Umbilics : static properties and shear-induced displacements

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Classification
Physics Abstracts
14.82

UMBILICS : STATIC PROPERTIES AND SHEAR-INDUCED DISPLACEMENTS

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(*Reçu le 8 février 1973*)

Résumé. — Appliqué sur une lamelle orientée de cristal liquide nématique, un champ électrique peut, dans certaines conditions, créer des défauts ponctuels appelés « ombilics ». Nous étudions leurs structures et nous montrons comment un écoulement dans la lamelle induit un déplacement de ces défauts.

Abstract. — We study the structure of umbilical « defects » which should appear under certain conditions in a nematic slab in an electric field. We show that a shear flow can induce a displacement of these defects.

1. **Degenerate Fredericks transition.** — A slab contains a nematic monocrystal with a negative dielectric (or magnetic) anisotropy (Fig. 1). The unperturbed configuration is chosen to be homeotropic (by a suitable treatment of the surfaces). A static electric (or magnetic) field, parallel to the optical axis can (above a threshold value) distort the structure. This situation is reminiscent of the Fredericks transition [1]. However, the nature of the distorsion is very particular : the optical axis tends to lie parallel to the surfaces to minimize the magnetic (or electric) energy, but no direction is preferred in this plane. We may describe the direction of tilt by a two dimensional unit vector $\mathbf{C}(x, y)$. The amplitude of the tilt can be measured by a real number $S(x, y, z) = |\mathbf{n}_\perp|$, where the ordinary director is $\mathbf{n} = (n_z, n_x, n_y) = (n_z, \mathbf{n}_\perp)$.

When $\mathbf{C}$ varies slowly with x, y, we may assume S to be essentially identical to its value $S(z, E)$ for an undistorted situation ($\mathbf{C}$ = constant vector). Thus $S(z, E)$ can be calculated while the $\mathbf{C}$ direction is unknown. In the ordinary Fredericks transition [1], we had a twofold degeneracy (since $\mathbf{n}$ and $-\mathbf{n}$ were equivalent) this allowed for two kinds of domains and for walls between them [4]. But, in this new case, we have an infinite degeneracy for the $\mathbf{C}$ direction in the x, y plane. And, for slow variation it is possible to define a two dimensional continuum elasticity for the $\mathbf{C}$ vector. The free energy of distorsion should be of the form :

$$F_{/\text{unit volume}} = \tfrac{1}{2} L_1[\text{div } \mathbf{C}]^2 + \tfrac{1}{2} L_2[(\mathbf{C}.\nabla)\,\mathbf{C}]^2 . \quad (1)$$

When $U \gg U_t$ (the threshold value for the electric potential applied to the electrodes), S is equal to one except in two thin layers, near the surfaces, of thickness $\sim \xi \left(\xi = \frac{U_t}{U}\frac{d}{\pi} \ll d\right.$ the thickness of the slab). In this limit K_1 is associated with splay distorsions : $K_1 = L_1$ and K_3 to bend distorsions : $K_3 = L_2$.

When $U \neq U_t$, $S \ll 1$ and the situation is rather different.

With $\mathbf{n}_\perp = S(z)\,\mathbf{C}(x, y)$, the Frank energy can be written :

$$F_{/\text{unit volume}} = F(S) + \tfrac{1}{2} K_1 S^2(z)\,[\text{div } \mathbf{C}]^2 + \tfrac{1}{2} K_2 S^2(z)\,[(\mathbf{C}.\nabla)\,\mathbf{C}]^2 . \quad (2)$$

Thus for the slab, the elastic constant for splay distorsions is $L_1 = K_1 < S^2(z) >$ while that for the bend distorsions is now $L_2 = K_2 < S^2(z) >$. The mean value $< S^2(z) >$ is defined by :

$$< S^2(z) > = \frac{1}{d}\int_{-d/2}^{+d/2} S^2(z)\,dz . \quad (3)$$

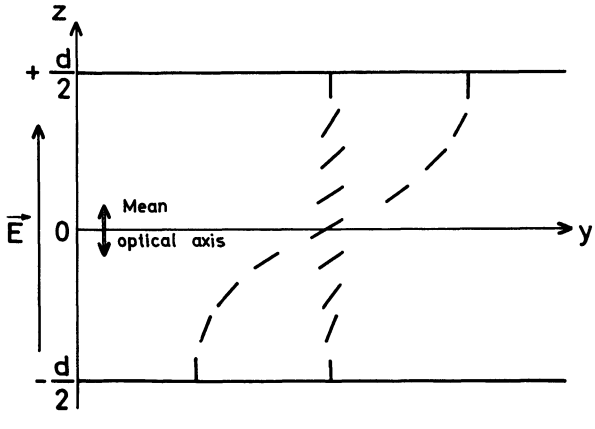

FIG. 1. — Nematic slab under an electric field.

In the first order approximation

$$S(z) = S_M(U) \cos\left(\frac{\pi}{d} z\right), \quad < S^2(z) > = \frac{1}{2} S_M^2(U).$$

The peak amplitude $S_M(U)$ can be calculated with the elastic energy $F(S)$ and the electric energy $F_{elec}(S)$. These two functions are given by :

$$\int_{slab} F(S)\, dz =$$

$$= \int \left[\frac{1}{2} K_3 \left(\frac{dS}{dz}\right)^2 + \frac{1}{2} K_1 \left(S \frac{dS}{dz}\right)^2 + 0(S^6)\right] dz$$

$$= \left(\frac{\pi^2 K_3}{4 d}\right)\left(1 + \frac{1}{4}\frac{K_1}{K_3} S_M^2\right) S_M^2 + 0(S_M^6) \qquad (4)$$

and [3] :

$$\int_{slab} F_{elec}(S)\, dz =$$

$$= \frac{1}{2}\left(\frac{U^2 \varepsilon_0 \varepsilon_1}{d}\right)\left[\frac{1}{d}\int_{slab} \frac{dz}{\left(1 - \frac{\Delta\varepsilon}{\varepsilon_1} S^2\right)}\right]^{-1} \qquad (5)$$

$$= \frac{1}{2}\left(\frac{U^2 \varepsilon_0 \varepsilon_1}{d}\right)\left(1 - \frac{1}{2}\frac{\Delta\varepsilon}{\varepsilon_1} S_M^2 - \frac{1}{8}\left(\frac{\Delta\varepsilon}{\varepsilon_1}\right)^2 S_M^4\right) + 0(S_M^6)$$

$\Delta\varepsilon = \varepsilon_1 - \varepsilon_2$; ε_1 and ε_2 are the dielectric constants measured parallel and perpendicular to the optical axis respectively and U is the electric potential applied to the electrodes.

In a virtual deformation with constant potential U,

$$\left(\int_{slab} F(S)\, dz\right) - \left(\int_{slab} F_{elec}(S)\, dz\right)$$

should be an extremum [3] for any variations of S_M. This requires

$$\left(1 - \frac{U^2}{U_t^2}\right) + \frac{1}{2}\left(\frac{K_1}{K_3} - \frac{\Delta\varepsilon}{\varepsilon_1}\frac{U^2}{U_t^2}\right) S_M^2 + 0(S_M^4) = 0$$

where the threshold potential value is :

$$U_t = \pi\left(\frac{K_3}{\varepsilon_0 \mid \Delta\varepsilon \mid}\right)^{1/2}. \qquad (6)$$

And for $(U - U_t)/U_t \ll 1$

$$S_M^2(U) = \frac{2(U^2 - U_t^2)}{U_t^2\left(\frac{K_1}{K_3} - \frac{\Delta\varepsilon}{\varepsilon_1}\right)}. \qquad (7)$$

Thus, we know the critical behaviour of L_1 and L_2 in the limit $U \neq U_t$.

Even in these situations, it is necessary to bear in mind that the assumption stated above does not hold when **C** is not smoothly varying. This is the reason why in section 2 we shall come back to a more general situation where S is function of z but also of x and y.

2. **Static structures of the umbilics.** — In the limit $U \neq U_t$, we want to study the point defects which appear in the slab and look like Frank defects [2]. These singular points have been called « umbilics » (Fig. 3). In contrast with Frank defects, their core is continuous, which allows for very accurate calculations. In order to describe the core, we should now consider the transverse part of the director **n** to be given by :

$$\mathbf{n}_\perp = S\mathbf{C} = a(r) \cos\left(\frac{\pi}{d} z\right) \mathbf{C}(\Phi). \qquad (8)$$

The $\mathbf{C}(\Phi)$ function will give the projected structure of the defect while $a(r)$ will describe the continuous core.

We first average the energy over the slab :

$$< F >_z = \frac{1}{d}\int_{slab} F(r, \Phi, z)\, dz.$$

Then :

$$< F_{elas} >_z = \frac{1}{4} K_1 [\text{div}\,(a\mathbf{C})]^2 + \frac{1}{4} K_2 [\text{curl}\,(a\mathbf{C})]^2 +$$

$$+ \left(\frac{\pi^2 K_3}{4 d^2}\right)\left(1 + \frac{1}{4}\frac{K_1}{K_3} a^2\right) . a^2 + 0(a^6) \qquad (9)$$

$$< F_{elec} >_z = \text{constant} + \left(\frac{\pi^2 K_3}{4 d^2}\right)\left(\frac{U^2}{U_t^2}\right) \times$$

$$\times \left(1 + \frac{1}{4}\frac{\Delta\varepsilon}{\varepsilon_1} a^2\right) a^2 + 0(a^6).$$

The only changes with section 1 concern the two first terms of $< F_{elas} >_z$. In the second order terms, we have disregarded the contribution of the r and Φ variations, these variations being smooth compare with the z variations. For a constant potential virtual deformation, $< F_{elas} >_z - < F_{elec} >_z$ should have an extreme value. In the one constant approximation ($K_1 = K_2 = K_3$), this requires for the **C** vector :

$$\Delta\mathbf{C} = \lambda\mathbf{C}. \qquad (10)$$

Equation which is equivalent to $\Delta\theta = 0$, where θ is the angle between **C** and the x axis. Thus,

$$\theta = p\Phi + \theta_0 \qquad (11)$$

p is the strength of the defect. Since **C** and $-$ **C** are not equivalent, p must be an integer (while for the screw disclinations of Frank, p may be half an integer). Keeping these solutions for **C** in the general case (*) ($K_1 \neq K_2 \neq K_3$), $a(r)$ is solution of the equation :

$$\frac{d^2 a}{dr^2} + \frac{1}{r}\frac{da}{dr} + \left(\chi^2 - \frac{1}{r^2}\right) a = \left(\frac{\chi}{a_\infty}\right)^2 a^3. \qquad (12)$$

(*) This is a rather good approximation as pointed by Frank [2].

With

$$\chi^2 K(p, \theta_0) = \left(\frac{\pi^2 K_3}{d^2}\right)\left(\frac{U^2}{U_t^2} - 1\right) ;$$

$$\left(\frac{\chi}{a_\infty}\right)^2 K(p, \theta_0) = \left(\frac{\pi^2 K_3}{2 d^2}\right)\left(\frac{K_1}{K_3} - \frac{U^2}{U_t^2}\frac{\Delta\varepsilon}{\varepsilon_1}\right) \quad (13)$$

U_t the threshold potential being defined by (6).

$K(p, \theta_0)$ being some combination of elastic constants which depends on the nature of the defect.

The eq. (12) has been previously solved numerically and the associated energy per unit length for vortex lines in helium calculated [6] (Fig. 2). The energy is roughly proportional to $K(p, \theta_0)$.

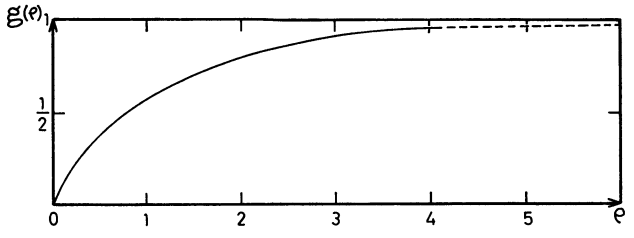

FIG. 2. — Solution of eq. (12) $g(r) = a(r)/a_\infty$; $\rho = \chi r$; a_∞ and χ are defined by eq. (13).

For umbilics $p = 1$, $\theta = \Phi + \theta_0$ and C_r and C_Φ are constant. Then, $K(1, \theta_0) = K_1 \cos^2 \theta_0 + K_2 \sin^2 \theta_0$; thus, the stable structure is

$$\theta_0 = 0 , \quad K(p, \theta_0) = K_1 \quad \text{if} \quad K_1 < K_2$$

splay umbilic (Fig. 3)

$$\theta_0 = \frac{\pi}{2}, \quad K(p, \theta_0) = K_2 \quad \text{if} \quad K_1 > K_2 \quad (14)$$

chiral umbilic (Fig. 3)

For umbilics $p = -1$,

$$K(-1, \theta_0) =$$

$$= < K_1 \cos^2 (2\Phi - \theta_0) + K_2 \sin^2 (2\Phi - \theta_0) >$$

$$= \frac{K_1 + K_2}{2}$$

and the projected structure is rather different with a higher associated energy than umbilics $p = +1$, since $(K_1 + K_2)/2$ is always larger than the smallest of K_1 and K_2.

The size ζ of the core is essentially given by :

$$\zeta = \chi^{-1} = \left(\frac{d^2 K(p, \theta_0)}{\pi^2 K_3}\right)^{1/2} \frac{U_t}{(U^2 - U_t^2)^{1/2}} \sim$$

$$\sim \left(\frac{d}{\pi}\right)\left(\frac{U_t^2}{U^2 - U_t^2}\right)^{1/2} . \quad (15)$$

The core spreads out for $U \neq U_t$ and we cannot describe the umbilics in this limit with the energy (1).

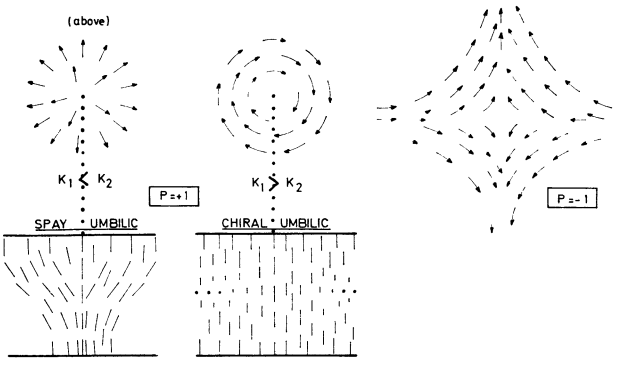

FIG. 3. — Projected structure of defects, $p = \pm 1$. The arrows indicate the different structure of the defect as we observe it from above or from below.

3. **Displacement induced by a shear flow.** — F. Brochard [4] has described the static structure of walls which can appear in the Fredericks transition of a nematic thin layer. She shows how a slight tilt of the magnetic field gets them moving to enlarge the favoured domains. We expect to find a similar displacement, of these walls or of the umbilics when a shear flow is produced in the slab since it generally removes the degeneracy between different orientations of the **C** director.

3.1 METHOD OF CALCULATION OF THE VELOCITY. — The velocity of the walls (or umbilics) can be evaluated from the energy loss by friction. We consider only the case when the defect is weakly perturbed by the flow. Then, we may still use our static results for the shape of the umbilics (or the walls). Moreover, we take into account only the z variation of the flow velocity : in the xy plane, a soft variation of the static structure should be coupled to a soft variation of the velocity. Hence, the velocity is given by the equation :

$$\eta_2 v_{\perp,zz} + \alpha_2 \frac{\partial}{\partial z}\left(\frac{\partial \mathbf{n}_\perp}{\partial t}\right) = 0 . \quad (16)$$

And for a shear flow, the velocity tensor

$$A_{ij} = \tfrac{1}{2}(v_{i,j} + v_{j,i})$$

is given by :

$$A_{zi} \neq \left(\frac{-\alpha_2}{2\eta_2}\right)\left(\frac{\partial v_i}{\partial t}\right)\left(\cos\left(\frac{\pi}{d} z\right) - \frac{2}{\pi}\right) + s\delta_{ik} \quad (17)$$

where :

$$\mathbf{n}_\perp \neq \mathbf{v} \cos\left(\frac{\pi}{d} z\right) ; \quad |\mathbf{v}| \ll 1 .$$

$s = V/2d$; V is the velocity of the upper glass surface in the k direction, the lower being at rest.

$2\eta_2 = \alpha_4 + \alpha_5 - \alpha_2$; the α_i being the Leslie coefficients of viscosity.

Then the entropy source for $| n_\perp | \ll 1$ is :

$$\int \dot{T}S \, d\tau \neq \gamma_1^* \int \left[\left(\frac{\partial n_x}{\partial t} \right)^2 + \left(\frac{\partial n_y}{\partial t} \right)^2 \right] d\tau + 4 \alpha_2 s \int \frac{\partial n_k}{\partial t} d\tau = 0 \quad (18)$$

with [4] :

$$\gamma_1^* = \gamma_1 - \frac{\alpha_2^2}{\eta_2} \left(1 - \frac{8}{\pi^2} \right). \quad (19)$$

It is clear that such a theory can only be applied in the immediate neighbourhood of U_t so that, as it is assumed, the variation of the velocity in the xy plane may be neglected.

3.2 A DIGRESSION ON WALLS. — Let us first study the case of torsional walls in a conventional Fredericks transition [4], [5]. We shall return to the more complex case of the umbilics later. With the use of the static structure calculated in reference [4] and of eq. (16) and (18), we find :

$$n_y = 0 ; \quad v_y = 0 ; \quad n_x = \theta(y - C_w t) \cos\left(\frac{\pi}{d} z \right). \quad (20)$$

And C_w, the velocity of the wall induced in the y direction by the shear flow is given by :

$$C_w = \frac{16 \alpha_2}{\pi \gamma_1^*} \frac{(\frac{3}{2}) s'}{\chi_2 a_\infty} \quad (21)$$

χ_2 and a_∞ are defined by relations (13) and s' is the projection of the shear rate s on the x direction.

Let us remark that the velocity C_w of the wall is normal to the shear inducing flow and depends upon the sign of the torsion via the sign of $\mathbf{n}$. It is also interesting to note that the effect of the shear flow on the walls can be used to balance the magnetic displacement described in [4].

3.3 EFFECT OF THE FLOW ON THE UMBILICS. — A chiral umbilic ($K_1 > K_2$) can be seen as kind of closed torsional wall. To derive the response to shear flows, the same method can be used. The static structure has been calculated in paragraph 2 : $n_r = 0$;

$$n_\Phi = a(r) \cos\left(\frac{\pi}{d} z \right)$$

where $a(r)$ is solution of eq. (12). With a shear flow in the x direction, we get from eq. (18) :

$$\gamma_1^* \int \left(\frac{\partial n_\Phi}{\partial t} \right)^2 d\tau + 4 \alpha_2 s \int \left(\frac{\partial n_x}{\partial t} \right) d\tau = 0 . \quad (22)$$

Thus the velocity C_{ch} should be in the y direction : $n_\Phi(y - C_{ch} t, x, z)$ and,

$$\gamma_1^* C_{ch} \int \left(\frac{\partial n_\Phi}{\partial r} \right)^2 \sin^2 \Phi \, d\tau + 4 \alpha_2 s \int \left(\frac{\partial n_\Phi}{\partial r} \right) \sin^2 \Phi \, d\tau = 0 . \quad (23)$$

Using reduced functions

$$g = \frac{a(r)}{a_\infty} \quad \text{and} \quad \rho = \chi_2 r , \quad \chi_2 = \chi(K(p, \theta_0) = K_2)$$

$$C_{ch} = - \left(\frac{16 \alpha_2}{\pi \gamma_1^*} \right) \left(\frac{s}{\chi_2 a_\infty} \right) \frac{\int_0^\infty \left(\frac{\partial g}{\partial \rho} \right) \rho \, d\rho}{\int_0^\infty \left(\frac{\partial g}{\partial \rho} \right)^2 \rho \, d\rho} . \quad (24)$$

The two integrals can be evaluated numerically [6] and

$$| C_{ch} | = \left(\frac{4.6 s}{\chi_2 a_\infty} \right) \left(\frac{16 \alpha_2}{\pi \gamma_1^*} \right). \quad (25)$$

The sign of the velocity changes with the sign of the torsion.

For a splay umbilic ($K_1 < K_2$), $n_\Phi = 0$ and

$$n_r = a(r) \cos\left(\frac{\pi}{d} z \right) ;$$

the velocity C_{sp} and the shear flow velocity should be in the same direction (bearing in mind that the sign of C_{sp} depends upon the sign of n_r).

$$| C_{sp} | = \frac{4.6 s}{\chi_1 a_\infty} \frac{16 \alpha_2}{\pi \gamma_1^*} . \quad (26)$$

We should note that the critical variation of the velocities C with the potential is the same for walls and umbilics ($C \propto (U^2 - U_t^2)^{-1}$).

For the room temperature nematic MBBA (at 23 °C)

$$\gamma_1 \neq 1.3 \text{ p} ; \quad \gamma_1^* \neq 1.1 \text{ p} ; \quad \alpha_2 \neq 1 \text{ p} ;$$

$$\varepsilon_1 \neq 4.7 ; \quad \varepsilon_2 \neq 5.4 .$$

Thus :

$$C \sim 10 d \left(\frac{U_t^2}{U^2 - U_t^2} \right) s$$

with $d \neq 100$ μm and

$$\left(\frac{U^2 - U_t^2}{U_t^2} \right) \neq 0.2 ,$$

$C \sim V$ (the velocity of the upper glass surface).

An easy measurable value for C is 1 μm/s.

4. **Experimental remarks.** — It should be easy to observe optically the umbilics and their displacements [5]. The shear can be produced by an oscillating glass surface. C is proportional not only to V but also to $(U^2 - U_t^2)^{-1}$ and d. Thus, choosing appropriate values for U and d, we can distinguish the velocity C of the umbilics from the shear velocity V even when they are both in the same direction. The curve $g(r) = a(r)/a_\infty$ may be deduced from optical measure-

ments applying the calculation of H. Gruler [3] to our case : The nematic liquid crystal is uniaxial and a normally incident monochromatic light beam will be split inside the slab into an ordinary and an extraordinary beam. The ordinary beam travels through the crystal with its electric field vector normal to the optical axis (**n**) and with, in the whole thickness, a constant refractive index N_0. While the extraordinary beam sees an effective refractive index given by :

$$N_{\text{eff}} = \frac{1}{d}\int_{-d/2}^{+d/2} N(z)\,\mathrm{d}z \tag{27}$$

where

$$\begin{aligned} N(z) &= N_0 N_e[N_e^2 n_z^2 + N_0^2 n_\perp^2]^{-1/2} \\ &= N_0\left[1 + \left(\frac{N_0^2 - N_e^2}{N_e^2}\right) n_\perp^2\right]^{-1/2} \end{aligned} \tag{28}$$

N_e is the extraordinary refractive index.

This gives a phase difference δ between the two transmitted beams :

$$\begin{aligned} \delta &= \frac{d}{\lambda}(N_0 - N_{\text{eff}}) \neq \left(\frac{N_0}{4\lambda}\right)\left(\frac{N_0^2 - N_e^2}{N_e^2}\right) da^2(r) \\ &= \left(\frac{N_0}{4\lambda}\right)\left(\frac{N_0^2 - N_e^2}{N_e^2}\right)(a_\infty^2\, d).g^2(r)\,. \end{aligned} \tag{29}$$

Placing the sample between crossed polarizers and illuminating with monochromatic light, one observes a black cross and concentric dark rings. Using these rings, one should evaluate the function $g(r)$.

Acknowledgments. — I have benefited from discussions with the members of Orsay Group on Liquid Crystals. I would like to acknowledge particularly the continued interest and assistance of Professor De Gennes. I take also the opportunity to thank G. Ågren for his help in the computational part of this study.

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$g(\rho)$ is solution of the equation :

$$\frac{\mathrm{d}^2 g}{\mathrm{d}\rho} + \frac{1}{\rho}\frac{\mathrm{d}g}{\mathrm{d}\rho} + \left(1 - \frac{1}{\rho^2}\right) g - g^3 = 0\,.$$

For the numerical evaluation of $g(r)$ and of the two integrals, I am indebted to G. Ågren.