

# Critical Splay-Bend Deformation of Nematic Films

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In thin nematic films the director field  $\mathbf{n}$  may only depend on  $z$ , the normal to the film plane. There are two stable configurations with less than all three types of deformation present, the pure twist and the pure splay-bend. For the pure twist under the additional influence of an external field normal to the twist plane the range of stability is well known already. For the pure splay-bend the critical equation is derived here under the additional influence of an external field normal to the splay-bend plane. It comes out as an eigenvalue problem which can be solved using Ritz' method. Numerical solutions are presented for  $K_1=K_3$ .

## § 1. Introduction

Liquid crystal films with a director field  $\mathbf{n}$  depending only on one coordinate  $z$  normal to the plane of the film are important in technical devices. Critical transitions are observed in a homogeneous magnetic or electric field if the field orientation has been suitably chosen. Well known are the various geometries of the Frederiks transition<sup>1</sup> in originally single crystalline layers with strong anchoring of the director on the plane walls of the film. After twisting a homogeneously textured film by the angle  $\Delta\varphi$ , a critical field  $\mathbf{H} = (0, 0, H)$  normal to the film plane destroys the pure twist. After Leslie<sup>2</sup> one gets

$$\mu_0 \chi_a (H d)^2 + (2 K_2 - K_3) \Delta\varphi^2 = K_1 \pi^2. \quad (1)$$

An analogous relation holds for an electrical voltage  $U$  between the film walls. Using  $\Delta\varphi = \pi/2$  we obtain the Schadt-Helfrich cell<sup>3</sup>.

The conditions for the existence of a critical transition remain fulfilled as long as the external field produces no torque in the subcritical range. From Eq. (1) we see that even without any external field a critical  $\Delta\varphi$  can be obtained, if  $K_2 > K_3/2$ . To avoid the appearance of disclinations or walls in the subcritical range requires  $\Delta\varphi < \pi/2$  resp.  $K_2 > 2 K_1 + K_3/2$ . This is a condition which hardly can be observed.

The pure twist is not the only stable deformation of a director field  $\mathbf{n}(z)$  with less than all three types of deformation present. The second stable configuration of this kind is a pure splay-bend deformation without twist. Here  $\text{rot } \mathbf{n}$  has to be normal to  $\mathbf{n}$  all over the film. This case should be obtained by starting with a constant director field. By

rotating the wall angles by  $\pm \vartheta_1$  in opposite directions one first would form a pure splay-bend deformation in the  $x$ - $z$  plane. After increasing  $\vartheta_1$  beyond a critical value the director will break out into the third dimension. Here again a homogeneous external field parallel or perpendicular to the  $y$  axis can be added without the conditions for a critical transition being lost.

Another kind of deformation in  $\mathbf{n}(z)$ , namely a pure twist-bend without splay could be realized by

$$\mathbf{n}(z) = [\sin \vartheta_0 \cos \varphi(z), \sin \vartheta_0 \sin \varphi(z), \cos \vartheta_0].$$

However it can be shown that such a field is not stable.

In this paper the critical parameters of a pure splay-bend deformation shall be found including the influence of an external field in  $y$  direction. This task will lead to an eigenvalue problem. Approximate solutions will be obtained by applying the Ritz method<sup>4</sup>. Finally the question of an experimental realization of the boundary conditions required for observing the critical transition shall be discussed.

## § 2. General Formulation of the Problem

The problem to be solved here may be defined as follows. Let us start with a plane nematic layer of thickness  $d$ . The director field  $\mathbf{n} = (n_x, n_y, n_z)$  may be homogeneous and may form an angle  $\vartheta_0$  with the  $z$  axis which is normal to the layer. We adjust the  $x$  and  $y$  axis so that  $n_y = 0$  first. Now the director at the boundaries  $z = \pm d/2$  will be rotated by  $\pm \vartheta_1$  in opposite directions within the  $x$ - $z$  plane. By this way the layer undergoes a splay-bend deformation. One has to determine the critical angle  $\vartheta_{1c}$ , at which the director will leave the  $x$ - $z$  plane. The critical angle  $\vartheta_{1c}$  will depend on  $\vartheta_0$ .

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For a director field  $\mathbf{n}(z)$  in equilibrium the continuum theory requires the total torque density  $\mathbf{I}'(z)$ , which is caused by the molecular field  $\mathbf{h}(z)$  acting upon  $\mathbf{n}(z)$ , to be zero:

$$\mathbf{I}' = \mathbf{n} \times \mathbf{h} = 0 \quad (2)$$

where

$$\mathbf{h} = \mathbf{h}^S + \mathbf{h}^T + \mathbf{h}^B. \quad (3)$$

The splay, twist, and bend components are defined by the following equations<sup>5</sup>

$$\mathbf{h}^S = K_1 \nabla D \quad \text{with} \quad D = \text{div } \mathbf{n}, \quad (4)$$

$$\mathbf{h}^T = K_2 \{ -A \text{rot } \mathbf{n} - \text{rot}(A \mathbf{n}) \} \quad (5)$$

with  $A = \mathbf{n} \text{rot } \mathbf{n}$ ,

$$\mathbf{h}^B = K_3 \{ \mathbf{B} \times \text{rot } \mathbf{n} + \text{rot}(\mathbf{B} \times \mathbf{n}) \} \quad (6)$$

with  $\mathbf{B} = \mathbf{n} \times \text{rot } \mathbf{n}$ .

Hereby  $n_y$ ,  $n_y'$ , and  $n_y''$  (' for  $d/dz$ ) are treated as small quantities so that only the linear approximation needs to be considered. In addition we make use of the normalizing condition

$$n_x^2 + n_z^2 = 1. \quad (7)$$

The  $y$  component of Eq. (2) gives

$$n_x''/n_x = \kappa_1 n_z''/n_z. \quad (8)$$

To be short we define

$$\begin{aligned} \kappa_1 &= K_1/K_3; \quad f = 1 + (\kappa_1 - 1)n_x^2, \\ \kappa_2 &= K_2/K_3; \quad g = 1 + (\kappa_2 - 1)n_x^2. \end{aligned} \quad (9)$$

The  $z$  component of Eq. (2) gives

$$\frac{d}{dz} (g n_y') - \frac{1}{n_x} \cdot \frac{d}{dz} (g n_x') \cdot n_y = 0. \quad (10)$$

The  $x$  component of Eq. (2) gives a differential equation, which is the sum of (8) and (10) and therefore can be forgotten.

When we write  $n_x = \sin \vartheta(z)$ ,  $n_z = \cos \vartheta(z)$  we have attended to Eq. (7). Then from Eq. (8) we obtain

$$\frac{d}{dz} [f(z) \vartheta'^2] = 0. \quad (11)$$

The explicit solution with the boundary conditions taken into account is

$$\vartheta(z) = \vartheta_0 - \vartheta_1 + 2 \vartheta_1 I(z)/I(d/2) \quad (12)$$

where

$$I(z) = \int_{-d/2}^z dz / \sqrt{f(z)}. \quad (13)$$

Then we also know  $n_x(z)$  and its derivatives. So Eq. (10) can be reduced to a linear homogeneous differential equation of second order in  $n_y(z)$ .

Here no simple statement can be found to fulfill this differential equation. But it comes out as Euler's differential equation of the variation problem:

$$I = \frac{1}{2} \int_{-d/2}^{+d/2} [g n_y'^2 + p n_y^2] dz = \text{Extr!} \quad (14)$$

with the boundary conditions  $n_y(\pm d/2) = 0$  (boundary value problem of the first kind). For shortness we have used

$$p(z) = -\frac{1}{n_x} \frac{d}{dz} (g n_x'). \quad (15)$$

The search for a critical equation analogous to Eq. (1) leads us to the problem of calculating the lowest eigenvalue parameter  $\vartheta_1$ , for which a non trivial solution  $n_y(z) \neq 0$  is allowed. For this task the Ritz method<sup>4</sup> shall be applied.

In this method the unknown function  $n_y(z)$  is replaced by

$$n_y(z) = \sum_{k=1}^n c_k v_k(z) \quad (16)$$

where the  $c_k$  are free coefficients. For  $v_k(z)$  one makes a good choice of so called comparison functions which have to fulfill all boundary conditions and which shall be similar to the exact eigenfunctions. For demands of a reasonable accuracy it is often sufficient to use only  $v_1(z)$ , if skilfully chosen. From  $dI(c_1)/dc_1 = 0$  we obtain the eigenvalue equation

$$\int_{-d/2}^{+d/2} (g v_1'^2 + p v_1^2) dz = 0. \quad (17)$$

Instead of  $\vartheta_1 = \vartheta_{1c}$  we use as an eigenvalue

$$\lambda = 2 \vartheta_1 / \pi. \quad (18)$$

So  $n_x$ ,  $g$ , and  $h$  are functions of  $z$  and  $\lambda$ . However as long as  $n_x$  contains elliptical integrals, as can be seen from Eq. (12), the efforts for obtaining solutions of (17) are too expensive. In § 3 we shall present a special case where numerical calculations can be obtained with a pocket computer.

Beforehand, however, let us discuss the influence of a homogeneous external field, for example a magnetic field  $\mathbf{H}$ , on the general formulation of the problem.

In order to conserve the critical conditions,  $\mathbf{H}$  can only be parallel or normal to the  $y$  axis. In the

latter case again the calculation would be too cumbersome. Therefore let us restrict to  $\mathbf{H} = (0, H, 0)$ . Its contribution to the torque density  $\mathbf{F}$  is

$$\mathbf{F}_H = \mu_0 \chi_a (\mathbf{n} \cdot \mathbf{H}) (\mathbf{n} \times \mathbf{H}) = \mu_0 \chi_a H^2 n_y \begin{pmatrix} -n_z \\ 0 \\ n_x \end{pmatrix}. \quad (19)$$

So Eq. (8) remains unchanged and in Eq. (10)  $p(z)$ , defined by Eq. (15), has to be extended by the term  $\mu_0 \chi_a H^2 / K_3$ .

### § 3. Special Solutions and Discussion

For  $\kappa_1 = 1$  Eq. (11) has the simple solution

$$\vartheta(z) = \vartheta_0 + \pi \lambda z/d. \quad (20)$$

So also  $g$  and  $p$  are known as simple functions of  $z$  and  $\lambda$ . As a comparison function we choose

$$v_1(z) = \cos(\pi z/d). \quad (21)$$

Now the integration of Eq. (17) can be performed and we obtain the critical equation.

$$\kappa_2 = 1 + 2(1 - \lambda^2 - \sigma)/\tau \quad (22)$$

where we have used the abbreviations

$$\sigma = \frac{\mu_0 \chi_a}{K_3} \left( \frac{Hd}{\pi} \right)^2 \quad (23)$$

and

$$\tau = \cos 2\vartheta_0 \cdot \frac{\sin \pi \lambda}{\pi \lambda} \cdot \frac{1 - 5\lambda^2}{1 - \lambda^2} - \lambda^2 - 1. \quad (24)$$

In Fig. 1, which holds for  $\sigma = 0$ , you find several graphs of the function  $\lambda(\kappa_2)$  with  $\vartheta_0$  between  $0^\circ$

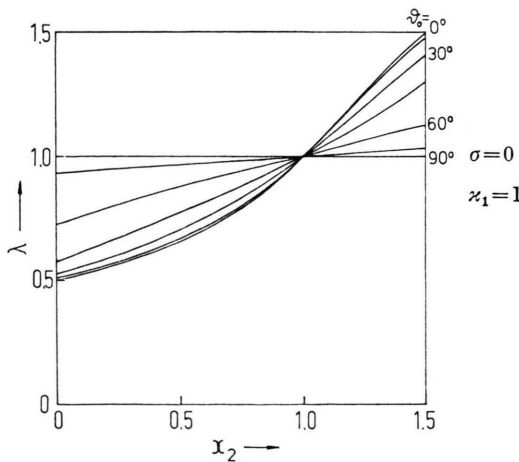


Fig. 1. Critical splay-bend deformation  $\lambda = 2\vartheta_1/\pi$  as a function of  $\kappa_2 = K_2/K_3$  at constant  $\kappa_1 = 1$  without a magnetic field ( $\sigma = 0$ ). The parameter  $\vartheta_0$  varies from  $0^\circ$  to  $90^\circ$ .

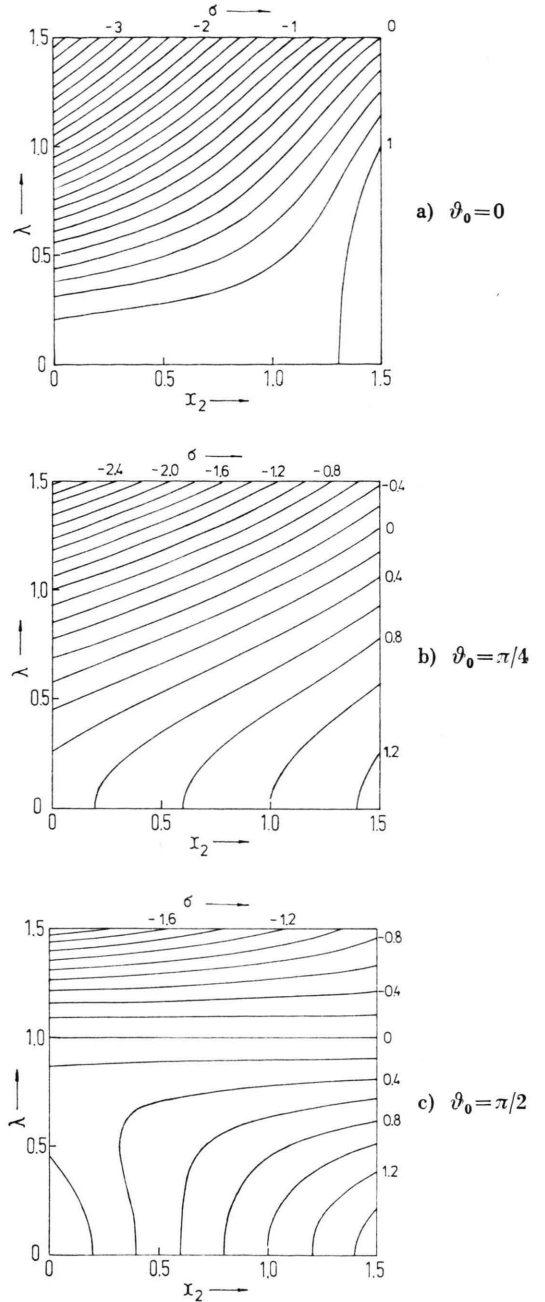


Fig. 2. Critical splay-bend deformation  $\lambda = 2\vartheta_1/\pi$  as a function of  $\kappa_2 = K_2/K_3$  at constant  $\kappa_1 = 1$ . Parameter is  $\sigma (\sim H^2)$ .

and  $90^\circ$  as a parameter. Applied to the special case  $\kappa_1 = 1$  and  $\kappa_2 = 0.5$  (nearly the data for MBBA) these graphs say: With a homeotropic orientation at the beginning ( $\vartheta_0 = 0^\circ$ ) one obtains the lowest eigenvalue  $\lambda = 0.65$  corresponding to a critical angle  $\vartheta_{1c} = 58.5^\circ$ . With a homogeneous orientation at the

beginning ( $\vartheta_0 = 90^\circ$ ), on the other hand,  $\lambda = 1$  and  $\vartheta_{1c} = 90^\circ$ , which is independent of  $\kappa_2$  in this case. Here the migration into the third dimension is only feasible after the "peaked" structure (Zipfelstruktur) has been formed. In the "peaked" structure the layer obeys homeotropic wall conditions and the director is turned by  $\pi$  when going from wall to wall. For symmetry reasons this structure remains indifferent against rotations around the  $z$  axis.

Figure 2 contains three more diagrams in which the influence of an external field is shown for different initial orientations  $\vartheta_0 = 0, \pi/4$ , and  $\pi/2$ . The parameter  $\sigma$  [Eq. (22)] can be positive or negative depending on the sign of  $\chi_a$ . In general with increasing  $\sigma$  the critical parameter  $\lambda$  will decrease. A special situation can be observed for  $\vartheta_0 = \pi/2$ . Here for instance at  $\lambda = 0$  and  $\kappa_2 = 0.35$  the layer can be forced into an overcritical field by applying  $\sigma = 0.35$ . This is one of the Frederiks transitions<sup>1</sup> into a deformation of pure twist. With increasing  $\lambda$  the layer returns to the subcritical state of pure splay-bend deformation at  $\lambda = 0.35$ . But by further increasing  $\lambda$  the layer again becomes overcritical at  $\lambda \geq 0.61$ . A similar behaviour can be found for  $\vartheta_0 = 0$  when  $\sigma > 1$  (not shown in this diagram).

The critical Eq. (22) includes the limiting case  $\lambda = 0$ . For it alone the critical conditions can be strongly derived without needing Ritz' approximation. This problem simply concerns the generalization of two Frederiks transitions with  $\vartheta_0$  as a free parameter. One gets

$$\mu_0 \chi_a (Hd)^2 = \pi^2 (K_3 \cos^2 \vartheta_0 + K_2 \sin^2 \vartheta_0). \quad (25)$$

However the same relation, namely  $\sigma = g(\sin \vartheta_0)$ , we derive from Equation (22). So for  $\lambda = 0$  our comparison function is identical with the true eigenfunction.

In order to test the grade of approximation, obtained in Eq. (22) using only one comparison function, a second comparison function  $v_2(z) = \cos 3\pi z/d$  has been introduced. Spot checks have resulted a decrease in  $\lambda$  of less than one percent. So the graphs in Fig. 1 approach the exact shape pretty well and present the qualitative behaviour in a correct manner.

Within certain limits also the case  $\kappa_1 = 0$  can be easily calculated using Ritz' method. Here  $n_x$  becomes a linear function of  $z$  and as a good comparison function we can choose  $v_1(z) = 1 - 4z^2/d^2$ . As soon as  $n_x$  becomes  $\pm 1$ , however, a splay-wall singularity appears. This makes a discussion difficult. Anyway computer calculations are planned for the whole range  $0 < \kappa_1 < 1$ , so that a discussion of this unrealistic case will not be necessary now.

Finally let us discuss by what way the special boundary conditions could be realized experimentally. First we could think of only changing the external field while the wall angles ( $\vartheta_0 + \vartheta_1$ ) and ( $\vartheta_0 - \vartheta_1$ ) are kept constant. Oblique wall angles could be enforced, for instance, by inclined vaporization of the walls. A possibility how to increase the wall angles gradually with time cannot be seen at the moment. However a similar condition can be accomplished using Poiseuille flow of a homeotropic layer. Here the velocity gradient is largest near the walls producing a rotation of the director towards flow alignment. The middle part of the layer undergoes an increasing splay-bend deformation with increasing flow rate. Experiments of this kind have been performed in our laboratory and the results will be published soon<sup>6</sup>. They have shown that at a critical flow rate the splay-bend deformation is transformed into a screw like deformation.

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<sup>5</sup> P. G. de Gennes, *The Physics of Liquid Crystals*, Oxford 1974, p. 68.

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