similar to the structural transformation between Bloch and Ising walls in magnetic systems [8]. Such transitions may occur in nematics confined to cavities with small characteristic lengths, in materials where  $B$ , the coefficient of the cubic term in the Landau expansion, is small [9], and near surfaces under the influence of strong fields. The characteristic length scale of elastic distortions near surfaces due to the influence of fields is the field coherence length  $\xi_F$ . We expect our results to hold, at least approximately, for field induced distortions [10] if  $d$  is replaced by  $\xi_F$ . This suggests that fields comparable to  $E_c \simeq \sqrt{(B/\epsilon_0\Delta\epsilon)}$  or  $H_c \simeq \sqrt{(B/\mu_0\Delta\chi)}$  can induce a configurational transition in the layer of nematic of thickness  $\xi_F$  near the anchoring surface. Such a transition may be related to recent experimental observations of surface melting [11–13] and light scattering studies of liquid crystals in silica gels [14–15]. Study of the effects of surface and field terms is currently under way.

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