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Twisting of liquid crystals

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We discuss a one-parameter family of general solutions of the hydrostatic equations for liquid crystals. For certain values of the parameter, the energy may take on extremal values. We discuss special features of such solutions. Configurations similar to those considered naturally occur in liquid crystals of cholesteric type, suggesting that some such state has a relatively low energy.

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1. Introduction

Generally, liquid crystal molecules are large and relatively rigid, one dimension being large compared with the others. In the phases to be considered, the molecules tend to be parallel to their neighbours, being relatively free to move so as to maintain the parallelism. Many unusual phenomena observed in them are discussed by Brown & Shaw (1957). Continuum theories of these involve a vector field $\mathbf{h}(\mathbf{x})$; loosely, the direction of the molecular axis. We assume, as is customary, that the length of $\mathbf{h}$ is invariable,

$$\mathbf{h}.\mathbf{h} = 1, \tag{1.1}$$

and that these liquids are incompressible. We consider the hydrostatic theory, as presented by Ericksen (1962*a*). We exclude the so-called smectic state, for which the equations to be used are inappropriate. The theory involves a stored energy function W, interpretable as Helmholtz free energy per unit volume, of the form

$$W = W(\mathbf{h}, \nabla\mathbf{h}). \tag{1.2}$$

It is subject to the condition that it be unaffected by rigidly rotating the material. Formally,

$$W(\mathbf{R}\mathbf{h}, \mathbf{R}\nabla\mathbf{h}\mathbf{R}^T) = W(\mathbf{h}, \nabla\mathbf{h}), \tag{1.3}$$

where $\mathbf{R}$ is any rotation matrix,

$$\mathbf{R}^{-1} = \mathbf{R}^T, \quad \det\mathbf{R} = 1. \tag{1.4}$$

As is discussed by Ericksen (1961), this implies that

$$A_{ij} \equiv h_i \frac{\partial W}{\partial h_j} + h_{i,k}\frac{\partial W}{\partial h_{j,k}} + h_{k,i}\frac{\partial W}{\partial h_{k,j}} = A_{ji}. \tag{1.5}$$

Further, derivatives of W with respect to its arguments transform as tensors of obvious type. For liquid crystals of nematic or cholesteric type, as defined, for example, by Frank (1958), $\mathbf{h}$ is physically indistinguishable from $-\mathbf{h}$, so

$$W(\mathbf{h}, \nabla\mathbf{h}) = W(-\mathbf{h}, -\nabla\mathbf{h}). \tag{1.6}$$

Liquid crystals of nematic type are further distinguished by the fact that (1.4) can be replaced by

$$\mathbf{R}^{-1} = \mathbf{R}^{T}, \quad \det \mathbf{R} = \pm 1, \tag{1.7}$$

these consisting of molecules which are symmetric with reflexions in planes parallel and perpendicular to **h**, or of racemic mixtures of asymmetric molecules. Possibly because of physical considerations mentioned by Frank (1958), the mathematical theory of cases consistent with (1.6) has received most attention.

In terms of W, the stress tensor **t**, generally asymmetric, is given by

$$t_{ij} = -p\delta_{ij} - w_{kj} h_{k,i}, \tag{1.8}$$

where

$$w_{kj} = \partial W / \partial h_{k,j} \tag{1.9}$$

and p is an arbitrary pressure. It can be considered as a Lagrangian multiplier, introduced because of the constraint of incompressibility.

As might be expected from the fact that **t** is asymmetric, there is a couple stress tensor **l**, given by

$$l_{ik} = e_{ijm} h_j w_{mk}. \tag{1.10}$$

Clearly

$$l_{ik} h_i = 0; \tag{1.11}$$

that is, the couple stress vector acting on any surface is perpendicular to **h**.

We assume there are no external body forces, in which case the equilibrium equations are

$$t_{ik,k} = 0, \tag{1.12}$$

$$w_{ik,k} - (\partial W / \partial h_i) = \lambda h_i, \tag{1.13}$$

λ being an arbitrary scalar, a Lagrangian multiplier corresponding to the constraint (1.1). Here (1.11) can be satisfied by satisfying (1.13) and setting

$$p + W = a = \text{const.} \tag{1.14}$$

Then (1.1) and (1.13) yield four equations in the four unknowns **h** and λ.

As is mentioned by Ericksen (1962*b*), it is straightforward to obtain a general solution of (1.3), giving W as an essentially arbitrary function of certain invariants of **h** and $\nabla\mathbf{h}$. Using this, one could, in a straightforward way, verify the solution to be presented. We employ a different approach, which seems briefer.

2. The solution

What we wish to show is that a field of the form

$$\mathbf{h} = (\cos\theta, \sin\theta, 0), \tag{2.1}$$

$$\theta = bx_3 + c \tag{2.2}$$

is a solution, b and c being arbitrary constants. The parameter c is of no great import, but introducing it facilitates analysis. For analysis, we assume $b \neq 0$. We still have a solution for $b = 0$, when $\mathbf{h} = \text{const}$. To verify this, it suffices to consider W linear in $\nabla\mathbf{h}$. Such forms are special cases of the forms considered by Frank (1958).

From (1.2), W reduces to a function of

$$\theta = bx_3 + c, \quad \theta' = d\theta / dx_3 = b. \tag{2.3}$$

Changing c amounts to applying a rotation about the x_3-axis, so (1.3) implies that W is independent of c. This is equivalent to saying that it is independent of θ, so

$$W = f(b) = \text{const.} \tag{2.4}$$

Similarly, the scalar

$$u = h_{i,j}(\partial W/\partial h_{i,j}) = h_i'(\partial W/\partial h_{i,3}) = u(b) = \text{const.} \tag{2.5}$$

Thus

$$\left(W - h_i'\frac{\partial W}{\partial h_{i,3}}\right)' = \left[\frac{\partial W}{\partial h_i} - \left(\frac{\partial W}{\partial h_{i,3}}\right)'\right] h_i' = 0. \tag{2.6}$$

Similarly,

$$\partial W/\partial h_{3,3} = g(b), \tag{2.7}$$

this quantity transforming as a scalar under such rotations. By considering 180° rotations about the x_3-axis, we see that

$$\partial W/\partial h_3 = k(\mathbf{h},\mathbf{h}') = k(-\mathbf{h}, -\mathbf{h}'). \tag{2.8}$$

On the other hand, 180° rotations about an axis parallel to $\mathbf{h}'$ yield

$$\partial W/\partial h_3 = k(\mathbf{h},\mathbf{h}') = -k(-\mathbf{h}, -\mathbf{h}'). \tag{2.9}$$

From (2.7), (2.8) and (2.9),

$$(\partial W/\partial h_{3,3})' = \partial W/\partial h_3 = 0. \tag{2.10}$$

From (2.6) and (2.10), there is some scalar λ such that

$$\left(\frac{\partial W}{\partial h_{i,j}}\right)_{,j} - \frac{\partial W}{\partial h_i} = \left(\frac{\partial W}{\partial h_{i,3}}\right)' - \frac{\partial W}{\partial h_i} = \lambda h_i, \tag{2.11}$$

the vector on the left being perpendicular to $\mathbf{h}'$ and the x_3-axis, both of which are perpendicular to $\mathbf{h}$. This suffices to show that $\mathbf{h}$ is a solution.

It is of interest to determine the forms of the stress and couple stress tensors. For simplicity, we henceforth restrict our attention to cases where (1.6) applies, so that, generally

$$\frac{\partial W}{\partial h_i}(\mathbf{h},\nabla\mathbf{h}) = -\frac{\partial W}{\partial h_i}(-\mathbf{h}, -\nabla\mathbf{h}), \quad \frac{\partial W}{\partial h_{i,k}}(\mathbf{h},\nabla\mathbf{h}) = -\frac{\partial W}{\partial h_{i,k}}(-\mathbf{h}, -\nabla\mathbf{h}). \tag{2.12}$$

Now

$$v_i = \epsilon_{ijk}\frac{\partial W}{\partial h_{m,k}}h_{m,j} = \epsilon_{i3k}\frac{\partial W}{\partial h_{m,k}}h_m' = v_i(\mathbf{h},\mathbf{h}') \tag{2.13}$$

is unaffected if the signs of $\mathbf{h}$ and $\mathbf{h}'$ be reversed. Such a change, combined with a 180° rotation about the x_3-axis, leaves $\mathbf{h}$ and $\mathbf{h}'$ unaltered, but should take $\mathbf{v} \to -\mathbf{v}$. Thus

$$\mathbf{v}(\mathbf{h},\mathbf{h}') = -\mathbf{v}(\mathbf{h},\mathbf{h}') = 0. \tag{2.14}$$

By essentially the same argument,

$$\epsilon_{i3k}(\partial W/\partial h_{m,k})\,h_m = 0. \tag{2.15}$$

From (2.13) and (2.15), it follows easily that

$$\frac{\partial W}{\partial h_{1,1}} = \frac{\partial W}{\partial h_{1,2}} = \frac{\partial W}{\partial h_{2,1}} = \frac{\partial W}{\partial h_{2,2}} = 0. \tag{2.16}$$

For this, the assumption (1.6) is important, as can be seen by considering a W proportional to $\nabla . \mathbf{h}$.

By essentially the same argument used to obtain (2.8) and (2.9), we find that

$$(\partial W/\partial h_{3,i})\,h_i = (\partial W/\partial h_{i,3})\,h_i = 0. \tag{2.17}$$

Turning to (1.5), we find, using (2.10) and (2.16), that

$$\partial W/\partial h_{3,3} = 0. \tag{2.18}$$

Using (1.8), (1.9), (1.14), (2.4), (2.5) and (2.16), we find that the stress tensor is given by

$$\mathbf{t} = -p\mathbf{1} + \left\|\begin{matrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -u(b) \end{matrix}\right\|, \tag{2.19}$$

where p is an arbitrary constant. Thus, for these solutions, it is symmetric and constant, consisting of a hydrostatic pressure superposed on a uni-axial tension or compression in the direction of the x_3-axis.

Now (2.17) and (2.18) imply that, for some choice of α and β,

$$\partial W/\partial h_{3,i} = \alpha h'_i, \quad \partial W/\partial h_{i,3} = \beta h'_i. \tag{2.20}$$

Using (2.1), (2.2) and (2.5)

$$u(b) = \beta \mathbf{h}'.\mathbf{h}' = \beta b^2. \tag{2.21}$$

Similarly, α, transforming as a scalar under rotations about the x_3-axis, depends only on b. Using (1.10) to calculate the couple stress tensor, we find that

$$\left.\begin{aligned} bl_{11} &= -\alpha b^2 \sin^2\theta = -\alpha (h'_1)^2, \\ bl_{12} &= bl_{21} = \alpha b^2 \sin\theta\cos\theta = -\alpha h'_1 h'_2, \\ bl_{22} &= -\alpha b^2 \cos^2\theta = -\alpha (h'_2)^2, \\ l_{13} &= l_{23} = l_{32} = l_{31} = 0, \\ bl_{33} &= \beta b^2 = u(b), \end{aligned}\right\} \tag{2.22}$$

or, more briefly,

$$bl_{ij} = -\alpha h'_i h'_j + u(b)\,\delta_{i3}\,\delta_{j3}. \tag{2.23}$$

On the planes $x_3 = \text{const.}$, the couple stress vector thus is in the direction of the x_3-axis. It is noteworthy that it, the twist per unit length b, and the uni-axial stress $u(b)$, are simply related by (2.22), independent of the form of W. Intuitively, it seems natural to think of the couple l_{33} as producing the twist, the accompanying normal stress being loosely similar to that occurring in torsion of non-linear elastic or viscoelastic materials. For cylindrical surfaces with generators parallel to the x_3-axis, the couple stress vector is, as always, perpendicular to $\mathbf{h}$, also perpendicular to the x_3-axis. It will vanish on planes with $\mathbf{h}$ as normal and be greatest on planes perpendicular to this. Intuitively, it would seem that the effect of releasing this would be to produce curvature in the planes $x_3 = \text{const.}$ in which $\mathbf{h}$ lies.

By considering special forms of W of the type

$$W = f_1(\mathbf{h}.\nabla\times\mathbf{h}) + f_2(\mathbf{h}.\nabla\times\mathbf{h})\,h_{i,j}h_{j,i}, \tag{2.24}$$

it can be seen that α and u can be essentially arbitrary functions of b for liquid crystals of cholesteric type. For liquid crystals of nematic type, $x_3 \to -x_3$ is an admissible symmetry transformation. It then follows that, for this type,

$$\left.\begin{aligned} W &= f(b) = f(-b), \\ \alpha(b) &= \alpha(-b), \quad u(b) = u(-b). \end{aligned}\right\} \tag{2.25}$$

3. Extremal twists

The solutions considered are especially simple when b is such as to give W an extremal value, so that

$$dW/db = 0. \tag{3.1}$$

We call such twists *extremal*. For liquid crystals of nematic type, (2.25) implies that $b = 0$ is extremal. Physically, there is some reason to think that W is then a minimum. That is, these seem to occur naturally in configurations where $\mathbf{h}$ is nearly constant. Within the context of the Oseen–Frank theory, which presumes W to be quadratic in $\nabla\mathbf{h}$, Ericksen (1966) derives corresponding inequalities to be satisfied by moduli. Not infrequently, the uniform pattern is marred by imperfections, involving lines on which $\mathbf{h}$ is undefined, surrounded by regions in which $\mathbf{h}$ varies rapidly. These are discussed by Frank (1958).

Liquid crystals of cholesteric type naturally occur in orientation patterns which, at least locally, resemble those here described. The value of the naturally occurring twist seems to be characteristic of a given material, though it is influenced by such factors as temperature and concentration of solutions. For various polypeptide solutions, Robinson, Ward & Beevers (1958) report observations in which the order of magnitude of b ranges from zero to $10^3\,\text{cm}^{-1}$. In data which I have seen for other materials, e.g. those of Cano & Chatelain (1964), values of the order of $10^5\,\text{cm}^{-1}$ seem more common. In the observed patterns, surfaces corresponding to the planes $x_3 = \text{const.}$ sometimes have appreciable curvature.

At least tentatively, it would seem reasonable to identify the twist with an extremal twist for which the energy is a relative minimum. Since the comparison is with similarly twisted states alone, this leaves open the possibility that there are orientation patterns, not included among the solutions here considered, with still lower energy. The problem of settling stability questions of this general type is interesting, but beyond the scope of this investigation.

For analysis of extremal twists, we again assume $b \neq 0$. Considering W as a function of $\mathbf{h}$ and $\nabla\mathbf{h}$, we have

$$\frac{\partial W}{\partial h_i}\frac{\partial h_i}{\partial b} + \frac{\partial W}{\partial h_{i,3}}\frac{\partial h_i'}{\partial b} = 0,$$

where

$$b\,\partial h_i/\partial b = b x_3\, dh_i/d\theta = x_3 h_i',$$

$$b\frac{\partial h_i'}{\partial b} = b\frac{\partial}{\partial b}\left(\frac{dh_i}{d\theta}b\right) = b\frac{dh_i}{d\theta} + b^2 x_3\frac{d^2h_i}{d\theta^2}$$

$$= h_i' + x_3 h_i''.$$

Thus (3.1) gives

$$x_3\left[\frac{\partial W}{\partial h_i}h_i' + \frac{\partial W}{\partial h_{i,3}}h_i''\right] = -\frac{\partial W}{\partial h_{i,3}}h_i' = -u$$

$$= x_3 W' = 0. \tag{3.2}$$

Thus, for the extremal twists, the stress reduces to a uniform hydrostatic pressure and the planes $x_3 = \text{const.}$ are free of couple stress. Whether other surfaces are free of couple stress depends on the form of W, as can be seen by studying special forms of W, e.g. those given by (2.24). Intuitively, one might expect that relaxing such couples would tend to lower the energy. However, it seems difficult to make any precise statements about this.

Analytically, it is clear that the twist need not be extremal. It is well known that solid single crystals, in contact with liquid crystals, tend to produce a definite orientation in the liquid near the interface. In some cases at least, **h** is tangent to a plane interface, on which it is essentially uniform. By using pairs of single crystals as wrenches, one might thus produce a range of values of the twist.

As far as I know, there are no static measurements of stress or couple stress in liquid crystals. Until this is done, contact between theory and experiment will remain rather tenuous.

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