Atti Accademia Nazionale Lincei Classe Scienze Fisiche Matematiche Naturali

Rendiconti Lincei
Matematica e Applicazioni

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Disclinations and hedgehogs in nematic liquid crystals with variable degree of orientation

Atti della Accademia Nazionale dei Lincei. Classe di Scienze Fisiche, Matematiche e Naturali. Rendiconti Lincei. Matematica e Applicazioni, Serie 9, Vol. **1** (1990), n.3, p. 275–280.

Accademia Nazionale dei Lincei

<http://www.bdim.eu/item?id=RLIN_1990_9_1_3_275_0>

Atti della Accademia Nazionale dei Lincei. Classe di Scienze Fisiche, Matematiche e Naturali. Rendiconti Lincei. Matematica e Applicazioni, Accademia Nazionale dei Lincei, 1990.

Rend. Mat. Acc. Lincei
s. 9, v. 1:275-280 (1990)

Fisica matematica. — *Disclinations and hedgehogs in nematic liquid crystals with variable degree of orientation.* Nota di EPIFANIO G. VIRGA, presentata (*) dal Corrisp. G. CAPRIZ.

ABSTRACT. — There is enough evidence to re-examine disclinations and hedgehogs, the singularities often observed in nematic liquid crystals, in the light of a new theory that allows for local changes in the degree of orientation.

KEY WORDS: Liquid crystals; Disclinations; Hedgehogs; Degree of orientation.

RIASSUNTO. — *Singolarità di linea e di punto in cristalli liquidi nematici con grado d'orientamento variabile.* Si esaminano le singolarità di linea e di punto, che spesso sono presenti nei cristalli liquidi, alla luce di una nuova teoria di Ericksen in cui si ammette che il grado d'orientamento del cristallo possa variare nello spazio.

THE CLASSICAL THEORY

A nematic liquid crystal is a fluid optically uniassic. The optical axis is described by a vector $\boldsymbol{n}$ of $\mathcal{S}^2$, the unit sphere of the three-dimensional Euclidean space. In the classical theory of Oseen [1] and Frank [2], the free energy of a nematic liquid crystal that occupies the region $\mathcal{B}$ is given by

$$\mathcal{F}_F[\boldsymbol{n}] := \int_{\mathcal{B}} \sigma_F(\boldsymbol{n}, \nabla \boldsymbol{n}), \tag{1}$$

where $\boldsymbol{n}: \mathcal{B} \to \mathcal{S}^2$ and

$$\sigma_F(\boldsymbol{n}, \nabla\boldsymbol{n}) := k_1(\operatorname{div}\boldsymbol{n})^2 + k_2(\boldsymbol{n}\cdot\operatorname{curl}\boldsymbol{n})^2 + k_3|\boldsymbol{n}\times\operatorname{curl}\boldsymbol{n}|^2 + \\ +(k_2+k_4)(tr(\nabla\boldsymbol{n})^2 - (\operatorname{div}\boldsymbol{n})^2), \tag{2}$$

$k_1, \dots, k_4$ being material moduli. For simplicity, in this paper I put

$$k_1 = k_2 = k_3 = \varkappa > 0, \qquad k_4 = 0. \tag{3}$$

Hence (1) becomes

$$\mathcal{F}_F[\boldsymbol{n}] := \varkappa \int_{\mathcal{B}} |\nabla \boldsymbol{n}|^2, \tag{4}$$

the formula I employ in the following for $\mathcal{F}_F$.

Moreover, I assume that the *strong anchoring* condition applies on $\partial\mathcal{B}$:

$$\boldsymbol{n}|_{\partial\mathcal{B}} = \boldsymbol{n}_0, \tag{5}$$

where $\boldsymbol{n}_0 : \partial\mathcal{B} \to \mathcal{S}^2$ is a prescribed smooth field.

(*) Nella seduta del 21 aprile 1990.

The minimizers of $\mathcal{F}_F$ subject to (5) are the *stable orientations* of the liquid crystal.

Disclinations and *hedgehogs* are singularities of $\boldsymbol{n}$ often observed in experiments. Disclination is the general name for a singularity of $\boldsymbol{n}$ occurring along a line. Hedgehog refers to a point singularity around which $\boldsymbol{n}$ is approximately radial. Hedgehogs are well explained by the classical theory, but disclinations are not quite.

Capillary tubes

Consider a capillary tube full of nematic liquid crystal, and suppose that $\boldsymbol{n}$ is parallel to the normal on the mantle of the tube. Thus in (5) we take $\boldsymbol{n}_0 = \boldsymbol{e}_r$, where $\boldsymbol{e}_r$ is the radial unit vector orthogonal to $\boldsymbol{e}_z$, the unit vector parallel to the axis of the tube. If the tube is sufficiently long, the problem is essentially two-dimensional: one expects the minimizer of (4) to be independent of z, the co-ordinate parallel to the axis. Moreover, one guesses that the stable orientation is just the planar radial field:

$$\boldsymbol{n} = \boldsymbol{e}_r . \tag{6}$$

Disclinations compatible with that exhibited by (6) along the axis of the tube have indeed been observed. Nevertheless, while (6) solves the Euler equation for $\mathcal{F}_F$, it does not even make $\mathcal{F}_F$ finite. The puzzle was solved by Cladis and Kléman [3], who showed that the stable orientation $\boldsymbol{n}$ lies everywhere in the plane $(\boldsymbol{e}_r, \boldsymbol{e}_z)$, it is parallel to $\boldsymbol{e}_z$ only along the axis of the tube, and it is parallel to $\boldsymbol{e}_r$ only on the mantle. This field is actually *continuous*: the disclination observed in experiments should be interpreted as the sign that $|\nabla \boldsymbol{n}|$ is maximum along the axis of tube, though everywhere finite.

Toward a new theory

The way toward a deeper explaination of disclinations in nematic liquid crystals did not end with the work of Cladis and Kléman. De Gennes [4, 5] 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 expressing how close a liquid crystal gets to its isotropic phase, came then on the scene. In [6] Fan employed a degree of orientation variable with position: he allowed the liquid crystal to become isotropic whenever the classical theory predicts a singularity of $\boldsymbol{n}$ with infinite energy (see also [7]). Recently, Ericksen [8] has extended Fan's remarks and set up a general theory for both statics and dynamics of liquid crystals with variable degree of orientation.

The new theory

The values of s range in the interval $]-1/2, 1[$. The lower bound of s represents the state of microscopic order in which all molecules are orthogonal to $\boldsymbol{n}$, but otherwise disordered. The upper bound of s corresponds to the state of perfect microscopic order in which all molecules lie parallel to $\boldsymbol{n}$. The isotropic phase of the liquid crystal, in which $\boldsymbol{n}$ is deprived of any meaning, corresponds to $s = 0$. In Ericksen's new theory the free energy per unit volume depends also on s and ∇s:

$$\mathcal{F}_E[s, \boldsymbol{n}] := \int_{\mathcal{B}} \sigma_E(s, \nabla s, \boldsymbol{n}, \nabla \boldsymbol{n}) \,. \tag{7}$$

I do not exploit here the general formula for σ_E (see [8]); rather, I resort to an approximation that somehow parallels (3):

$$\mathcal{F}_E[s, \boldsymbol{n}] := \varkappa s_0^{-2} \int_{\mathcal{B}} \{k|\nabla s|^2 + s^2 |\nabla \boldsymbol{n}|^2 + w_0\} \,, \tag{8}$$

where $k > 0$ and $s_0 \in]0, 1[$ are constants and $w_0 :]-1/2, 1[\rightarrow \mathbb{R}$ is a smooth function such that

$$w_0(s) = 0 \quad \text{only for} \quad s = s_0 \,, \tag{9}$$

$$\lim_{s \to -1/2} w_0(s) = \lim_{s \to 1} w_0(s) = +\infty \,. \tag{10}$$

Besides (5) I impose the boundary condition

$$s|_{\partial \mathcal{B}} = s_0 \,. \tag{11}$$

It follows from (8), (4), and (11) that

$$\mathcal{F}_E[s_0, \boldsymbol{n}] = \mathcal{F}_F[\boldsymbol{n}] \,. \tag{12}$$

Thus the new theory reduces to the old when the degree of orientation reduces to a constant.

An approximation

Another boundary condition for s has sofar been considered:

$$\left.\frac{\partial s}{\partial \nu}\right|_{\partial \mathcal{B}} = 0 \,, \tag{13}$$

where ν denotes the outer unit normal to $\partial \mathcal{B}$ (see *e.g.* [9] and [10]). I employ (11) instead of (13), because, the former, unlike the latter, is compatible with neglecting w_0 in (8), which simplifies the analysis a great deal. In fact, if (13) is imposed on s and w_0 is neglected in (8), $\mathcal{F}_E$ is minimum for $s \equiv 0$ and arbitrary $\boldsymbol{n}$, that is when $\mathcal{B}$ is full of the isotropic phase.

Of course, whether to neglect w_0 it is not merely a question of convenience. Regardless of the boundary condition for s, this approximation should also base on physical grounds. When w_0 prevails over $s^2 |\nabla \boldsymbol{n}|^2$, by (9), $\mathcal{F}_E$ is minimum only if $s \equiv s_0$; hence, by (12), the classical theory need not be emended; conditions (11) and (13) are both satisfied. This is not the case for many polymeric liquid crystals. Apart from an opinion, I produce an indirect reason that is supported by repeated observations of *domains* (see [11] and [12]). Domains are adjacent regions with different values of $\boldsymbol{n}$, separated by surfaces that are likely to consist of the isotropic phase. It has long been known that domains are not compatible with the classical theory. Hence for polymers we may exclude that w_0 prevail over $s^2 |\nabla \boldsymbol{n}|^2$. Accordingly, it is not a too crude approximation to neglect w_0, provided (11) is enforced. Under these hypotheses, for a special boundary-value problem Ambrosio and I [13] have predicted domains when k is less than a critical value.

Henceforth $\mathcal{F}_E$ will be the functional

$$\mathcal{F}_E[s, \boldsymbol{n}] := \varkappa s_0^{-2} \int_{\mathcal{B}} \{k|\nabla s|^2 + s^2 |\nabla \boldsymbol{n}|^2\}, \tag{14}$$

subject to (5) and (11).

Disclinations

I wish to re-examine within the new theory the problem of finding the stable orientation of a nematic liquid crystal in a capillary tube. Let R be the radius of the tube. We take $\boldsymbol{n}$ as

$$\boldsymbol{n} = \cos\varphi \boldsymbol{e}_r + \sin\varphi \boldsymbol{e}_z, \tag{15}$$

where φ depends only on r, the radial co-ordinate, and satisfies

$$\varphi(R) = 0. \tag{16}$$

Accordingly, we assume that s depends only on r and

$$s(R) = s_0. \tag{17}$$

Thus, it follows from (14) that the free energy per unit length of the tube is

$$\mathcal{F}_d[s, \varphi] := 2\pi\varkappa s_0^{-2} \int_0^R \{ks'^2 + s^2(\varphi'^2 + \cos^2\varphi/r^2)\}\, r dr. \tag{18}$$

In a forthcoming paper [14] Mizel, Roccato and I study in detail the minimizers of $\mathcal{F}_d$ subject to (16) and (17). Here I show only that for k sufficiently small the new theory provides a better understanding of disclinations in capillary tubes. Precisely, we shall see that for $k < 4$ there is a solution of the Euler equations for $\mathcal{F}_d$ that resembles (6) and possesses less energy than the solution found by Cladis and Kléman.

The Euler equations for $\mathcal{F}_d$ are

$$k(rs')' = sr(\varphi'^2 + \cos^2\varphi/r^2), \tag{19}$$

$$(rs^2\varphi')' = -s^2 r^{-1} \cos\varphi \sin\varphi. \tag{20}$$

Clearly $\varphi \equiv 0$ solves (20) and (16); then (19) becomes

$$k(rs'' + s') = s/r \tag{21}$$

There is only one solution of (21) and (17) bounded in $[0, R]$:

$$\hat{s}(r) = s_0 (r/R)^{1/\sqrt{k}}. \tag{22}$$

For $s = \hat{s}$ and $\varphi \equiv 0$ (18) yields

$$\mathcal{F}_d[\hat{s}, 0] = 2\pi\varkappa\sqrt{k}. \tag{23}$$

On the other hand, the solution of Cladis and Kléman reads (see [3])

$$\begin{cases} \hat{\varphi}(r) = 2 \operatorname{arctg} r/R - \pi/2 \\ s \equiv 0; \end{cases} \tag{24}$$

its energy is

(25) $$\mathcal{F}_d[s_0, \hat{\varphi}] = 4\pi\varkappa .$$

Thus

(26) $$\mathcal{F}_d[\hat{s}, 0] \leqslant \mathcal{F}_d[s_0, \hat{\varphi}] \quad \text{if and only if} \quad k \leqslant 4 .$$

Since (24) does not solve eqs. (19) and (20), (26) simply proves that the pair $(\hat{s}, 0)$ fails to minimize $\mathcal{F}_d$ when $k > 4$. The argument illustrated above is merely heuristic. In [14] Mizel, Roccato and I prove that a solution of (19) and (20) sharing many qualitative features of (24) minimizes $\mathcal{F}_d$ for $k > 1$, and that $(\hat{s}, 0)$ minimizes $\mathcal{F}_d$ for $k < 1$.

Hedgehogs

Now I turn attention to hedgehogs. Suppose that $\mathcal{B}$ is a ball of radius R and that on $\partial\mathcal{B}$ $\boldsymbol{n}$ is parallel to the normal. It is easy to see that the spherical radial field

(27) $$\boldsymbol{n} = \boldsymbol{e}_\rho$$

solves the Euler equations for $\mathcal{F}_F$. A few years ago Brezis, Coron and Lieb [15] proved that (27) actually minimizes $\mathcal{F}_F$. In the light of the above remarks about disclinations, a question comes naturally: *Do* $\boldsymbol{n} = \boldsymbol{e}_\rho$ *and* $s \equiv s_0$ *minimize* $\mathcal{F}_E$? We see now that the answer is *no.*

Taking $\boldsymbol{n}$ as in (27) and assuming that s depends only on ρ, the spherical radial coordinate, and

(28) $$s(R) = s_0 ,$$

we give (14) the form

(29) $$\mathcal{F}_e[s] := 4\pi\varkappa s_0^{-2} \int_0^R \{k\rho^2 s'^2 + 2s^2\}\, d\rho .$$

The Euler equation for $\mathcal{F}_e$ is

(30) $$k(\rho^2 s')' = 2s .$$

There is only one solution of (30) and (28) bounded in $[0, R]$:

(31) $$\tilde{s}(\rho) = s_0 (\rho/R)^{\alpha(k)} \quad \text{where} \quad \alpha(k) = (\sqrt{1 + 8/k} - 1)/2 .$$

The energy of this solution is

(32) $$\mathcal{F}_e[\tilde{s}] = 4\pi\varkappa R f(k) \quad \text{where} \quad f(k) = k\alpha(k) .$$

On the other hand, if $s \equiv s_0$ (29) yields

(33) $$\mathcal{F}_e[s_0] = 8\pi\varkappa R .$$

Since $f(k) < 2$ for all $k > 0$, it follows from (32) and (33) that

(34) $$\mathcal{F}_e[\tilde{s}] < \mathcal{F}_e[s_0] .$$

Thus (27) does not minimize $\mathcal{F}_E$.

Conclusion

We have learnt that in nematic liquid crystals with variable degree of orientation a disclination may consist of the isotropic phase and may not, according to the value of k, but a hedgehog does always consist of the isotropic phase, irrespective of k.

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