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Résumé. — Un champ tridirectionnel est employé comme modèle pour un fluide général anisotrope. La densité de l'énergie élastique est décrite par un polynôme invariant dans les composantes du tenseur de torsion. Les termes de l'énergie de surface sont dérivés à l'aide des conditions de compatibilité pour le champ tridirectionnel. Le modèle est appliqué aux cholestériques de pas grand et petit, pour $^3$He-A, et pour les nématiques biaxes.

Abstract. — A tripod field is used as model for a general anisotropic fluid. The elastic energy density is expanded as invariant polynomial in the components of the contortion tensor. Surface energy terms are derived from compatibility conditions for the tripod field. The model is applied to cholesteric liquid crystals of large and small pitch, to $^3$He-A, and to biaxial nematic liquid crystals.

1. Introduction. — The elastic energy density due to curvature strain was formulated phenomenologically by Frank [1] for a directional medium of local axial symmetry. In the present work, the elastic energy density for mesomorphic phases of continuous translational symmetry, but arbitrarily broken rotational symmetry is established. Following Kléman’s proposals [2], I first consider a medium of orthonormal tripods. As in the early papers of Cosserat [3], the contortion tensor is used as measure for curvature strain. The elastic energy density is expressed as polynomial in the components of this tensor of correct local point symmetry. In the absence of defects, the contortion tensor must satisfy compatibility conditions. It is these conditions which allow to express part of the energy density as divergence of a vector field, resulting in surface terms or ‘nilpotent energies’. In case of constant boundary conditions the tripod field carries a topological quantum number, the degree of the mapping, which is proportional to the volume integral over the determinant of the contortion tensor. The theory is applied to cholesteric liquid crystals, where for large pitch it yields the Frank energy [1], for small pitch Volovik’s large scale continuous theory of cholesterics [4], and to $^3$He-A. For the elastic energy of the recently discovered biaxial liquid crystals [5], 12 bulk elastic constants are required.

2. Elastic energy density. — The directional medium is described by a field of orthonormal frames $(\hat{b}_1(x), \hat{b}_2(x), \hat{b}_3(x))$. Each tripod is obtained from a fixed triad of orthonormal vectors $(\hat{e}_1, \hat{e}_2, \hat{e}_3)$ by a rotation:

$$\hat{b}_i(x) = \hat{e}_i R_j^i(x),$$

(1)

where $R$ is an orthogonal $3 \times 3$-matrix. Summation over repeated indices is assumed implicitly. As measure for curvature strain serves the contortion tensor $K$ of components

$$K_{ij} = \frac{1}{2} \epsilon_{ijk} R_{jk}^l \partial_l R_{ki};$$

(2)

$\epsilon_{ijk}$ are the components of the completely antisymmetric third rank tensor. $K$ contains all information about changes of the tripod field in linear approximation; when proceeding from $x$ to $x + \Delta x$, the vectors $\hat{b}_i$ are rotated by the axial vector $\Omega$ of components $\Omega_i = \Delta x_i K_{ij}$, so that $\Delta \hat{b}_i = \Omega \times \hat{b}_i$.

When no defects are present, the contortion tensor is restricted by the condition

$$\oint db_i = \oint \Omega \times b_i = 0$$

(3)

for integration about any closed contour. Here the components of $\Omega$ are differential forms

$$\Omega_j = dx_i K_{ij}.$$  

(4)

After application of Stokes’ theorem this leads to the compatibility conditions (see for instance [2])

$$J_{ikmn} = \epsilon_{ilm} (K_{kl,j} - K_{lj,k}) + (K_{km} K_{ln} - K_{ln} K_{km}) = 0.$$  

(5)
In case of a weakly distorted anisotropic fluid, the elastic energy density $F(x)$ is formulated as polynomial in the components of $K$. For simplicity, higher order derivatives, as in the work of Nehring and Saupe [6], will not be included here. This polynomial must be invariant under the operations of the point group of the medium, applied about $x$, the symmetry axes depending on the moving frame. Therefore it is convenient to write the polynomial in terms of components

$$H_{rs} = K_{ij} R_{ir} R_{js}$$

of $K$ in the moving frame, and to compose it of linearly independent homogeneous invariant polynomials $p_n^m(H_{rs})$ of degree $q$:

$$F(x) = \sum_{q,n} c_n^{(q)} p_n^m(H_{rs}).$$

The coefficients $c_n^{(q)}$ are the elastic constants. For the components $H_{rs}$ one obtains

$$H_{rs} = -\frac{1}{2} \varepsilon_{xij} b_r \vDash (\hat{\varepsilon}_b \hat{b}_s),$$

where $\vDash = (b_r \vDash)$ denotes the directional derivative along axis $b_r$ of the moving tripod.

$H$ transforms according to a polar vector with respect to the first index, according to an axial vector with respect to the second.

For fixed $(r, s, t) \in \text{cycl} (1, 2, 3)$ the following relation results from the compatibility conditions (5):

$$H_{rr} H_{ss} - H_{ss} H_{rr} = \frac{1}{2} \text{div} b_m \sum_{p=r} \varepsilon_{mpq} H_{qr}$$

$$= \frac{1}{2} \text{div}(b_r \text{div} b_r + b_s \times \text{curl} b_s).$$

This term transforms like $x^2$. Hence the number of surface terms or « nilpotent energies » in the elastic energy density is equal to the number of linearly independent polynomials which can be composed of $x^2$, $y^2$ and $z^2$, and which are invariant under the point group of the medium.

3. Uniaxial systems. — Linear combinations of $H$ transforming according to the irreducible representations of the symmetry group $D_\infty$ are presented in Table I. For uniaxial systems the invariants can be expressed in terms of the local symmetry axis $l = b_3$ and the vector $v$ of components $v_i = b_i \vDash b_3$ (such that $v \cdot b_3 = -H_{33}$). For superfluid $^3\text{He}$-A, $v$ is proportional to the superfluid velocity. The Mermin-Ho relation [2, 7]

$$[\text{curl } v]_i = \frac{1}{2} \varepsilon_{ijk} l.(\hat{\varepsilon}_l \vDash \hat{\varepsilon}_k)$$

is an immediate consequence of the compatibility conditions (5).

Note that the integral

$$N = \frac{1}{4\pi} \int_S \text{curl } v \cdot dF$$

about a closed surface $S$ yields the index $N$ of all point singularities of the vector field $l$ enclosed by $S$.

The first degree invariant polynomials are the linear combinations transforming according to $\Sigma^+$. The second degree invariant polynomials are linear combinations of the direct products of each representation with itself (Table II). There are two surface terms, $J_4$ and $J_5$, transforming as $z^2$ and $x^2 + y^2$, respectively.

Table II. — Polynomials in the components of $H$ invariant under $D_\infty$.

First degree :

$$I_1 = H_{11} + H_{22} = -l \cdot \text{curl } l$$

$$I_2 = H_{33} = -l \cdot v.$$

Second degree :

$$J_1 = (H_{12} - H_{21})^2 = (\text{div } l)^2$$

$$J_2 = (H_{11} + H_{22})^2 = (l \cdot \text{curl } l)^2$$

$$J_3 = H_{33}^2 + H_{23}^2 = (l \times l)^2$$

$$J_4 = H_{11} H_{22} - H_{21} H_{12} = l \cdot \text{curl } v =$$

$$= \frac{1}{2} \text{div} (l \text{div } l + l \times l)$$

$$J_5 = (H_{33} H_{11} - H_{13} H_{33}) + (H_{23} H_{33} - H_{33} H_{23})$$

$$= v \cdot \text{curl } l = (l \times v) + \frac{1}{2} \text{div} (l \text{div } l + l \times l)$$

$$J_6 = (H_{11} + H_{22}) H_{33} = (l \cdot \text{curl } l) (l \cdot v)$$

$$J_7 = (H_{33})^2 = (l \cdot v)^2$$

$$J_8 = H_{13}^2 + H_{23}^2 = (l \times v)^2 = v^2 - (l \cdot v)^2.$$

In a small scale theory (large pitch) a cholesteric liquid crystal is viewed as a nematic liquid crystal, but lacking inversion symmetry, and thus of point group $D_\infty$. The symmetry axis points along the director. Parametrizing the rotations $R(x)$ by Eulerian angles $(\theta(x), \phi(x), \psi(x))$, one finds

$$v = -(\nabla \psi) - (\nabla \phi) \cos \theta.$$ (12)
leaving only the well-known splay, twist and bend curvature strains, apart from the surface term $J_4$. In a large scale theory as proposed by Volovik [4], in lowest order of the pitch the director field is written as $b_1(x) \cos \chi(x) + b_2(x) \sin \chi(x)$ with $V_\chi = q_0 I$, $q_0 I$ denoting the pitch wave vector. Volovik inserted this form of the director field into the Frank (small scale) elastic energy and averaged over the rapidly varying phase $\chi$. By the averaging procedure the system obtains a local cylinder symmetry $D_{\infty}$ of symmetry axis $I$. So all terms of table II should contribute to the elastic energy density. However, since $I$ is gradient of a phase, curl $I$ vanishes, leaving for the second degree bulk energies those found by Volovik, namely $J_1$, $J_7$, $J_8$. The symmetry analysis does not remove the linear term $l v$. The elastic constant of this term vanishes on the assumption of a stable local pitch, so that in first order enlarging the pitch length ($l v > 0$ for a right-hand cholesteric helix) costs the same energy as diminishing it ($l v < 0$). The surface term in the large scale theory is $1/2 \text{div} (\text{div} I)$. Note that the large scale theory has only a limited range of applicability [4].

For superfluid $^3$He-A the order parameter is the second rank tensor $\mathbf{A} = \hat{d} \otimes \mathbf{q}$, where $\hat{d}$ is a real unit vector and $\mathbf{q} = b_1 + i b_2$ a complex vector related to the orbital motion of the Cooper pairs. The orbital part of the gradient energy depends on the spatial variation of $\mathbf{q}$ for which the contortion tensor is a natural measure. This energy is invariant under rotations about $I$ (gauge invariance), under the inversion $\mathbf{q} \rightarrow - \mathbf{q}$ (if simultaneously $\hat{d}$ is transformed to $- \hat{d}$), and under complex conjugation $(\mathbf{q} \rightarrow \mathbf{q}^*)$ which amounts to a reflexion in the plane spanned by $b_1$ and $b_2$. In total the local symmetry group is $D_{\infty h}$ for which the invariant polynomials are those of second degree in table II, in agreement with reference [7], although the surface term $J_5$ seems not to be recognized as such in the literature.

### 4. Biaxial systems.

Biaxial systems are the biaxial nematic liquid crystals [5] of symmetry $D_{2h}$, but also for cholesteric liquid crystals biaxial models (of symmetry $D_2$) exist [9, 10], the three inequivalent axes being the director, the helix axis, and the binormal. The irreducible representations of $D_2$ according to which the components of $H$ transform, are listed in table III. For symmetry $D_2$ there are three first degree invariants, namely $H_{11}$, $H_{22}$, $H_{33}$. Those of second degree are also invariant under $D_{2h}$. They are of the form $H_{ij} H_{ji} - H_{ij} H_{ji}$ (no summation here over repeated indices). For comparison with uniaxial symmetry different linear combinations of the invariants seem favourable. All the invariants for the small scale theory of cholesteric liquid crystals ($D_{\infty h}$ plus gauge invariance) are also invariants for symmetry $D_2$ ($I_1$, $J_1$, $J_7$, $J_8$ of table II). Since the gauge invariance is broken, also invariants $I_2$, $J_5$ to $J_8$ of table II occur. The additional invariants of table IV come from the fact that rotations about axes $b_1$ and $b_2$ are inequivalent. The corresponding elastic constants for these latter should be small compared to the former in case of weak biaxiality. For biaxial nematic liquid crystals 12 bulk terms and three surface terms ($J_4$, $J_5$, $J_{15}$) contribute to the curvature elastic energy density.

Table III. — Components of $H$ transforming according to irreducible representations of $D_2$

| $A_1$ | $H_{11}$; $H_{22}$; $H_{33}$ |
| $B_1$ | $H_{12}$; $H_{21}$ |
| $B_2$ | $H_{23}$; $H_{32}$ |
| $B_3$ | $H_{31}$; $H_{13}$ |

Table IV. — Additional invariant polynomials in case of biaxial symmetry ($D_2$)

Notation: $u$ is a vector of components $u_k = b_{2k}, \partial \partial_{b_1} I$. $w$ has components $w_k = I, \partial \partial_{b_1} I$.

\[
H_{r1} = - b_{r1} u, \quad H_{r2} = - b_{r2} w, \quad H_{r3} = - b_{r3} v, \quad r = 1, 2, 3.
\]

First degree:

\[
I_3 = H_{11} - H_{22} = (b_1 - u - b_2 - w).
\]

Second degree:

\[
J_9 = H_{12}^2 - H_{33}^2 = (I \partial \partial_{b_1} I)(b_1 - u - b_2 - w),
J_{19} = H_{13}^2 - H_{22}^2 = (I \partial \partial_{b_1} I)(b_1 - u - b_2 - w),
J_{11} = H_{11} + H_{22} + H_{33},
J_{12} = H_{21}^2 - H_{32}^2 = (I \partial \partial_{b_1} I)(b_1 - u - b_2 - w),
J_{13} = (H_{11} - H_{22})H_{33} = (I \partial \partial_{b_1} I)(b_1 - u - b_2 - w),
J_{14} = H_{13}^2 - H_{23}^2 = (I \partial \partial_{b_1} I)(b_1 - u - b_2 - w),
J_{15} = (H_{11} - H_{22} - H_{33}) - (H_{13} - H_{23} - H_{32}),
= b_2 \partial \partial_{b_1} I - b_2 \partial \partial_{b_1} I
\]

\[
N = \frac{1}{(4 \pi)^3} \int_V \text{det} K d^3 x
\]

is an integer and counts how often the tripods sweep.
over the image sphere as one moves through all of physical space. This « degree of the mapping » (see for instance [12]) can also be expressed as [11]

\[ N = \frac{1}{(4 \pi)^2} \int \mathbf{v} \cdot \text{curl} \mathbf{v} \, d^3 \mathbf{x}. \]  

Relation (14) is applicable to systems of uniaxial symmetry, in which case \( N \) denotes the Hopf-index, and also to cholesteric liquid crystals even if the director field is not constant at the boundary, but forms a homogeneous helix. Simultaneously \( \det K \) is an invariant third degree polynomial for systems whose point group contains only proper rotations (like \( D_2 \)). Since the integer \( N \) does not change upon continuous variations of the rotation field \( R \), this invariant polynomial does not contribute to the Euler-Lagrange equations for the minimalization of the curvature energy, and thus constitutes a third order « nilpotent » energy.

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References