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New variational problems in the statics of liquid crystals — Source link

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NEW VARIATIONAL PROBLEMS IN THE STATICS OF LIQUID CRYSTALS

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Introduction. Liquid crystals are anisotropic fluids that exhibit a preferred direction, possibly different at each place. The preferred direction is simply the *optical axis* of the material, that we describe by a unit vector $\mathbf{n}$. Most liquid crystals present different phases as the temperature varies. We restrict attention to only one of these phases: our development concerns *nematic* liquid crystals. We assume the region of space occupied by a liquid crystal as given and we denote it by $\mathcal{B}$. Thus $\mathbf{n}$ is a field of $\mathcal{B}$ onto $\mathcal{S}^2$, the unit sphere of the translation space of the three-dimensional Euclidean space $\mathcal{E}$. Formally,

$$\mathcal{B} \subset \mathcal{E} \ , \ \mathbf{n} : \mathcal{B} \to \mathcal{S}^2 \ , \ \mathcal{S}^2 := \{\mathbf{u} \in \mathcal{V} | \ |\mathbf{u}| = 1\}, \qquad \text{where } \mathcal{V} := \mathcal{E} - \mathcal{E}.$$

As $\mathcal{B}$ we take a *fit region*, that is a set which is regularly open, bounded, of finite perimeter, and of negligible boundary (see [1]). The optical axis is somehow prescribed on a part of the reduced boundary of $\mathcal{B}$:

$$\mathbf{n}|_{\mathcal{S}} = \mathbf{n}_0, \quad \mathbf{n}_0 : \mathcal{S} \to \mathcal{S}^2, \quad \mathcal{S} \subset \partial^*\mathcal{B}. \tag{1}$$

The reduced boundary $\partial^*\mathcal{B}$ of the fit region $\mathcal{B}$ is the subset of the topological boundary $\partial\mathcal{B}$ where the outer unit normal $\boldsymbol{\nu}$ to $\mathcal{B}$ is defined. Various orientations of $\mathbf{n}$ can be induced on $\partial^*\mathcal{B}$ by *rubbing* it properly.

The stable equilibrium configurations of the optical axis in a liquid crystal minimize the *free energy*, that according to FRANK's theory [2] is the functional

$$\mathcal{F}_F[\mathbf{n}] := \int_{\mathcal{B}} \sigma_F(\mathbf{n}, \nabla\mathbf{n}), \tag{2}$$

subject to (1). In (2) σ_F is the real function defined by

$$\begin{aligned} \sigma_F(\mathbf{n}, \nabla\mathbf{n}) : = k_1(\text{div } \mathbf{n})^2 + k_2(\mathbf{n} \cdot \text{curl } \mathbf{n})^2 + k_3|\mathbf{n} \wedge \text{curl } \mathbf{n}|^2 + \\ + (k_4 + k_2)(tr(\nabla\mathbf{n})^2 - (\text{div } \mathbf{n})^2), \end{aligned} \tag{3}$$

where k_1, k_2, k_3, and k_4 are constants.

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If we set $k_1 = k_2 = k_3 = \kappa_F$ and $k_4 = 0$, σ_F reduces to

$$\sigma_F = \kappa_F |\nabla \mathbf{n}|^2. \tag{4}$$

This simple formula for σ_F is to be used in this paper. The minimizers of $\mathcal{F}_F$ may possibly not be smooth mappings: in particular, they could be discontinuous somewhere in $\mathcal{B}$. The discontinuous minimizers of $\mathcal{F}_F$ are called *defects*. They take different names according to the space dimension of the sites where their discontinuities occur. For example, there are *hedgehogs*, *disclinations*, and *textures* for which the discontinuities occurs on points, lines, and surfaces, respectively. Hedgehogs and disclinations are observed quite often in ordinary liquid crystals, while textures are not. Experiments concerning textures in polymeric liquid crystals are still widely disputed (cf. e.g. [3]). FRANK's functional explains hedgehogs fairly well, but it provides a defective explanation for disclinations and none whatsoever for textures. A new mathematical theory to explain defects in a unified setting has been proposed by ERICKSEN in 1989 [4]. It is the aim of this paper to show by example the need for such a theory and the answers it provides to the problems that FRANK's theory left unsolved.

Hedgehogs. Suppose that $\mathcal{B}$ is a ball and that $\mathbf{n}_0$ is just the unit outer normal:

$$\mathbf{n}|_{\partial\mathcal{B}} = \boldsymbol{\nu}. \tag{5}$$

Here, of course, $\partial\mathcal{B} = \partial^*\mathcal{B}$. One expects that the minimizer of $\mathcal{F}_F$ subject to (5) is the radial field:

$$n_R(p) := \frac{1}{\rho(x)}(p-0), \quad \rho(x) := |p-0|, \tag{6}$$

where 0 is the center of the ball. Though this is indeed so, a rigorous proof was given only in 1986 by BREZIS, CORON and LIEB [5]. There are point defects different from that exhibited by (6), but they are set aside in this paper.

The name "hedgehog" strictly refers to any point singularity resembling 0 in (6).

Disclinations. Suppose that $\mathcal{B}$ is a circular cylinder of heigh 2ℓ and radius R:

$$\mathcal{B} = \{p \in \mathcal{E} | -\ell < (p-0)\cdot\mathbf{e}_z < \ell, \quad 0 < (p-0)\cdot\mathbf{e}_r < R\}, \tag{7}$$

where 0 is a point of $\mathcal{E}$, $\mathbf{e}_z$ is a unit vector directed along the axis of the cylinder, and $\mathbf{e}_r$ is the radial unit vector orthogonal to $\mathbf{e}_z$. We denote by z and r the coordinates of $p \in \mathcal{B}$ along $\mathbf{e}_z$ and $\mathbf{e}_r$, respectively: $z(p) := (p-0)\cdot\mathbf{e}_z$, $r(p) := (p-0)\cdot\mathbf{e}_r$. We prescribe $\mathbf{n}$ on the lateral boundary of $\mathcal{B}$ as the unit outer normal:

$$\mathbf{n}|_{\partial_R\mathcal{B}} = \mathbf{e}_r, \quad \partial_R\mathcal{B} := \{p \in \partial\mathcal{B} | r = R\}, \tag{8}$$

and we leave $\mathbf{n}$ unrestricted on the bases of $\mathcal{B}$. It is not hard to see that $\mathcal{F}_F$ attains its minimum in the class of orientations that have the form (cf. also [12]):

$$\mathbf{n} = \cos\varphi(r)\mathbf{e}_r + \sin\varphi(r)\mathbf{e}_z, \tag{9}$$

where $\varphi : [0, R] \to \left[0, \frac{\pi}{2}\right]$ is a mapping subject to

$$\varphi(R) = 0. \tag{10}$$

One expects that the minimizer of $\mathcal{F}_F$ would be the field with $\varphi \equiv 0$, which indeed is discontinuous along the axis of the cylinder. Actually, FRANK himself proved that this field solves the Euler-Lagrange equations associated to $\mathcal{F}_F$, but it possesses *infinite* energy, despite to the fact that disclinations resembling it have been often observed. This puzzle was solved by CLADIS and KLÉMAN [6] who showed that the minimizer of $\mathcal{F}_F$ is a field that lies everywhere in the plane $(\mathbf{e}_r, \mathbf{e}_z)$, it is parallel to $\mathbf{e}_z$ only along the axis of the cylinder, and it is parallel to $\mathbf{e}_r$ only on the lateral boundary of the cylinder. Formally,

$$\varphi_{CK}(r) := \frac{\pi}{2} - 2\tan^{-1}\left(\frac{r}{R}\right), \quad r \in [0, R]. \tag{11}$$

Inserting (11) into (9) yields a *continuous* field. The disclination observed in experiments should be interpreted as a sign that $|\nabla\mathbf{n}|$ attains its maximum along the axis of the cylinder, though it is everywhere finite.

All the experiments I referred to have been performed in capillary tubes (cf. e.g. [7], [8]).

Toward a new theory. The way toward a deeper understanding of disclinations in nematics did not end with the work of CLADIS and KLÉMAN. DE GENNES [9] proposed a theory to describe the change of liquid crystals into isotropic fluids that was modelled after the general theory of LANDAU for phase transitions. The *degree of orientation* s, a scalar that expresses how close a liquid crystal gets to its isotropic phase, came on the scene at that time. FAN [10] employed a degree of orientation variable in space to *tame* the singularities of $\mathbf{n}$: he allowed the liquid crystal to become isotropic wherever the classical theory predicts a singularity of $\mathbf{n}$ with infinite energy. ERICKSEN [4] has pursued FAN's line of though and has set up a general theory for both the statics and dynamics of liquid crystals with variable degree of orientation.

The new theory. The scalar s ranges in the interval $\left[-\frac{1}{2}, 1\right]$. It measures the degree of orientation of the molecules that make up the material. The molecules are elongated in our preferred direction. The lower bounds of s represents the state of microscopic order in which all molecules in a macroscopic site are orthogonal to $\mathbf{n}$, but otherwise disordered. The upper bound of s corresponds to the state of perfect microscopic order in which all molecules are parallel to $\mathbf{n}$. Both these cases are ideal: they never occur in real specimens.

In the isotropic phase of a liquid crystal $\mathbf{n}$ is deprived of any meaning: the molecules are completely disordered. The value $s = 0$ corresponds to such a microscopic state.

In the new theory s and $\mathbf{n}$ are fields defined thus:

$$s : \mathcal{B} \to \left[-\frac{1}{2}, 1\right], \quad \mathbf{n} : \mathcal{B} \setminus \mathcal{S}(s) \to \mathcal{S}^2, \tag{12}$$

where

$$\mathcal{S}(s) := \{p \in \mathcal{B} | s(p) = 0\} \tag{13}$$

is the *singular set* of the pair $(s, \mathbf{n})$. If $\mathcal{S}(s) \neq \emptyset$, we say that the pair $(s, \mathbf{n})$ is *singular*, otherwise we say that it is *regular*. The singular set of a pair $(s, \mathbf{n})$ is the set where discontinuities of $\mathbf{n}$ may occur. Thus, defects in liquid crystals are to be interpreted as *localized transitions to the isotropic phase*.

The free energy is the functional

$$\mathcal{F}_E[s, \mathbf{n}] := \int_{\mathcal{B}} \{\sigma_E(s, \nabla s, \mathbf{n}, \nabla \mathbf{n}) + \sigma_0(s)\}, \tag{14}$$

where σ_E and σ_0 are constitutive functions. I do not employ here the most general formula that ERICKSEN has proposed for σ_E in [4], I rather select a special instance of it that somehow parallels (4):

$$\sigma_E = \kappa_E\{k|\nabla s|^2 + s^2|\nabla \mathbf{n}|^2\}, \tag{15}$$

where κ_E and k are positive material moduli, both depending on the temperature T. Of course, when $s \equiv s_0$ (15) reduces to (4) with $\kappa_F = \kappa_E s_0^2$. The function σ_0 is often given the form

$$\sigma_0 = \frac{1}{2}as^2 - \frac{1}{3}bs^3 + \frac{1}{4}cs^4, \tag{16}$$

where a, b and c are non-negative moduli, of which only a depends on T. Equation (16) was derived by DOI [15] within his molecular theory for polymeric liquid crystals. The main features of σ_0 are illustrated in Figure 1 for five different values of T.

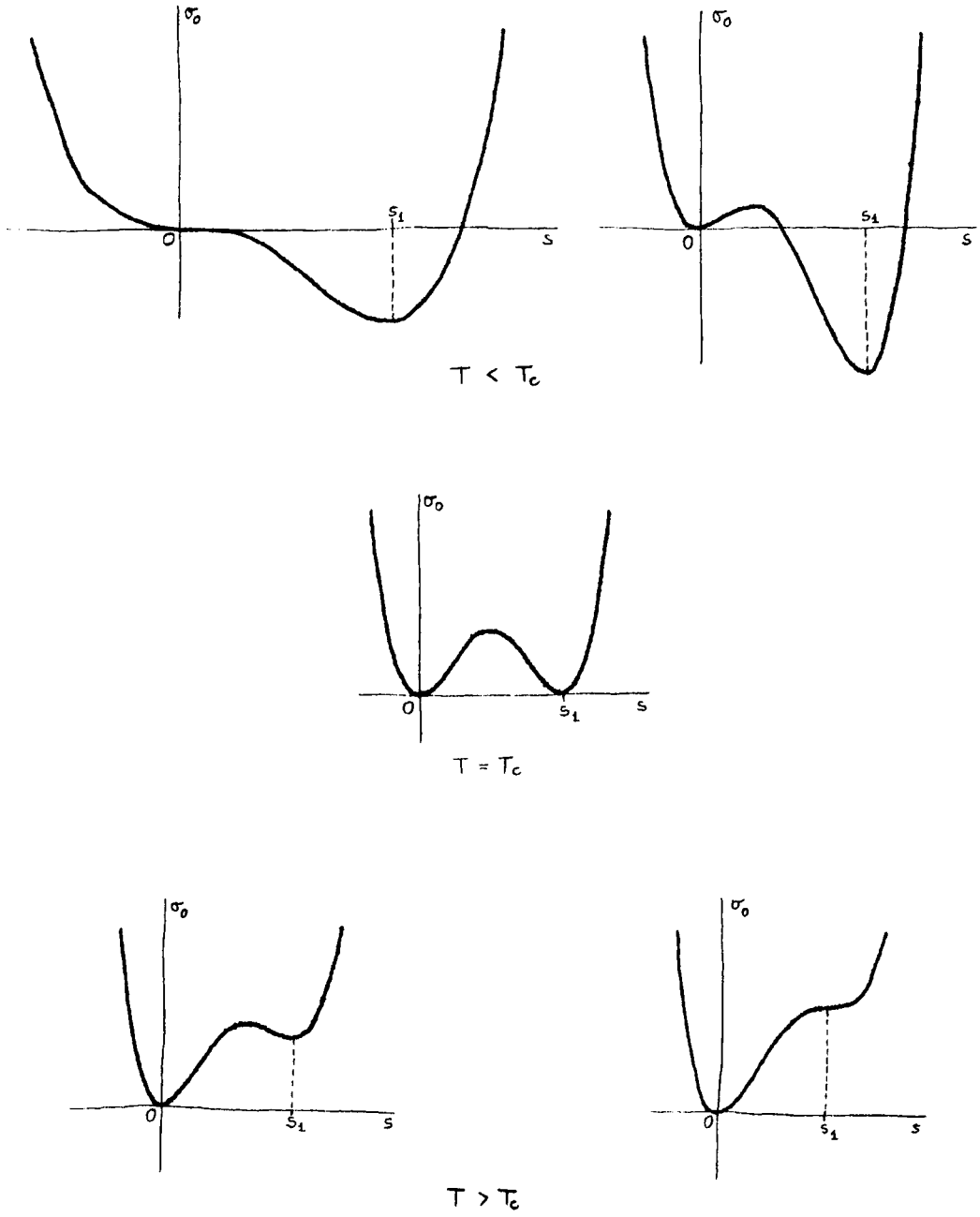

Figure 1

In the above graphs s_1 is a function of T: it is the degree of orientation of the equilibrium anisotropic phase, when both s and $\mathbf{n}$ are constant. The critical temperature T_c is the temperature above which s_1 is no longer the minimizer of σ_0.

Orders of magnitude. For ordinary liquid crystals there is experimental evidence that σ_0 prevails over σ_E by orders of magnitude (cf. [11]). Thus one should expect that the new theory systematically reduces to the classical one when $T < T_c$, since σ_0 is minimized only if $s \equiv s_1$. There are at least two objections to this conclusion. First, there is no evidence that σ_0 prevails over σ_E for polymeric liquid crystals, for which the new theory

is also, if not principally, intended. Second, if T is sufficiently close to T_c, σ_0, though prevailing over σ_E, is unlikely to dictate the value of s everywhere, since $\sigma_0(0)$ and $\sigma_0(s_1)$ do not differ much.

In any event, we feel free to explore also the variational problems that arise when σ_0 is neglected in (14).

Boundary conditions. While several methods have been devised to induce a specific orientation of $\mathbf{n}$ on $\partial^*\mathcal{B}$, there is no way that I know of to prescribe s on $\partial^*\mathcal{B}$. The problems I will review here have been solved under different hypotheses, whose sole justification is their simplicity. Thus, hedgehogs and disclinations have been accommodated into the new theory, by assuming that $s = s_1$ on $\partial^*\mathcal{B}$ or on part of it and by neglecting σ_0. Textures, which are not explained by the classical theory, are shown to fit into the new one, by *not* prescribing s on $\partial^*\mathcal{B}$ and by employing a simplified formula for σ_0.

More about hedgehogs. Let $\mathcal{B}$ be a ball of radius R whose center is 0. We prescribe $\mathbf{n}$ on $\partial\mathcal{B}$ as in (5) and, moreover, we require that

$$s|_{\partial\mathcal{B}} = s_1. \tag{17}$$

THEOREM (TORTORELLI and VIRGA [12], VIRGA [16]). *The functional*

$$\mathcal{F}_0[s, \mathbf{n}] := \int_{\mathcal{B}} \{k|\nabla s|^2 + s^2|\nabla \mathbf{n}|^2\}, \tag{18}$$

subject to $(5)_1$ *and (17), attains its minimum for* $\mathbf{n} = \mathbf{n}_R$ *(cf. (6)) and* $s(p) = s_R(\rho(p))$ *for all* $p \in \mathcal{B}$, *where* ρ *is defined as in* $(6)_2$ *and*

$$s_R(\rho) := s_1 \left(\frac{\rho}{R}\right)^{\alpha(k)}, \quad \alpha(k) := \frac{1}{2}\left(\sqrt{1 + \frac{8}{k}} - 1\right). \tag{19}$$

REMARK. *Note that* $\mathcal{S}(s) = \{0\}$ *for all values of* k.

More about disclinations. Let $\mathcal{B}$ be the cylinder defined in (7). We prescribe $\mathbf{n}$ on the lateral boundary $\partial_R\mathcal{B}$ of $\mathcal{B}$ as in $(8)_1$ and moreover, we require that

$$s|_{\partial_R\mathcal{B}} = s_1, \tag{20}$$

where $\partial_R\mathcal{B}$ is defined as in $(8)_2$.

THEOREM (TORTORELLI and VIRGA [12]). *The functional $\mathcal{F}_0$ subject to $(8)_1$ and (20) attains its minimum when* $\mathbf{n}$ *has the form (9) and $s(p)$ depends only on $r(p)$ for all $p \in \mathcal{B}$.*

THEOREM (MIZEL, ROCCATO and VIRGA [13]). *If $k \leqq 1$, $\mathcal{F}_0$ subject to $(8)_1$ and (20) is minimized by the pair*

$$\hat{s}_R(r) := s_1 \left(\frac{r}{R}\right)^{1/\sqrt{k}} \quad \text{and } \varphi = 0. \tag{21}$$

If $k > 1$, the pair that minimizes $\mathcal{F}_0$ is regular.

REMARK. *Note that the singular set of the minimizer is the axis of the cylinder for $k \leqq 1$, while it is empty for $k > 1$. FRANK's original solution for disclinations has thus been legitimazed by the new theory. For $k > 1$ the function φ that gives the minimizer of $\mathcal{F}_0$ is much like φ_{CK}, while s is far from being constant (cf. [13]). Figure 2 illustrates the minimizing s for different values of k.*

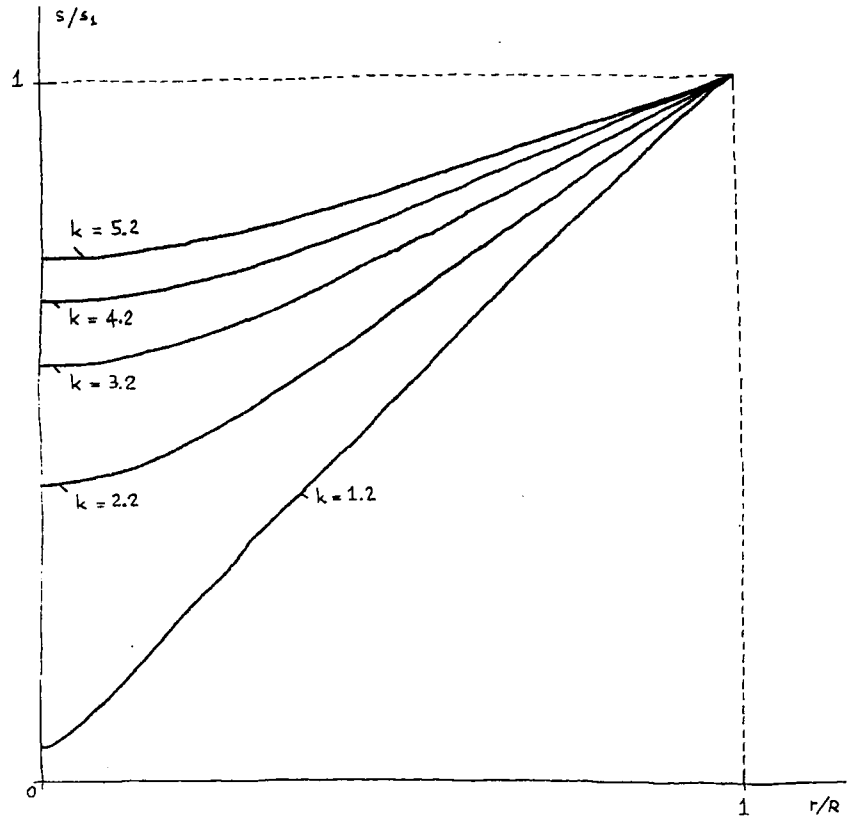

Figure 2

The graph in Figure 3 shows the minimum of $\mathcal{F}_0$ as a function of k. There the asymptothe corresponds to the value taken by $\mathcal{F}_0$ when $s \equiv s_1$ and $\varphi = \varphi_{CK}$.

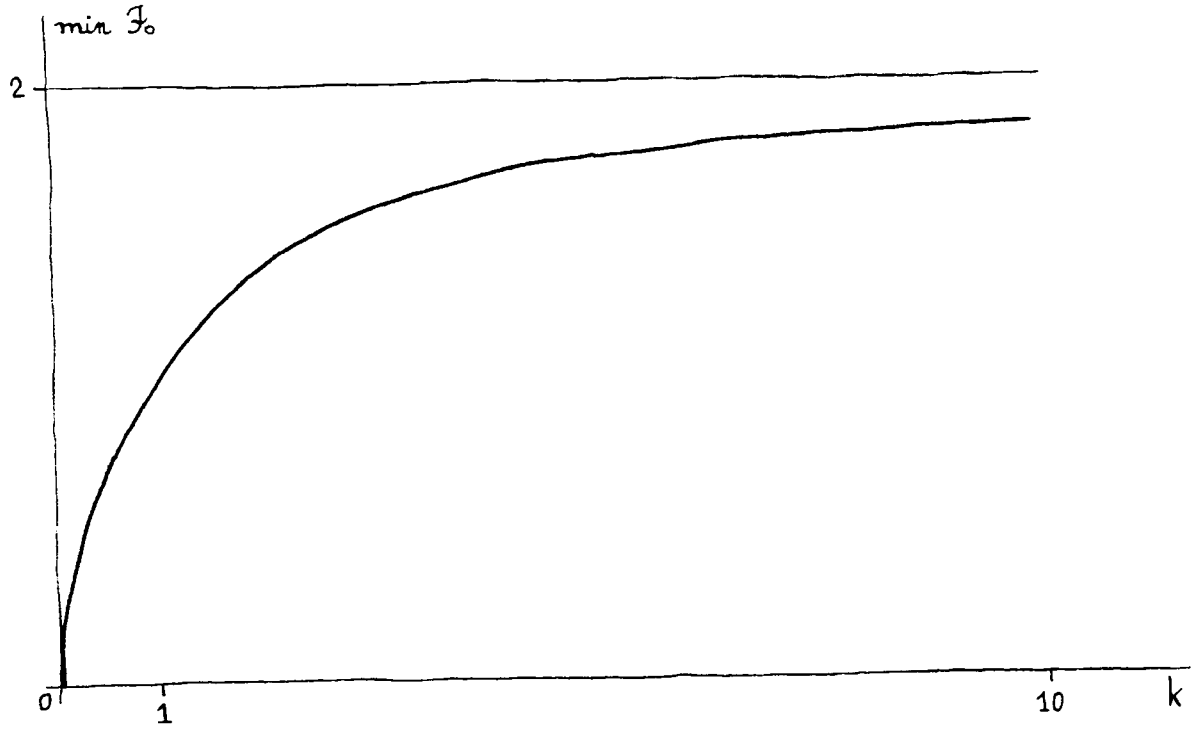

Figure 3

News about textures. It has long been known that surface defects are not explained by the classical theory. In my opinion this has deferred researchers from interpretating the defects observed in some polymeric liquid crystal as textures. By a simple example we show here that textures can indeed minimize $\mathcal{F}_E$. Let $\mathcal{B}$ be the region between two parallel plates, 2ℓ apart:

$$\mathcal{B} = \{p \in \mathcal{E} | -\ell < (p-0)\cdot\mathbf{e} < \ell, \quad 0 < (p-0)\cdot\mathbf{e}_1 < \ell_1, \quad 0 < (p-0)\cdot\mathbf{e}_2 < \ell_2\}, \tag{22}$$

where $0 \in \mathcal{E}$ and $\mathbf{e}, \mathbf{e}_1, \mathbf{e}_2$ are mutually orthogonal unit vectors. We denote by x the coordinate of p along $\mathbf{e}$: $x(p) := (p-0)\cdot\mathbf{e}$. The plates that bound $\mathcal{B}$ are at $x = -\ell$ and $x = \ell$; we call them $\mathcal{S}^-$ and $\mathcal{S}^+$, respectively. There we prescribe $\mathbf{n}$, thus:

$$\mathbf{n}|_{\mathcal{S}^-} = \cos\alpha_0\mathbf{e}_1 - \sin\alpha_0\mathbf{e}_2, \quad \mathbf{n}|_{\mathcal{S}^+} = \cos\alpha_0\mathbf{e}_1 + \sin\alpha_0\mathbf{e}_2, \tag{23}$$

where $\alpha_0 \in]-\frac{\pi}{2}, \frac{\pi}{2}[$ (see Figure 4).

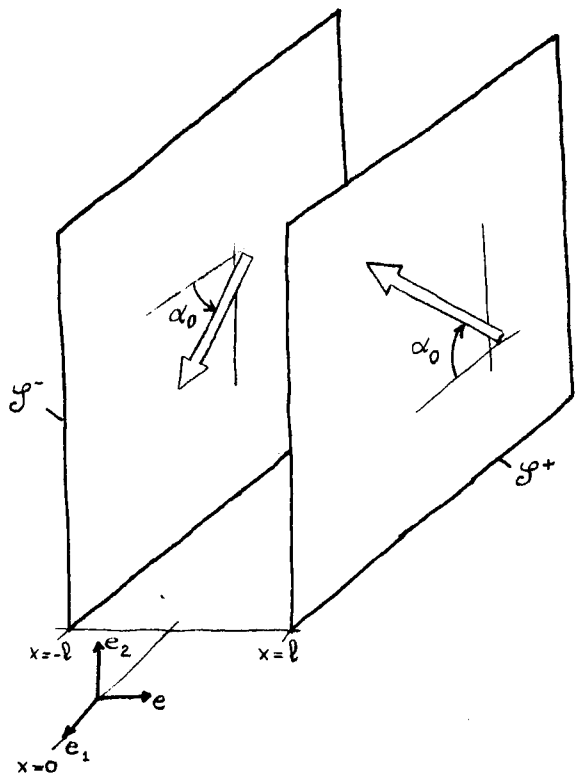

Figure 4

The degree of orientation is not prescribed on any part of $\partial^*\mathcal{B}$. For simplicity, the function σ_0 in $\mathcal{F}_E$ is replaced by

$$\psi(s) := \kappa_E h(s - s_1)^2, \tag{24}$$

where both h and s_1 are positive constants. Thus the free energy reduces to the functional

$$\mathcal{F}[s, \mathbf{n}] := \kappa_E \int_{\mathcal{B}} \{k|\nabla s|^2 + s^2|\nabla \mathbf{n}|^2 + h(s - s_1)^2\}. \tag{25}$$

THEOREM (VIRGA [14]). *The functional $\mathcal{F}$ is minimized when $s(p) = \hat{s}(x(p))$ and*

$$\mathbf{n} = \cos\alpha \mathbf{e}_1 + \sin\alpha \mathbf{e}_2, \tag{26}$$

where $\hat{s} : [-\ell, \ell] \to [-\frac{1}{2}, 1]$ is an even function such that $\hat{s}(x) \leqq s_1$ for all $x \in [-\ell, \ell]$ and $\alpha : [-\ell, \ell] \setminus \mathcal{S}(s) \to [-\frac{\pi}{2}, \frac{\pi}{2}]$ is an odd function.

THEOREM (VIRGA [14]). *For given α_0 and h, let k_c be the zero of the function*

$$f(k) := \sqrt{\frac{k}{h\ell^2}} \tanh \sqrt{\frac{h\ell^2}{k}} - \frac{\alpha_0^2}{\alpha_0^2 + h\ell^2}. \tag{27}$$

If $k \leqq k_c$, then $\mathcal{F}$ is minimized by a $\hat{s}$ vanishing at $x = 0$ and

$$\alpha(x) = \begin{cases} \alpha_0 & \text{if } x \in]0, \ell] \\ -\alpha_0 & \text{if } x \in [-\ell, 0[\end{cases}. \tag{28}$$

If $k > k_c$, then $\mathcal{F}$ is minimized by

$$\hat{s} = \frac{s_1}{1 + \frac{\alpha_0^2}{h\ell^2}} =: s_0 \quad \text{and} \quad \alpha(x) = \frac{\alpha_0}{\ell} x. \tag{29}$$

REMARK. *Note that for $k \leqq k_c$ a texture with two adjacent domains minimizes $\mathcal{F}$: $\mathbf{n}$ is constant on both sides of the mid plane $x = 0$ and jumps by the angle $2\alpha_0$ across it.*

Figure 5 shows the graph of k_c as a function of $h\ell^2$ for $\alpha_0 = \pi/2$.

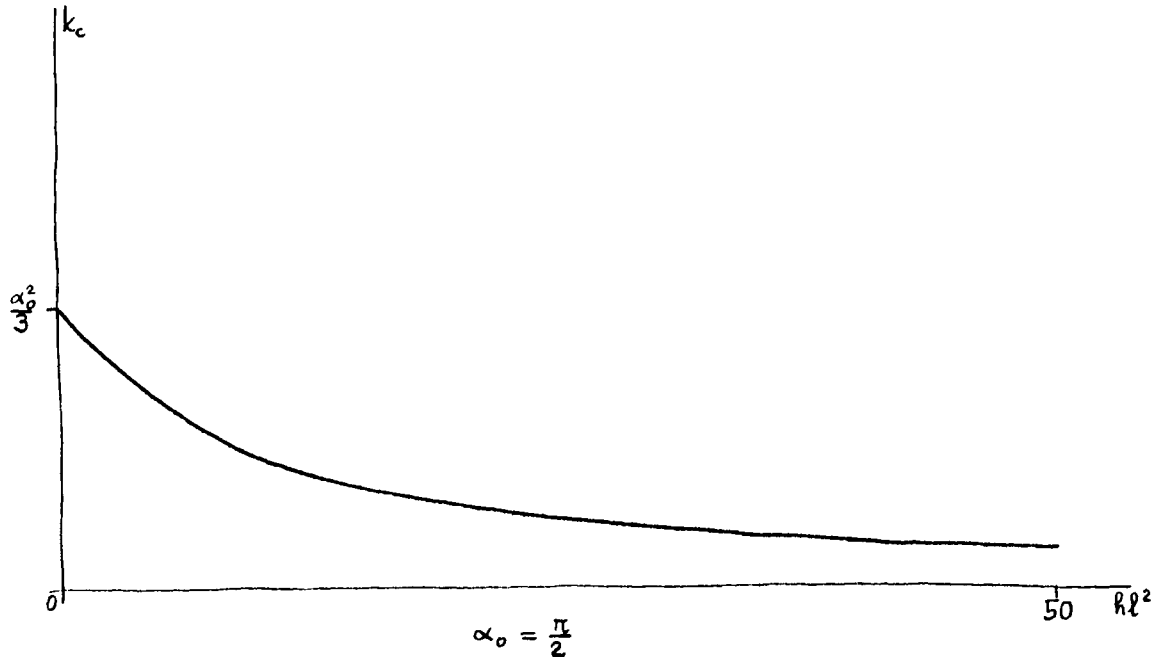

Figure 5

It is proved in [14] that $k_c = \frac{\alpha_0^2}{3}$ when $h = 0$ and $k_c \approx \frac{\alpha_0^4}{h\ell^2}$ when $h \to \infty$.

Furthermore, when $k \leqq k_c$, $\hat{s}|_{[0,\ell]}$ is an increasing function that vanishes at $x = 0$ and

$$\hat{s}(\ell) = s_1 \left\{ 1 - \sqrt{1 - \tanh^2 \sqrt{\frac{h\ell^2}{k}}} \right\}. \tag{30}$$

A computation shows that

$$s_0 < \hat{s}(\ell) \quad \text{for } k = k_c \text{ and for all } h \in [0, \infty[. \tag{31}$$

Thus, decreasing k, we cause the degree of orientation to suddenly increase at the plates, when $k = k_c$ (cf. [14] for further details).

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