

## Theory of orientational elasticity

S. Stallinga and G. Vertogen

*Institute for Theoretical Physics, University of Nijmegen, Toernooiveld, 6525 ED Nijmegen, The Netherlands*

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In order to describe the local orientation of a macroscopic medium with broken rotational symmetries, an orientational field that consists of three orthonormal vectors is introduced. Next, the deformation free-energy density is constructed and a detailed account is given of the form and number of the appearing surface terms. It appears that the general expression involves 39 bulk elastic constants and 24 surface elastic constants for nonchiral materials, whereas the property of chirality introduces an additional number of six bulk elastic constants and three surface elastic constants. The influence of discrete and continuous symmetries on the independence of these elastic constants is considered.

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### I. THE ORIENTATIONAL FIELD

The forms of the free-energy densities of orientational deformations in nematic liquid crystals with uniaxial [1–5] and biaxial symmetry [6–10] and in smectic liquid crystals [11,12] are well known. All these deformation free-energy densities are derived from *a priori* symmetry considerations. The aim of the present paper is to formulate a theory of orientational elasticity without any *a priori* symmetry considerations, i.e., a theory analogous to the theory of positional elasticity [13]. The advantage of such a theory is that all possible effects of biaxiality, polarity, and chirality are taken into account. The deformation free-energy density of a material with any symmetry group is then obtained by *a posteriori* sym-

metry requirements. As opposed to the theories of Liu [8] and Trebin [9] the present approach makes use of the instrument of tensor calculus in order to facilitate the analysis of the form and number of the appearing bulk and surface terms. Their approach also differs from the present one in some results concerning the surface terms.

The orientation of a given material point is fixed with respect to a space-fixed frame ( $\hat{e}_x, \hat{e}_y, \hat{e}_z$ ) by defining a local frame attached to that point. The axes of this local frame are given by the three orthonormal vectors  $\mathbf{l}(\mathbf{r})$ ,  $\mathbf{m}(\mathbf{r})$ , and  $\mathbf{n}(\mathbf{r})$ . The orthonormality requirements impose six constraints on the nine components of  $\mathbf{l}(\mathbf{r})$ ,  $\mathbf{m}(\mathbf{r})$ , and  $\mathbf{n}(\mathbf{r})$ . A suitable representation of these local vectors is in terms of the three Eulerian angles  $\phi(\mathbf{r})$ ,  $\theta(\mathbf{r})$ , and  $\psi(\mathbf{r})$ :

$$\mathbf{l} = (\cos \theta \cos \phi \cos \psi - \sin \phi \sin \psi, \cos \theta \sin \phi \cos \psi + \cos \phi \sin \psi, -\sin \theta \cos \psi), \quad (1a)$$

$$\mathbf{m} = (-\cos \theta \cos \phi \sin \psi - \sin \phi \cos \psi, -\cos \theta \sin \phi \sin \psi + \cos \phi \cos \psi, \sin \theta \sin \psi), \quad (1b)$$

$$\mathbf{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta). \quad (1c)$$

The local body-fixed frame and the space-fixed frame are connected by an orthogonal transformation, whose matrix elements  $R_{i\alpha}$  with  $i = 1, 2, 3$  and  $\alpha = x, y, z$  are given by

$$\mathbf{l} = R_{1\alpha} \hat{e}_\alpha, \quad (2a)$$

$$\mathbf{m} = R_{2\alpha} \hat{e}_\alpha, \quad (2b)$$

$$\mathbf{n} = R_{3\alpha} \hat{e}_\alpha. \quad (2c)$$

It follows directly that

$$R_{1\alpha} = l_\alpha, \quad (3a)$$

$$R_{2\alpha} = m_\alpha, \quad (3b)$$

$$R_{3\alpha} = n_\alpha. \quad (3c)$$

The orthonormality of the vectors  $\mathbf{l}$ ,  $\mathbf{m}$ , and  $\mathbf{n}$  is represented by

$$R_{i\alpha} R_{j\alpha} = \delta_{ij} \quad (4)$$

and the completeness by

$$R_{i\alpha} R_{i\beta} = \delta_{\alpha\beta}. \quad (5)$$

N.B. Repeated indices imply summation. For the sake of clearness, Roman indices denote 1, 2, or 3, whereas Greek indices stand for  $x, y, z$ .

### II. THE DEFORMATION FREE-ENERGY DENSITY

The deformation free-energy density  $f_d(\mathbf{r})$  of an arbitrary orientational field is defined as the difference between the free-energy density  $f(\mathbf{r})$  of the spatially varying orientational field ( $\mathbf{l}(\mathbf{r})$ ,  $\mathbf{m}(\mathbf{r})$ ,  $\mathbf{n}(\mathbf{r})$ ) and the free en-

ergy density  $f_0$  of the uniformly oriented medium:

$$f_d(\mathbf{r}) = f(\mathbf{r}) - f_0. \quad (6)$$

Consequently  $f_d(\mathbf{r})$  is a function of the spatial derivatives of the orientational field. If the distortion of the orientational field is sufficiently small, the free-energy density  $f_d(\mathbf{r})$  can be approximated by

$$\begin{aligned} f_d(\mathbf{r}) = & A_{\alpha\beta}(\mathbf{r})\partial_\alpha l_\beta(\mathbf{r}) + B_{\alpha\beta\gamma\delta}(\mathbf{r})\partial_\alpha l_\beta(\mathbf{r})\partial_\gamma l_\delta(\mathbf{r}) \\ & + C_{\alpha\beta\gamma\delta}(\mathbf{r})\partial_\alpha l_\beta(\mathbf{r})\partial_\gamma m_\delta(\mathbf{r}) \\ & + D_{\alpha\beta\gamma}(\mathbf{r})\partial_\alpha \partial_\beta l_\gamma(\mathbf{r}) + (\text{additional terms}), \end{aligned} \quad (7)$$

where the additional terms are obtained by cyclic permutations of the letters  $l$ ,  $m$ , and  $n$ . The appearing tensors such as  $A_{\alpha\beta}$ ,  $B_{\alpha\beta\gamma\delta}$ ,  $C_{\alpha\beta\gamma\delta}$ , and  $D_{\alpha\beta\gamma}$  must be constructed from the available tensors  $l_\alpha$ ,  $m_\alpha$ , and  $n_\alpha$ . Note that any appearing Kronecker tensor  $\delta_{\alpha\beta}$  can be expressed in terms of these three vectors, since they satisfy the completeness relation (5).

In order to determine the total number of linearly in-

dependent terms of the distortion free-energy density, i.e., the number of elastic constants, the three appearing classes of terms are considered separately.

(i) *The class of linear first order terms.* These terms have the form

$$a_\alpha b_\beta \partial_\alpha c_\beta \quad (8)$$

with  $a, b, c \in \{l, m, n\}$ . It follows from the orthonormality of  $l$ ,  $m$ , and  $n$  that

$$\begin{aligned} a_\alpha \partial_\beta b_\alpha &= \partial_\beta (a_\alpha b_\beta) - b_\alpha \partial_\beta a_\alpha \\ &= -b_\alpha \partial_\beta a_\alpha, \end{aligned} \quad (9)$$

and, in particular,

$$a_\alpha \partial_\beta a_\alpha = 0. \quad (10)$$

The expression (8) is antisymmetric in  $b$  and  $c$ . Consequently the class of linear first order terms consists of the following invariants:

$$\begin{aligned} D_{11} &= l_\alpha m_\beta \partial_\alpha n_\beta, & D_{12} &= l_\alpha n_\beta \partial_\alpha l_\beta, & D_{13} &= l_\alpha l_\beta \partial_\alpha m_\beta, \\ D_{21} &= m_\alpha m_\beta \partial_\alpha n_\beta, & D_{22} &= m_\alpha n_\beta \partial_\alpha l_\beta, & D_{23} &= m_\alpha l_\beta \partial_\alpha m_\beta, \\ D_{31} &= n_\alpha m_\beta \partial_\alpha n_\beta, & D_{32} &= n_\alpha n_\beta \partial_\alpha l_\beta, & D_{33} &= n_\alpha l_\beta \partial_\alpha m_\beta. \end{aligned} \quad (11)$$

These nine invariants can also be expressed as

$$D_{ij} = \frac{1}{2} \varepsilon_{jkl} R_{i\alpha} R_{k\beta} \partial_\alpha R_{l\beta}, \quad (12)$$

where the Levi-Civita symbol is defined by

$$\varepsilon_{jkl} = \begin{cases} 1 & \text{if } jkl = 123, 231, 312 \\ -1 & \text{if } jkl = 132, 321, 213 \\ 0 & \text{otherwise.} \end{cases} \quad (13)$$

The invariants  $D_{ij}$  are just the negative of the components of the so-called contortion tensor [9] with respect to the local frame given by the three orthonormal vectors  $l$ ,  $m$ , and  $n$ .

(ii) *The class of quadratic first order terms.* These terms have the form

$$a_\alpha b_\beta c_\gamma d_\delta \partial_\alpha e_\beta \partial_\gamma f_\delta \quad (14)$$

with  $a, b, c, d, e, f \in \{l, m, n\}$ . These terms are nothing but the linearly independent products of the nine invariants given in (11). Therefore this class contains 45 different terms.

(iii) *The class of linear second order terms.* These terms have the form

$$\frac{1}{2} (a_\alpha b_\beta + b_\alpha a_\beta) c_\gamma \partial_\alpha \partial_\beta d_\gamma \quad (15)$$

with  $a, b, c, d \in \{l, m, n\}$ . Consequently this class consists of 54 terms.

A number of terms appearing in the distortion free en-

ergy density can be expressed as the sum of other terms and surface terms. The latter have the form of divergences and thus only contribute to the surface free energy according to Gauss's theorem. In the thermodynamic limit their contribution to the total free energy is negligible compared to the contribution of the remaining bulk terms. These surface terms appear in all three classes.

(i) The class of linear first order terms contains three surface terms. These terms are obtained from the following relations between six of the nine invariants:

$$\begin{aligned} \partial_\alpha l_\alpha &= \delta_{\alpha\beta} \partial_\alpha l_\beta \\ &= (l_\alpha l_\beta + m_\alpha m_\beta + n_\alpha n_\beta) \partial_\alpha l_\beta \\ &= D_{32} - D_{23}, \end{aligned} \quad (16a)$$

$$\partial_\alpha m_\alpha = D_{13} - D_{31}, \quad (16b)$$

$$\partial_\alpha n_\alpha = D_{21} - D_{12}. \quad (16c)$$

(ii) The class of quadratic first order terms appears to contain six surface terms. This can be shown by starting from the general form of a surface term being a linear combination of the terms in this class. The relevant term reads

$$S = \partial_\alpha (A_{\alpha\beta\gamma} \partial_\beta d_\gamma), \quad (17)$$

where  $d \in \{l, m, n\}$  and  $A_{\alpha\beta\gamma} = -A_{\beta\alpha\gamma}$ . It should be remarked here that the tensor  $A_{\alpha\beta\gamma}$ , which is symmetric in  $\alpha$  and  $\beta$ , can be expressed as a linear combination of terms belonging to the class of linear second order terms. As the tensor  $A_{\alpha\beta\gamma}$  must be composed of the local axes it follows directly that

$$A_{\alpha\beta\gamma} = (a_\alpha b_\beta - b_\alpha a_\beta) c_\gamma. \quad (18)$$

Consequently the surface terms belonging to this class can be expressed as

$$S = \partial_\alpha((a_\alpha b_\beta - b_\alpha a_\beta) c_\gamma \partial_\beta d_\gamma) \quad (19)$$

with  $a, b, c, d \in \{l, m, n\}$ . It follows directly that  $S$  depends on the quadratic first order terms in the following way:

$$\begin{aligned} S = & a_\alpha b_\beta \partial_\alpha c_\gamma \partial_\beta d_\gamma - a_\beta b_\alpha \partial_\alpha c_\gamma \partial_\beta d_\gamma + b_\beta c_\gamma \partial_\alpha a_\alpha \partial_\beta d_\gamma \\ & - a_\beta c_\gamma \partial_\alpha b_\alpha \partial_\beta d_\gamma + a_\alpha c_\gamma \partial_\alpha b_\beta \partial_\beta d_\gamma \\ & - b_\alpha c_\gamma \partial_\alpha a_\beta \partial_\beta d_\gamma. \end{aligned} \quad (20)$$

It seems that there are nine surface terms. Three of them, however, appear to be linearly dependent on the remaining surface terms. The six independent surface terms are

$$\begin{aligned} S_1 = & \partial_\alpha((n_\alpha l_\beta - n_\beta l_\alpha) n_\gamma \partial_\beta l_\gamma) \\ = & \partial_\alpha((\delta_{\alpha\gamma} - m_\alpha m_\gamma - l_\alpha l_\gamma) l_\beta \partial_\beta l_\gamma \\ & - (\delta_{\beta\gamma} - m_\beta m_\gamma - l_\beta l_\gamma) l_\alpha \partial_\beta l_\gamma) \\ = & \partial_\alpha(l_\beta \partial_\beta l_\alpha - l_\alpha \partial_\beta l_\beta) \\ & - \partial_\alpha((l_\alpha m_\beta - l_\beta m_\alpha) l_\gamma \partial_\beta m_\gamma), \end{aligned} \quad (21a)$$

$$\begin{aligned} S_2 = & \partial_\alpha((l_\alpha m_\beta - l_\beta m_\alpha) l_\gamma \partial_\beta m_\gamma) \\ = & \partial_\alpha(m_\beta \partial_\beta m_\alpha - m_\alpha \partial_\beta m_\beta) \\ & - \partial_\alpha((m_\alpha n_\beta - m_\beta n_\alpha) m_\gamma \partial_\beta n_\gamma), \end{aligned} \quad (21b)$$

$$\begin{aligned} S_3 = & \partial_\alpha((m_\alpha n_\beta - m_\beta n_\alpha) m_\gamma \partial_\beta n_\gamma) \\ = & \partial_\alpha(n_\beta \partial_\beta n_\alpha - n_\alpha \partial_\beta n_\beta) \\ & - \partial_\alpha((n_\alpha l_\beta - n_\beta l_\alpha) n_\gamma \partial_\beta l_\gamma), \end{aligned} \quad (21c)$$

$$\begin{aligned} S_4 = & \partial_\alpha((m_\alpha n_\beta - m_\beta n_\alpha) n_\gamma \partial_\beta l_\gamma) \\ = & \partial_\alpha(m_\alpha \partial_\beta l_\beta - m_\beta \partial_\beta l_\alpha), \end{aligned} \quad (21d)$$

$$\begin{aligned} S_5 = & \partial_\alpha((n_\alpha l_\beta - n_\beta l_\alpha) l_\gamma \partial_\beta m_\gamma) \\ = & \partial_\alpha(n_\alpha \partial_\beta m_\beta - n_\beta \partial_\beta m_\alpha), \end{aligned} \quad (21e)$$

$$\begin{aligned} S_6 = & \partial_\alpha((l_\alpha m_\beta - l_\beta m_\alpha) m_\gamma \partial_\beta n_\gamma) \\ = & \partial_\alpha(l_\alpha \partial_\beta n_\beta - l_\beta \partial_\beta n_\alpha). \end{aligned} \quad (21f)$$

The remaining three surface terms are

$$\begin{aligned} S_7 = & \partial_\alpha((l_\alpha n_\beta - l_\beta n_\alpha) n_\gamma \partial_\beta m_\gamma) \\ = & \partial_\alpha(l_\alpha \partial_\beta m_\beta - l_\beta \partial_\beta m_\alpha) = S_4, \end{aligned} \quad (22a)$$

$$\begin{aligned} S_8 = & \partial_\alpha((m_\alpha l_\beta - m_\beta l_\alpha) l_\gamma \partial_\beta n_\gamma) \\ = & \partial_\alpha(m_\alpha \partial_\beta n_\beta - m_\beta \partial_\beta n_\alpha) = S_5, \end{aligned} \quad (22b)$$

$$\begin{aligned} (a_\alpha b_\beta + b_\alpha a_\beta) c_\gamma \partial_\alpha \partial_\beta d_\gamma = & \partial_\alpha((a_\alpha b_\beta + b_\alpha a_\beta) c_\gamma \partial_\beta d_\gamma) - a_\alpha b_\beta \partial_\alpha c_\gamma \partial_\beta d_\gamma - a_\beta b_\alpha \partial_\alpha c_\gamma \partial_\beta d_\gamma \\ & - b_\beta c_\gamma \partial_\alpha a_\alpha \partial_\beta d_\gamma - a_\beta c_\gamma \partial_\alpha b_\alpha \partial_\beta d_\gamma - a_\alpha c_\gamma \partial_\alpha b_\beta \partial_\beta d_\gamma - b_\alpha c_\gamma \partial_\alpha a_\beta \partial_\beta d_\gamma. \end{aligned} \quad (26)$$

The general form of such a surface term can again be expressed as

$$S = \partial_\alpha(A_{\alpha\beta\gamma} \partial_\beta d_\gamma), \quad (27)$$

where the tensor  $A_{\alpha\beta\gamma}$  has the form

$$\begin{aligned} S_9 = & \partial_\alpha((n_\alpha m_\beta - n_\beta m_\alpha) m_\gamma \partial_\beta l_\gamma) \\ = & \partial_\alpha(n_\alpha \partial_\beta l_\beta - n_\beta \partial_\beta l_\alpha) = S_6, \end{aligned} \quad (22c)$$

as can be easily verified, e.g.,

$$\begin{aligned} \partial_\alpha(m_\alpha \partial_\beta l_\beta - m_\beta \partial_\beta l_\alpha) - \partial_\alpha(l_\alpha \partial_\beta m_\beta - l_\beta \partial_\beta m_\alpha) \\ = \partial_\alpha \partial_\beta (m_\alpha l_\beta - m_\beta l_\alpha) = 0. \end{aligned} \quad (23)$$

Clearly the expressions for the surface terms can be simplified by considering the linear combinations  $S_1 + S_2$ ,  $S_2 + S_3$ , and  $S_3 + S_1$  instead of  $S_1$ ,  $S_2$ , and  $S_3$ . Then the general expression for the surface terms appearing in the class of quadratic first order terms can be summarized as

$$\begin{aligned} S_{ij} = & \partial_\alpha(R_{i\beta} \partial_\beta R_{j\alpha} - R_{i\alpha} \partial_\beta R_{j\beta}) \\ = & \partial_\alpha R_{i\beta} \partial_\beta R_{j\alpha} - \partial_\alpha R_{i\alpha} \partial_\beta R_{j\beta} \\ = & (\delta_{\beta\gamma} \delta_{\alpha\delta} - \delta_{\alpha\beta} \delta_{\gamma\delta}) \partial_\alpha R_{i\beta} \partial_\gamma R_{j\delta} \\ = & (R_{k\alpha} R_{l\beta} \partial_\alpha R_{i\beta}) (R_{l\gamma} R_{k\delta} \partial_\gamma R_{j\delta}) \\ & - (R_{k\alpha} R_{k\beta} \partial_\alpha R_{i\beta}) (R_{l\gamma} R_{l\delta} \partial_\gamma R_{j\delta}) \\ = & (\varepsilon_{kim} \varepsilon_{ljn} - \varepsilon_{lim} \varepsilon_{kjn}) D_{lm} D_{kn}. \end{aligned} \quad (24)$$

This means that the six independent surface terms can be written as

$$\partial_\alpha(l_\beta \partial_\beta l_\alpha - l_\alpha \partial_\beta l_\beta) = 2(D_{23} D_{32} - D_{22} D_{33}), \quad (25a)$$

$$\partial_\alpha(m_\beta \partial_\beta m_\alpha - m_\alpha \partial_\beta m_\beta) = 2(D_{31} D_{13} - D_{33} D_{11}), \quad (25b)$$

$$\partial_\alpha(n_\beta \partial_\beta n_\alpha - n_\alpha \partial_\beta n_\beta) = 2(D_{12} D_{21} - D_{11} D_{22}), \quad (25c)$$

$$\begin{aligned} \partial_\alpha(l_\beta \partial_\beta m_\alpha - l_\alpha \partial_\beta m_\beta) = & D_{12} D_{33} + D_{21} D_{33} - D_{31} D_{23} \\ & - D_{13} D_{32}, \end{aligned} \quad (25d)$$

$$\begin{aligned} \partial_\alpha(m_\beta \partial_\beta n_\alpha - m_\alpha \partial_\beta n_\beta) = & D_{23} D_{11} + D_{32} D_{11} - D_{12} D_{31} \\ & - D_{21} D_{13}, \end{aligned} \quad (25e)$$

$$\begin{aligned} \partial_\alpha(n_\beta \partial_\beta l_\alpha - n_\alpha \partial_\beta l_\beta) = & D_{31} D_{22} + D_{13} D_{22} - D_{23} D_{12} \\ & - D_{32} D_{21}. \end{aligned} \quad (25f)$$

Summarizing the class of quadratic first order terms consists of 39 bulk terms and six surface terms. Note that these surface terms disappear for orientational fields that only depend on one coordinate, because they are anti-symmetric in the spatial derivatives as follows from (19).

(iii) The class of linear second order terms consists of 54 terms that can all be reduced to the sum of quadratic first order terms and a surface term as follows from:

$$A_{\alpha\beta\gamma} = (a_\alpha b_\beta + b_\alpha a_\beta) c_\gamma, \quad (28)$$

i.e.,  $A_{\alpha\beta\gamma}$  is now symmetric in  $\alpha$  and  $\beta$ . It follows immediately that there are 18 independent surface terms. Their general form can also be expressed as

$$S_{ijk} = S_{jik} = \partial_\alpha(R_{i\alpha} D_{jk} + R_{j\alpha} D_{ik}). \quad (29)$$

Summarizing the class of linear second order terms consist of terms that can be related to the 39 bulk terms of the class of quadratic first order terms with the aid of 18 surface terms.

Concluding the deformation free-energy density of an arbitrary orientational field can be expressed as

$$f_d(\mathbf{r}) = k_{ij}D_{ij} + \frac{1}{2}K_{ijkl}D_{ij}D_{kl} + L_{ijk}S_{ijk}, \quad (30)$$

where the elastic constants satisfy the symmetry relations

$$K_{ijkl} = K_{klij}, \quad (31a)$$

$$L_{ijk} = L_{jik}. \quad (31b)$$

The first contribution to the deformation free-energy density is due to the linear first order terms and contains three surface terms. The second contribution originates from the quadratic first order terms and the linear second order terms and contains six surface terms, whereas the third contribution consists of 18 surface terms that are composed of linear second order terms and quadratic first order terms. Consequently the general expression of the deformation free-energy density of an arbitrary orientational field consists of six chiral bulk terms and 39 quadratic bulk terms.

### III. SYMMETRY AND THE NUMBER OF INDEPENDENT ELASTIC CONSTANTS

The different cases of symmetry can be examined by changing to new orthonormal local basis vectors  $\mathbf{l}'$ ,  $\mathbf{m}'$ , and  $\mathbf{n}'$  according to

$$\mathbf{l}' = T_{11}\mathbf{l} + T_{12}\mathbf{m} + T_{13}\mathbf{n}, \quad (32a)$$

$$\mathbf{m}' = T_{21}\mathbf{l} + T_{22}\mathbf{m} + T_{23}\mathbf{n}, \quad (32b)$$

$$\mathbf{n}' = T_{31}\mathbf{l} + T_{32}\mathbf{m} + T_{33}\mathbf{n}, \quad (32c)$$

or, shortly,

$$R'_{i\alpha} = T_{ij}R_{j\alpha}. \quad (33)$$

The orthogonal transformation matrix  $T_{ij}$  satisfies the relations

$$T_{ik}T_{jk} = T_{ki}T_{kj} = \delta_{ij} \quad (34)$$

and its determinant is denoted by  $T$ , where  $T = \pm 1$ . From the identity

$$\varepsilon_{ijk}T_{il}T_{jm}T_{kn} = T\varepsilon_{lmn}, \quad (35)$$

it follows that

$$\varepsilon_{ijk}T_{jm}T_{kn} = T\varepsilon_{lmn}T_{il}. \quad (36)$$

This means that the nine attendant invariants  $D'_{ij}$  are given by

$$D'_{ij} = T T_{ik}T_{jl}D_{kl}. \quad (37)$$

Consequently the new elastic constants  $k'_{ij}$ ,  $K'_{ijkl}$ , and  $L'_{ijk}$  are expressed according to

$$k'_{ij} = T T_{mi}T_{nj}k_{mn}, \quad (38a)$$

$$K'_{ijkl} = T_{mi}T_{nj}T_{pk}T_{ql}K_{mnpq}, \quad (38b)$$

$$L'_{ijk} = T T_{mi}T_{nj}T_{pk}L_{mnp}. \quad (38c)$$

Note that three elastic constants can always be made zero by choosing a suitable set of local basis vectors. Clearly the elastic constants do not change under a symmetry operation. This means in mathematical terms that a number of systems of local basis vectors lead to the same elastic constants, i.e.,

$$k'_{ij} = k_{ij}, \quad (39a)$$

$$K'_{ijkl} = K_{ijkl}, \quad (39b)$$

$$L'_{ijk} = L_{ijk}. \quad (39c)$$

These symmetry requirements impose constraints on the number of independent elastic constants, i.e., result in a reduction of their number.

#### A. The effect of discrete symmetry

By analogy with Landau and Lifshitz [13] the results for the seven crystal systems and their associated 32 crystallographic point groups are discussed. Note that this classification is only exhaustive for orientational fields in crystals. First of all the elastic constants  $K_{ijkl}$  are considered.

(i) *Triclinic system.* The point groups of this crystal system are 1 and  $\bar{1}$ . No constraints on the elastic constants  $K_{ijkl}$  are imposed. Their number equals 39, but three of them can be set equal to zero by making a suitable choice of the system of local basis vectors.

(ii) *Monoclinic system.* The point groups are 2,  $m$ , and  $2/m$ . Choose  $\mathbf{n}$  as the twofold axis or the normal to the mirror plane. Then the symmetry requirement reads

$$K_{ijkl} = (-1)^N K_{ijkl}, \quad (40)$$

where  $N$  is the number of indices with value 3 in  $\{ijkl\}$ . This means that all the  $K_{ijkl}$  with odd  $N$  vanish, i.e., the following 25 constants remain:

$$\begin{aligned} &K_{1111}, K_{2222}, K_{3333}, K_{1122}, K_{2233}, \\ &K_{3311}, K_{1212}, K_{2121}, K_{1221}, K_{2323}, \\ &K_{3232}, K_{2332}, K_{3131}, K_{1313}, K_{1331}, \\ &K_{1112}, K_{1121}, K_{2212}, K_{2221}, K_{3312}, \\ &K_{3321}, K_{3132}, K_{3123}, K_{1332}, K_{1323}. \end{aligned} \quad (41)$$

By a suitable choice of  $\mathbf{l}$  and  $\mathbf{m}$  one of these constants can be set equal to zero. Note that only 21 bulk terms appear due to the relations (25a), (25b), (25c), and (25d).

(iii) *Orthorhombic system.* The point groups are 222,  $2mm$ , and  $2/mmm$ . Choose  $\mathbf{l}$ ,  $\mathbf{m}$ , and  $\mathbf{n}$  as twofold axes or normals to the mirror planes. Using symmetry requirements of the type (40) the following 15 constants remain:

$$\begin{aligned} &K_{1111}, K_{1122}, K_{1212}, K_{2323}, K_{3131}, \\ &K_{2222}, K_{2233}, K_{2121}, K_{3232}, K_{1313}, \\ &K_{3333}, K_{3311}, K_{1221}, K_{2332}, K_{1331}. \end{aligned} \quad (42)$$

Due to the relations (25a), (25b), and (25c) only 12 bulk

terms appear in the deformation free-energy density.

(iv) *Trigonal system.* Before discussing the number of independent elastic constants of the crystal system it is convenient to introduce a new system of basis vectors, namely,

$$\xi = \frac{1}{\sqrt{2}}(l + im), \quad (43a)$$

$$\eta = \frac{1}{\sqrt{2}}(l - im). \quad (43b)$$

The third basis vector  $\mathbf{n}$  remains untouched. The nine attendant invariants are defined as

$$D_{\xi\xi} = i\xi_{\alpha}n_{\beta}\partial_{\alpha}\xi_{\beta}, \quad (44a)$$

$$D_{\eta\xi} = i\eta_{\alpha}n_{\beta}\partial_{\alpha}\xi_{\beta}, \quad (44b)$$

$$D_{z\xi} = in_{\alpha}n_{\beta}\partial_{\alpha}\xi_{\beta}, \quad (44c)$$

$$D_{\xi\eta} = i\xi_{\alpha}\eta_{\beta}\partial_{\alpha}n_{\beta}, \quad (44d)$$

$$D_{\eta\eta} = i\eta_{\alpha}\eta_{\beta}\partial_{\alpha}n_{\beta}, \quad (44e)$$

$$D_{z\eta} = in_{\alpha}\eta_{\beta}\partial_{\alpha}n_{\beta}, \quad (44f)$$

$$D_{\xi z} = i\xi_{\alpha}\xi_{\beta}\partial_{\alpha}\eta_{\beta}, \quad (44g)$$

$$D_{\eta z} = i\eta_{\alpha}\xi_{\beta}\partial_{\alpha}\eta_{\beta}, \quad (44h)$$

$$D_{zz} = in_{\alpha}\xi_{\beta}\partial_{\alpha}\eta_{\beta}. \quad (44i)$$

Consequently the elastic constants will now be labeled by  $\xi$ ,  $\eta$ , and  $z$  instead of by 1, 2, and 3. The advantage of the present procedure is that arbitrary rotations around the  $\mathbf{n}$  axis can be easily dealt with. A rotation through an angle  $\alpha$  around the  $\mathbf{n}$  axis results in the vectors

$$\xi' = e^{-i\alpha}\xi, \quad (45a)$$

$$\eta' = e^{i\alpha}\eta, \quad (45b)$$

$$\mathbf{n}' = \mathbf{n}, \quad (45c)$$

whereas a reflection in a plane perpendicular to  $\mathbf{m}$  gives

$$\xi' = \eta, \quad (46a)$$

$$\eta' = \xi, \quad (46b)$$

$$\mathbf{n}' = \mathbf{n}. \quad (46c)$$

The point groups of the trigonal system are  $3$ ,  $\bar{3}$ ,  $32$ ,  $3m$ , and  $\bar{3}m$ . Consider the first two point groups and choose  $\mathbf{n}$  as the threefold axis. Then only elastic constants remain having three indices with value  $\xi$  or three indices with value  $\eta$  or having the same number of indices with value  $\xi$  and  $\eta$ . These 15 constants are

$$\begin{aligned} &K_{zzzz}, K_{zz\xi\xi}, K_{zz\xi\eta}, K_{z\eta z\xi}, K_{z\eta\xi z}, \\ &K_{\eta z\xi z}, K_{\eta z z\xi}, K_{\eta\xi\eta\xi}, K_{\eta\xi\xi\eta}, K_{\xi\eta\xi\eta}, \\ &K_{\xi\xi\eta\eta}, K_{\eta\eta\eta z}, K_{\eta\eta z\eta}, K_{\xi\xi\xi z}, K_{\xi z z\xi}. \end{aligned} \quad (47)$$

Here one constant can be set equal to zero by a suitable choice of  $\mathbf{l}$  and  $\mathbf{m}$ . Next the last three point groups are considered. Choosing the twofold axis or normal to the mirror plane along  $\mathbf{m}$  the following five relations between the 15 elastic constants hold:

$$K_{z\eta\xi z} = K_{z\xi\eta z}, \quad (48a)$$

$$K_{zz\eta\xi} = K_{zz\xi\eta}, \quad (48b)$$

$$K_{\eta\xi\eta\xi} = K_{\xi\eta\xi\eta}, \quad (48c)$$

$$K_{\eta\eta z\eta} = K_{\xi\xi z\xi}, \quad (48d)$$

$$K_{\eta\eta\eta z} = K_{\xi\xi\xi z}. \quad (48e)$$

The number of independent elastic constants of the point groups  $32$ ,  $3m$ , and  $\bar{3}m$  is thus reduced from 15 to 10 by the additional symmetry. These constants do not only concern bulk terms but surface terms as well. In order to determine the number of relevant surface terms the relations (25) are rewritten in terms of the new representation:

$$\partial_{\alpha}(\xi_{\beta}\partial_{\beta}\xi_{\alpha} - \xi_{\alpha}\partial_{\beta}\xi_{\beta}) = 2(D_{\xi\xi}D_{zz} - D_{\xi z}D_{z\xi}), \quad (49a)$$

$$\partial_{\alpha}(\eta_{\beta}\partial_{\beta}\eta_{\alpha} - \eta_{\alpha}\partial_{\beta}\eta_{\beta}) = 2(D_{\eta\eta}D_{zz} - D_{\eta z}D_{z\eta}), \quad (49b)$$

$$\partial_{\alpha}(n_{\beta}\partial_{\beta}n_{\alpha} - n_{\alpha}\partial_{\beta}n_{\beta}) = 2(D_{\xi\xi}D_{\eta\eta} - D_{\eta\xi}D_{\xi\eta}), \quad (49c)$$

$$\begin{aligned} \partial_{\alpha}(\xi_{\beta}\partial_{\beta}\eta_{\alpha} - \xi_{\alpha}\partial_{\beta}\eta_{\beta}) &= D_{\eta z}D_{z\xi} + D_{z\eta}D_{\xi z} - D_{\eta\xi}D_{zz} \\ &\quad - D_{\xi\eta}D_{zz}, \end{aligned} \quad (49d)$$

$$\begin{aligned} \partial_{\alpha}(\eta_{\beta}\partial_{\beta}n_{\alpha} - \eta_{\alpha}\partial_{\beta}n_{\beta}) &= D_{\eta z}D_{\xi\eta} + D_{z\eta}D_{\eta\xi} - D_{\xi z}D_{\eta\eta} \\ &\quad - D_{z\xi}D_{\eta\eta}, \end{aligned} \quad (49e)$$

$$\begin{aligned} \partial_{\alpha}(n_{\beta}\partial_{\beta}\xi_{\alpha} - n_{\alpha}\partial_{\beta}\xi_{\beta}) &= D_{\eta\xi}D_{\xi z} + D_{\xi\eta}D_{z\xi} - D_{z\eta}D_{\xi\xi} \\ &\quad - D_{\eta z}D_{\xi\xi}. \end{aligned} \quad (49f)$$

Because of symmetry only two surface terms are left, namely, (49c) and (49d). Consequently the number of bulk terms equals 13 and 8, respectively.

(v) *Tetragonal system.* The point groups are  $4$ ,  $\bar{4}$ ,  $4/m$ ,  $422$ ,  $4mm$ ,  $\bar{4}2m$ , and  $4/mmm$ . Choosing  $\mathbf{n}$  as the fourfold axis the point groups  $4$  and  $\bar{4}$  are described in terms of the following 13 elastic constants:

$$\begin{aligned} &K_{zzzz}, K_{zz\xi\eta}, K_{zz\eta\xi}, K_{z\eta z\xi}, K_{z\eta\xi z}, \\ &K_{\eta z\xi z}, K_{\eta z z\xi}, K_{\eta\xi\eta\xi}, K_{\eta\xi\xi\eta}, K_{\xi\eta\xi\eta}, \\ &K_{\xi\xi\eta\eta}, K_{\xi\xi\xi\xi}, K_{\eta\eta\eta\eta}. \end{aligned} \quad (50)$$

One of these constants can be set equal to zero by a suitable choice of  $\mathbf{l}$  and  $\mathbf{m}$ . With the choice of  $\mathbf{l}$  and  $\mathbf{m}$  as the twofold axes or the normals to the mirror planes, the additional symmetry of the remaining point groups imposes the following relations between these 13 elastic constants:

$$K_{z\eta\xi z} = K_{z\xi\eta z}, \quad (51a)$$

$$K_{zz\eta\xi} = K_{zz\xi\eta}, \quad (51b)$$

$$K_{\eta\xi\eta\xi} = K_{\xi\eta\xi\eta}, \quad (51c)$$

$$K_{\eta\eta\eta\eta} = K_{\xi\xi\xi\xi}. \quad (51d)$$

Consequently only nine independent elastic constants remain. The symmetry gives rise to the same surface terms as those for the trigonal system. Thus the number of independent elastic constants that are required to describe the distortion free-energy density of the bulk is given by 11 and 7, respectively.

(vi) *Hexagonal system.* The attendant point groups are  $6$ ,  $\bar{6}$ ,  $6/m$ ,  $622$ ,  $6mm$ ,  $\bar{6}2m$ , and  $6/mmm$ . The 11 constants of the first two point groups are

$$\begin{aligned} &K_{zzzz}, K_{zz\xi\eta}, K_{zz\eta\xi}, K_{z\eta z\xi}, K_{z\eta\xi z}, K_{\eta z\xi z}, \\ &K_{\eta z z\xi}, K_{\eta\xi\eta\xi}, K_{\eta\xi\xi\eta}, K_{\xi\eta\xi\eta}, K_{\xi\xi\eta\eta}. \end{aligned} \quad (52)$$

One of them can be set equal to zero by a suitable choice of  $\mathbf{l}$  and  $\mathbf{m}$ . The additional symmetry imposes the three relations

$$K_{z\eta\xi z} = K_{z\xi\eta z}, \quad (53a)$$

$$K_{zz\eta\xi} = K_{zz\xi\eta}, \quad (53b)$$

$$K_{\eta\xi\eta\xi} = K_{\xi\eta\xi\eta}. \quad (53c)$$

Consequently the number of independent elastic constants of the last five point groups is equal to 8. The same surface terms as those for the trigonal and tetragonal systems are found meaning that the number of bulk terms equals 9 and 6 respectively, i.e., nine and six elastic constants, respectively, are required to describe the distortion of the bulk.

(vii) *Cubic system.* The point groups are 23,  $m\bar{3}$ , 432,  $4\bar{3}m$ , and  $m\bar{3}m$ . Cubic crystal systems have orthorhombic symmetry so it suffices to consider the effect of the additional symmetry on the elastic constants of the orthorhombic system. The threefold axis of the cubic system is then parallel to  $(\mathbf{l} + \mathbf{m} + \mathbf{n})/\sqrt{3}$ . This symmetry imposes the following relations between the elastic constants:

$$K_{1111} = K_{2222} = K_{3333}, \quad (54a)$$

$$K_{1122} = K_{2233} = K_{3311}, \quad (54b)$$

$$K_{1212} = K_{2323} = K_{3131}, \quad (54c)$$

$$K_{2121} = K_{3232} = K_{1313}, \quad (54d)$$

$$K_{1221} = K_{2332} = K_{3113}. \quad (54e)$$

Consequently the first two point groups lead to five elastic constants. The additional fourfold axes of the other three point groups impose the relations

$$K_{1212} = K_{2121}, \quad (55a)$$

$$K_{2323} = K_{3232}, \quad (55b)$$

$$K_{3131} = K_{1313}. \quad (55c)$$

This means that these point groups have four independent elastic constants. Only one surface term remains. Consequently the number of independent bulk elastic constants is given by 4 and 3, respectively.

Next the elastic constants  $k_{ij}$  are considered. Clearly only the crystal systems without inversion symmetry need to be considered as all the chiral elastic constants are zero for systems with inversion symmetry.

(a) *Triclinic system.* The point group 1 has nine chiral elastic constants. The three surface terms (16) lead to six bulk terms.

(b) *Monoclinic system.* Consider the point group 2 and choose  $\mathbf{n}$  along the twofold axis. The chiral elastic constants are

$$k_{12}, k_{21}, k_{11}, k_{22}, k_{33}. \quad (56)$$

Only the surface term (16c) remains, i.e., four bulk terms appear. Next consider the point group  $m$  and take  $\mathbf{n}$  along the normal to the mirror plane. The remaining constants are

$$k_{13}, k_{31}, k_{23}, k_{32}. \quad (57)$$

Now the two surface terms (16a) and (16b) are left. Consequently the point group  $m$  has two chiral bulk terms.

(c) *Orthorhombic system.* The point group 222 has three chiral elastic constants as follows directly from choosing  $\mathbf{l}$ ,  $\mathbf{m}$ , and  $\mathbf{n}$  along the twofold axes. These constants are

$$k_{11}, k_{22}, k_{33}. \quad (58)$$

There are no surface terms to reduce the number of bulk terms. The point group  $2mm$  has two chiral elastic constants, as follows directly by choosing  $\mathbf{l}$  and  $\mathbf{m}$  as the normals to the mirror planes. These constants are

$$k_{12}, k_{21}. \quad (59)$$

One surface term is relevant, namely the one given in (16c), i.e., there is one chiral bulk elastic constant.

(d) *Trigonal system.* The surface terms read in terms of the basis vectors  $\xi$ ,  $\eta$ , and  $\mathbf{n}$ ,

$$\partial_\alpha \xi_\alpha = i(D_{z\eta} - D_{\eta z}), \quad (60a)$$

$$\partial_\alpha \eta_\alpha = i(D_{\xi z} - D_{z\xi}), \quad (60b)$$

$$\partial_\alpha n_\alpha = i(D_{\eta\xi} - D_{\xi\eta}). \quad (60c)$$

The point group 3 has the following three chiral elastic constants:

$$k_{\eta\xi}, k_{\xi\eta}, k_{zz}, \quad (61)$$

where  $\mathbf{n}$  is taken along the threefold axis. Only the surface term (60c) remains, i.e., two chiral bulk terms appear. The additional symmetry of the point group 32 leads to the relation

$$k_{\eta\xi} = k_{\xi\eta} \quad (62)$$

whereas the surface term is absent, i.e., also here two chiral bulk terms are found. On the other hand, the additional symmetry of the point group  $3m$  imposes the relations

$$k_{zz} = 0, \quad (63a)$$

$$k_{\eta\xi} = -k_{\xi\eta}. \quad (63b)$$

Moreover the surface term remains, i.e., no chiral bulk terms appear in systems with point group  $3m$ .

(e) *Tetragonal system.* The point group 4 with  $\mathbf{n}$  along the fourfold axis has the following three chiral elastic constants:

$$k_{\eta\xi}, k_{\xi\eta}, k_{zz}. \quad (64)$$

Only the surface term (60c) is relevant leaving two chiral bulk constants. The additional symmetry of the point group 422 leads to the relation

$$k_{\eta\xi} = k_{\xi\eta}, \quad (65)$$

whereas the surface term disappears, meaning that two chiral bulk terms are present. The symmetry of the point group  $4mm$  leads to the additional relations

$$k_{zz} = 0, \quad (66a)$$

$$k_{\eta\xi} = -k_{\xi\eta}, \quad (66b)$$

whereas the surface term does not disappear here, i.e., this point group has no chiral bulk terms.

(f) *Hexagonal system.* The point group 6 with  $\mathbf{n}$  along the sixfold axis has the following three chiral elastic constants:

$$k_{\eta\xi}, k_{\xi\eta}, k_{zz}. \quad (67)$$

Further the surface term (60c) is relevant, i.e., two independent chiral bulk constants are present. The point group 622 has the additional relation

$$k_{\eta\xi} = k_{\xi\eta}, \quad (68)$$

whereas the surface term is absent, i.e., this point group also has two independent chiral bulk terms. The symmetry of the point group  $6mm$  only allows:

$$k_{zz} = 0, \quad (69a)$$

$$k_{\eta\xi} = -k_{\xi\eta}, \quad (69b)$$

whereas only the surface term remains, i.e., there are no chiral bulk terms here.

(g) *Cubic system.* The point group 23 has orthorhombic symmetry. The threefold axis parallel to  $(\mathbf{l} + \mathbf{m} + \mathbf{n})/\sqrt{3}$  imposes the relation

$$k_{11} = k_{22} = k_{33}. \quad (70)$$

Further the surface terms disappear. Consequently one chiral bulk term appears. The point group 432 leads to the same result.

Finally the elastic constants  $L_{ijk}$  of the remaining 18 surface terms are considered.

(i) *Triclinic system.* This symmetry does not impose any constraints, i.e., there are 18 elastic constants.

(ii) *Monoclinic system.* Choose  $\mathbf{n}$  as the twofold axis or normal to the mirror plane. Then the following elastic constants appear:

$$\begin{aligned} L_{113}, L_{223}, L_{333}, L_{123}, \\ L_{131}, L_{321}, L_{312}, L_{232}. \end{aligned} \quad (71)$$

Consequently there are eight surface terms of the considered type, i.e., due to the linear second order terms.

(iii) *Orthorhombic system.* Choose  $\mathbf{l}$ ,  $\mathbf{m}$ , and  $\mathbf{n}$  as the twofold axes and/or normals to the mirror planes. This means that the following elastic constants are found:

$$L_{123}, L_{231}, L_{312}, \quad (72)$$

i.e., there are three elastic constants.

(iv) *Trigonal system.* Choosing  $\mathbf{n}$  as the threefold axis the following elastic constants appear:

$$L_{\eta\xi z}, L_{\eta z \xi}, L_{\xi z \eta}, L_{zzz}, L_{\eta\eta\eta}, L_{\xi\xi\xi}. \quad (73)$$

Consequently the point groups 3 and  $\bar{3}$  give rise to six surface terms of the considered type. The additional symmetry of the point groups  $3m$ ,  $32$ , and  $\bar{3}2m$  leads to

$$L_{zzz} = 0, \quad (74a)$$

$$L_{\xi\eta z} = 0, \quad (74b)$$

$$L_{\eta z \xi} = -L_{\xi z \eta}, \quad (74c)$$

$$L_{\eta\eta\eta} = -L_{\xi\xi\xi}. \quad (74d)$$

Therefore these point groups have two independent surface terms.

(v) *Tetragonal system.* Choose  $\mathbf{n}$  as the fourfold symmetry axis of the point group 4. Then the following independent constants are found:

$$L_{\eta\xi z}, L_{\eta z \xi}, L_{\xi z \eta}, L_{zzz}. \quad (75)$$

The same result holds for the point groups  $\bar{4}$  and  $4/m$ . The additional symmetry of the point groups  $422$ ,  $42m$ ,  $\bar{4}2m$ , and  $4/mmm$  leads to

$$L_{zzz} = 0, \quad (76a)$$

$$L_{\xi\eta z} = 0, \quad (76b)$$

$$L_{\eta z \xi} = -L_{\xi z \eta}, \quad (76c)$$

meaning that only one independent surface term appears here.

(vi) *Hexagonal system.* Choosing  $\mathbf{n}$  along the sixfold axis it is found that the point groups 6,  $\bar{6}$ , and  $6/m$  lead to the independent constants

$$L_{\eta\xi z}, L_{\eta z \xi}, L_{\xi z \eta}, L_{zzz}, \quad (77)$$

i.e., their symmetry reduces the number of independent surface terms of the considered type to 4. The additional symmetry of the point groups  $622$ ,  $6mm$ ,  $\bar{6}2m$ , and  $6/mmm$  imposes the further conditions

$$L_{zzz} = 0, \quad (78a)$$

$$L_{\xi\eta z} = 0, \quad (78b)$$

$$L_{\eta z \xi} = -L_{\xi z \eta}, \quad (78c)$$

meaning that only one independent surface term remains.

(vii) *Cubic system.* It suffices to consider the effect of the threefold axis on the results of the orthorhombic system. Clearly it follows that

$$L_{123} = L_{231} = L_{312}. \quad (79)$$

This means that only one independent surface term is present.

## B. Continuous symmetries

Choose  $\mathbf{n}$  along the axis of continuous rotation symmetry. This symmetry requires that the invariants  $D_{ij}$ ,  $D_{ij}D_{kl}$ , and  $S_{ijk}$  do not depend on the Eulerian angle  $\psi$  and its spatial derivatives  $\partial_\alpha\psi$ . Consequently all the terms that are forbidden by hexagonal symmetry are also forbidden here, as these excluded terms depend on  $\psi$ . From the remaining terms, those terms that are composed of the invariants  $D_{iz}$  are also excluded, for the invariants  $D_{iz}$  depend on  $\partial_\alpha\psi$ . The independent chiral elastic constants are

$$k_{\eta\xi}, k_{\xi\eta}, \quad (80)$$

and the surface term (60c) is relevant, i.e., one chiral bulk term is present. The bulk elastic constants are

$$K_{z\eta z\xi}, K_{\xi\eta\xi\eta}, K_{\eta\xi\eta\xi}, K_{\eta\eta\xi\xi}, K_{\eta\xi\xi\eta}. \quad (81)$$

Only the surface term (49c) appears to be relevant, i.e., there are four bulk elastic constants. The remaining elastic constants relating to surface terms are

$$L_{\eta z\xi}, L_{\xi z\eta}. \quad (82)$$

The additional symmetry of a twofold rotation axis perpendicular to  $\mathbf{n}$  leads to

$$k_{\eta\xi} = k_{\xi\eta}, \quad (83a)$$

$$K_{\eta\xi\eta\xi} = K_{\xi\eta\xi\eta}, \quad (83b)$$

$$L_{\eta z\xi} = -L_{\xi z\eta}. \quad (83c)$$

As is well known these are the elastic constants of chiral nematics. Two independent surface terms appear, one

concerns the quadratic first order terms and the other the linear second order terms. In case a mirror plane perpendicular to  $\mathbf{n}$  is present, the chiral constant  $k_{\eta\xi}$  equals zero. Finally the additional symmetry of a mirror plane with normal perpendicular to  $\mathbf{n}$  is considered. Here it holds that

$$k_{\eta\xi} = -k_{\xi\eta}, \quad (84a)$$

$$K_{\eta\xi\eta\xi} = K_{\xi\eta\xi\eta}, \quad (84b)$$

$$L_{\eta z\xi} = -L_{\xi z\eta}. \quad (84c)$$

In this case a third surface term is present originating from the linear first order terms.

#### IV. CONCLUSION

Macroscopic media with broken rotational symmetries have to be described by an orientational tensor field. Using tensor analysis the general form of the elastic deformation free-energy density is derived. The general

TABLE I. The number of independent elastic constants for discrete symmetry. The number of surface elastic constants for the linear first order and quadratic first order classes are indicated separately. The international short notation is used to label the different crystallographic point groups.

Crystal system	Point group	$K_{ijkl}$		$k_{ij}$		$L_{ijk}$
		bulk	surface	bulk	surface	
triclinic	1	39	6	6	3	18
	$\bar{1}$	39	6			18
monoclinic	2	21	4	4	1	8
	$m$	21	4	2	2	8
	$2/m$	21	4			8
orthorhombic	222	12	3	3		3
	$2mm$	12	3	1	1	3
	$2/mmm$	12	3			3
trigonal	3	13	2	2	1	6
	$\bar{3}$	13	2			6
	$32$	8	2	2		2
	$3m$	8	2		1	2
	$\bar{3}m$	8	2			2
tetragonal	4	11	2	2	1	4
	$\bar{4}, 4/m$	11	2			4
	422	7	2	2		1
	$4mm$	7	2		1	1
	$\bar{4}2m, 4/mmm$	7	2			1
hexagonal	6	9	2	2	1	4
	$\bar{6}, 6/m$	9	2			4
	622	6	2	2		1
	$6mm$	6	2		1	1
	$\bar{6}2m, 6/mmm$	6	2			1
cubic	23	4	1	1		1
	$m\bar{3}$	4	1			1
	432	3	1	1		1
	$\bar{4}3m, m\bar{3}m$	3	1			1

TABLE II. The number of independent elastic constants for the three appearing classes of in case of continuous symmetry. The number of bulk and surface elastic constants for the first two classes are indicated seperately. The different symmetry groups are denoted by the Schoenflies symbols.

Point group	$K_{ijkl}$		$k_{ij}$		$L_{ijk}$
	bulk	surface	bulk	surface	
$C_\infty$	4	1	1	1	2
$C_{\infty h}$	4	1			2
$C_{\infty v}$	3	1		1	1
$D_\infty$	3	1	1		1
$D_{\infty h}$	3	1			1

expression appears to involve 39 bulk elastic constants and 24 surface elastic constants. In addition the chirality of the medium introduces six bulk elastic constants and three surface elastic constants. By a suitable choice of the local basis vectors of the orientational field three of the elastic constants can be set equal to zero. Symmetry requirements reduce the number of independent elastic constants. The effect of discrete and continuous symmetries are summarized in Tables I and II, respectively. Some of these results have also been found by Liu [8] and by Trebin [9]. There are, however, some discrepancies with their results. According to Liu the general form of the deformation free-energy density consists of 45 invariants, namely, 36 bulk terms and nine surface terms. This means that Liu claims 36 bulk elastic constants. However, a careful analysis of his surface terms shows that this claim is unjustified, as only six of the nine surface terms are mutually different. On the other hand, Trebin only finds the first three of the six surface terms (25). Further it should be remarked that neither Liu nor Trebin discusses the surface terms originating from the linear second order terms and that Liu does not consider the chiral terms. In the Appendix it is shown that the present results agree with the known results for systems with uniaxial and orthorhombic or biaxial symmetry, i.e., nematic liquid crystals.

Finally it should be mentioned that in cases where translational symmetries are also broken, e.g., the smectic mesophases, the deformations of the orientational and positional tensor field do not need to be independent. Consequently some orientational deformations can be neglected as being of higher order in the positional deformation variables than the elastic terms of the positional deformations.

## APPENDIX: SOME EXPLICIT VECTOR EXPRESSIONS

### 1. The case of uniaxial symmetry

The deformation free-energy density of an orientational field with uniaxial  $D_\infty$  symmetry reads

$$\begin{aligned}
 f_d = & k_{\eta\xi}(D_{\eta\xi} + D_{\xi\eta}) + \frac{1}{2}K_{\eta\xi\eta\xi}(D_{\eta\xi}D_{\eta\xi} + D_{\xi\eta}D_{\xi\eta}) \\
 & + K_{\eta\eta\xi\xi}D_{\eta\eta}D_{\xi\xi} + K_{\eta\xi\xi\eta}D_{\eta\xi}D_{\xi\eta} + K_{z\eta z\xi}D_{z\eta}D_{z\xi} \\
 & + L_{\eta z\xi}[\partial_\alpha(\eta_\alpha D_{z\xi} + n_\alpha D_{\eta\xi}) \\
 & - \partial_\alpha(\xi_\alpha D_{z\eta} + n_\alpha D_{\xi\eta})]. \tag{A1}
 \end{aligned}$$

From the following relations:

$$D_{\eta\xi} + D_{\xi\eta} = D_{11} + D_{22}, \tag{A2a}$$

$$D_{\eta\xi}D_{\eta\xi} + D_{\xi\eta}D_{\xi\eta} = \frac{1}{2}(D_{11} + D_{22})^2 - \frac{1}{2}(D_{12} - D_{21})^2, \tag{A2b}$$

$$D_{\eta\eta}D_{\xi\xi} = \frac{1}{4}(D_{11} - D_{22})^2 + \frac{1}{4}(D_{12} + D_{21})^2, \tag{A2c}$$

$$D_{\eta\xi}D_{\xi\eta} = \frac{1}{4}(D_{11} + D_{22})^2 + \frac{1}{4}(D_{12} - D_{21})^2, \tag{A2d}$$

$$D_{z\eta}D_{z\xi} = \frac{1}{2}D_{31}^2 + \frac{1}{2}D_{32}^2, \tag{A2e}$$

$$\eta_\alpha D_{z\xi} - \xi_\alpha D_{z\eta} = i(l_\alpha D_{31} - m_\alpha D_{32}), \tag{A2f}$$

$$n_\alpha D_{\eta\xi} - n_\alpha D_{\xi\eta} = i n_\alpha (D_{12} - D_{21}), \tag{A2g}$$

it follows that

$$\begin{aligned}
 f_d = & k_{\eta\xi}(D_{11} + D_{22}) + \frac{1}{4}[-K_{\eta\xi\eta\xi} + K_{\eta\xi\xi\eta} + K_{\eta\eta\xi\xi}](D_{12} - D_{21})^2 \\
 & + \frac{1}{4}[K_{\eta\xi\eta\xi} + K_{\eta\xi\xi\eta} + K_{\eta\eta\xi\xi}](D_{11} + D_{22})^2 + \frac{1}{2}K_{z\xi z\eta}(D_{31}^2 + D_{32}^2) \\
 & + K_{\eta\eta\xi\xi}(D_{12}D_{21} - D_{11}D_{22}) + iL_{\eta z\xi}\partial_\alpha[l_\alpha D_{32} - m_\alpha D_{31} + n_\alpha(D_{12} - D_{21})]. \tag{A3}
 \end{aligned}$$

The appearing terms can be expressed in vector notation by

$$\begin{aligned} D_{11} + D_{22} &= (l_\alpha m_\beta - l_\beta m_\alpha) \partial_\alpha n_\beta = \varepsilon_{\alpha\beta\gamma} n_\gamma \partial_\alpha n_\beta \\ &= \mathbf{n} \cdot (\nabla \times \mathbf{n}), \end{aligned} \quad (\text{A4a})$$

$$\begin{aligned} D_{12} - D_{21} &= l_\alpha n_\beta \partial_\alpha l_\beta - m_\alpha m_\beta \partial_\alpha n_\beta = -(l_\alpha l_\beta + m_\alpha m_\beta) \partial_\alpha n_\beta \\ &= -(\delta_{\alpha\beta} - n_\alpha n_\beta) \partial_\alpha n_\beta = -\partial_\alpha n_\alpha \\ &= -\nabla \cdot \mathbf{n}, \end{aligned} \quad (\text{A4b})$$

$$\begin{aligned} D_{31}^2 + D_{32}^2 &= (n_\alpha m_\beta \partial_\alpha n_\beta)^2 + (n_\alpha n_\beta \partial_\alpha l_\beta)^2 = n_\alpha n_\gamma (l_\beta l_\delta + m_\beta m_\delta) \partial_\alpha n_\beta \partial_\gamma n_\delta \\ &= n_\alpha n_\gamma \partial_\alpha n_\beta \partial_\gamma n_\beta = (n_\alpha \partial_\beta n_\alpha - n_\alpha \partial_\alpha n_\beta) (n_\gamma \partial_\beta n_\gamma - n_\gamma \partial_\gamma n_\beta) \\ &= (\varepsilon_{\alpha\beta\sigma} \varepsilon_{\mu\nu\tau} n_\alpha \partial_\mu n_\nu) (\varepsilon_{\gamma\beta\tau} \varepsilon_{\mu\nu\tau} n_\gamma \partial_\mu n_\nu) \\ &= [\mathbf{n} \times (\nabla \times \mathbf{n})]^2, \end{aligned} \quad (\text{A4c})$$

$$\begin{aligned} D_{12} D_{21} - D_{11} D_{22} &= \frac{1}{2} \partial_\alpha (n_\beta \partial_\beta n_\alpha - n_\alpha \partial_\beta n_\beta) \\ &= \frac{1}{2} \nabla \cdot [(\mathbf{n} \cdot \nabla) \mathbf{n} - \mathbf{n} (\nabla \cdot \mathbf{n})], \end{aligned} \quad (\text{A4d})$$

$$\begin{aligned} \partial_\alpha [l_\alpha D_{32} - m_\alpha D_{31}] &= \partial_\alpha [l_\alpha n_\beta n_\gamma \partial_\beta l_\gamma - m_\alpha n_\beta m_\gamma \partial_\beta n_\gamma] \\ &= -\partial_\alpha [(\delta_{\alpha\gamma} - n_\alpha n_\gamma) n_\beta \partial_\beta] = -\partial_\alpha [n_\beta \partial_\beta n_\alpha] \\ &= -\nabla \cdot [(\mathbf{n} \cdot \nabla) \mathbf{n}], \end{aligned} \quad (\text{A4e})$$

$$\partial_\alpha [n_\alpha (D_{12} - D_{21})] = -\nabla \cdot [\mathbf{n} (\nabla \cdot \mathbf{n})], \quad (\text{A4f})$$

where a right-handed space-fixed frame is used, while (A4d) immediately follows from Eq. (25c). Defining the chiral elastic constant, the elastic constants for splay, twist, and bend, and the two surface elastic constants by

$$k = k_{\eta\xi}, \quad (\text{A5a})$$

$$K_1 = -\frac{1}{2} K_{\eta\xi\eta\xi} + \frac{1}{2} K_{\eta\xi\xi\eta} + \frac{1}{2} K_{\eta\eta\xi\xi}, \quad (\text{A5b})$$

$$K_2 = \frac{1}{2} K_{\eta\xi\eta\xi} + \frac{1}{2} K_{\eta\xi\xi\eta} + \frac{1}{2} K_{\eta\eta\xi\xi}, \quad (\text{A5c})$$

$$K_3 = K_{z\xi z\eta}, \quad (\text{A5d})$$

$$K_4 = K_{\eta\eta\xi\xi}, \quad (\text{A5e})$$

$$K_5 = -2i L_{\eta z \xi}, \quad (\text{A5f})$$

respectively, the well known Frank expression for chiral uniaxial nematics follows:

$$\begin{aligned} f_d &= k \mathbf{n} \cdot (\nabla \times \mathbf{n}) + \frac{1}{2} K_1 (\nabla \cdot \mathbf{n})^2 + \frac{1}{2} K_2 [\mathbf{n} \cdot (\nabla \times \mathbf{n})]^2 + \frac{1}{2} K_3 [\mathbf{n} \times (\nabla \times \mathbf{n})]^2 + \frac{1}{2} K_4 \nabla \cdot [(\mathbf{n} \cdot \nabla) \mathbf{n} - \mathbf{n} (\nabla \cdot \mathbf{n})] \\ &\quad + \frac{1}{2} K_5 \nabla \cdot [(\mathbf{n} \cdot \nabla) \mathbf{n} + \mathbf{n} (\nabla \cdot \mathbf{n})]. \end{aligned} \quad (\text{A6})$$

The present choice of the elastic constants seems preferable to the existing one [3,4], as the given expression reflects the proper antisymmetry and symmetry in the spatial derivatives of the surface terms originating from the quadratic first order and the linear second order terms, respectively.

## 2. The case of orthorhombic symmetry

The deformation free-energy density of an orientational field with orthorhombic 222 symmetry reads

$$\begin{aligned} f_d &= k_{11} D_{11} + k_{22} D_{22} + k_{33} D_{33} + \frac{1}{2} K_{1111} D_{11}^2 + \frac{1}{2} K_{2222} D_{22}^2 + \frac{1}{2} K_{3333} D_{33}^2 + \frac{1}{2} K_{1212} D_{12}^2 \\ &\quad + \frac{1}{2} K_{2323} D_{23}^2 + \frac{1}{2} K_{3131} D_{31}^2 + \frac{1}{2} K_{2121} D_{21}^2 + \frac{1}{2} K_{3232} D_{32}^2 + \frac{1}{2} K_{1313} D_{13}^2 + K_{1122} D_{11} D_{22} \\ &\quad + K_{2233} D_{22} D_{33} + K_{3311} D_{33} D_{11} + K_{1221} D_{12} D_{21} + K_{2332} D_{23} D_{32} + K_{3113} D_{31} D_{13} + L_{123} \partial_\alpha (l_\alpha D_{23} + m_\alpha D_{13}) \\ &\quad + L_{231} \partial_\alpha (m_\alpha D_{31} + n_\alpha D_{21}) + L_{312} \partial_\alpha (n_\alpha D_{12} + l_\alpha D_{32}). \end{aligned} \quad (\text{A7})$$

Vector expressions for  $D_{11}$ ,  $D_{22}$ , and  $D_{33}$  are obtained by using (A4a) and the analogous relations

$$D_{22} + D_{33} = \mathbf{l} \cdot (\nabla \times \mathbf{l}), \quad (\text{A8a})$$

$$D_{33} + D_{11} = \mathbf{m} \cdot (\nabla \times \mathbf{m}). \quad (\text{A8b})$$

Then it follows that

$$D_{11} = \frac{1}{2} [\mathbf{m} \cdot (\nabla \times \mathbf{m}) + \mathbf{n} \cdot (\nabla \times \mathbf{n}) - \mathbf{l} \cdot (\nabla \times \mathbf{l})], \quad (\text{A9a})$$

$$D_{22} = \frac{1}{2} [\mathbf{n} \cdot (\nabla \times \mathbf{n}) + \mathbf{l} \cdot (\nabla \times \mathbf{l}) - \mathbf{m} \cdot (\nabla \times \mathbf{m})], \quad (\text{A9b})$$

$$D_{33} = \frac{1}{2} [\mathbf{l} \cdot (\nabla \times \mathbf{l}) + \mathbf{m} \cdot (\nabla \times \mathbf{m}) - \mathbf{n} \cdot (\nabla \times \mathbf{n})]. \quad (\text{A9c})$$

The remaining six invariants can be expressed as

$$D_{12} = l_\alpha n_\beta \partial_\alpha l_\beta = (l_\alpha n_\beta - l_\beta n_\alpha) \partial_\alpha l_\beta = -\varepsilon_{\alpha\beta\gamma} m_\gamma \partial_\alpha l_\beta = -\mathbf{m} \cdot (\nabla \times \mathbf{l}), \quad (\text{A10a})$$

$$D_{23} = -\mathbf{n} \cdot (\nabla \times \mathbf{m}), \quad (\text{A10b})$$

$$D_{31} = -\mathbf{l} \cdot (\nabla \times \mathbf{n}), \quad (\text{A10c})$$

$$D_{21} = -\mathbf{l} \cdot (\nabla \times \mathbf{m}) = \nabla \cdot \mathbf{n} - \mathbf{m} \cdot (\nabla \times \mathbf{l}), \quad (\text{A10d})$$

$$D_{32} = -\mathbf{m} \cdot (\nabla \times \mathbf{n}) = \nabla \cdot \mathbf{l} - \mathbf{n} \cdot (\nabla \times \mathbf{m}), \quad (\text{A10e})$$

$$D_{13} = -\mathbf{n} \cdot (\nabla \times \mathbf{l}) = \nabla \cdot \mathbf{m} - \mathbf{l} \cdot (\nabla \times \mathbf{n}), \quad (\text{A10f})$$

where use is made of (A4b) and analogous relations. Vector expressions for the three surface terms due to the quadratic first order terms as given by Eqs. (25a), (25b), and (25c) follow immediately from

$$D_{23}D_{32} - D_{22}D_{33} = \frac{1}{2} \nabla \cdot [(\mathbf{l} \cdot \nabla) \mathbf{l} - \mathbf{l}(\nabla \cdot \mathbf{l})], \quad (\text{A11a})$$

$$D_{31}D_{13} - D_{33}D_{11} = \frac{1}{2} \nabla \cdot [(\mathbf{m} \cdot \nabla) \mathbf{m} - \mathbf{m}(\nabla \cdot \mathbf{m})], \quad (\text{A11b})$$

$$D_{12}D_{21} - D_{11}D_{22} = \frac{1}{2} \nabla \cdot [(\mathbf{n} \cdot \nabla) \mathbf{n} - \mathbf{n}(\nabla \cdot \mathbf{n})]. \quad (\text{A11c})$$

The relevant three linear second order terms can be easily rewritten in terms of vector notation using the expressions (A10):

$$\begin{aligned} \partial_\alpha (m_\alpha D_{31} + n_\alpha D_{21}) &= -\nabla \cdot \left\{ \mathbf{m} [\mathbf{l} \cdot (\nabla \times \mathbf{n})] \right. \\ &\quad \left. + \mathbf{n} [\mathbf{l} \cdot (\nabla \times \mathbf{m})] \right\}, \quad (\text{A12a}) \end{aligned}$$

$$\begin{aligned} \partial_\alpha (n_\alpha D_{12} + l_\alpha D_{32}) &= -\nabla \cdot \left\{ \mathbf{n} [\mathbf{m} \cdot (\nabla \times \mathbf{l})] \right. \\ &\quad \left. + \mathbf{l} [\mathbf{m} \cdot (\nabla \times \mathbf{n})] \right\}, \quad (\text{A12b}) \end{aligned}$$

$$\begin{aligned} \partial_\alpha (l_\alpha D_{23} + m_\alpha D_{13}) &= -\nabla \cdot \left\{ \mathbf{l} [\mathbf{n} \cdot (\nabla \times \mathbf{m})] \right. \\ &\quad \left. + \mathbf{m} [\mathbf{n} \cdot (\nabla \times \mathbf{l})] \right\}. \quad (\text{A12c}) \end{aligned}$$

Define the three chiral elastic constants, the 12 quadratic first order bulk elastic constants, the three quadratic first order surface elastic constants, and the three linear second order surface elastic constants according to

$$k_1 = \frac{1}{2}(k_{22} + k_{33} - k_{11}),$$

$$k_2 = \frac{1}{2}(k_{33} + k_{11} - k_{22}),$$

$$k_3 = \frac{1}{2}(k_{11} + k_{22} - k_{33}),$$

$$K_1 = \frac{1}{2}(K_{2222} + K_{3333} - K_{1111}) - 2K_{2233} - 2K_{2332},$$

$$K_2 = \frac{1}{2}(K_{3333} + K_{1111} - K_{2222}) - 2K_{3311} - 2K_{3113},$$

$$K_3 = \frac{1}{2}(K_{1111} + K_{2222} - K_{3333}) - 2K_{1122} - 2K_{1221},$$

$$K_4 = \frac{1}{2}(K_{2222} + K_{3333} - K_{1111}),$$

$$K_5 = \frac{1}{2}(K_{3333} + K_{1111} - K_{2222}),$$

$$K_6 = \frac{1}{2}(K_{1111} + K_{2222} - K_{3333}),$$

$$K_7 = K_{2323} + 2K_{2233} + 2K_{2332}$$

$$- \frac{1}{2}(K_{2222} + K_{3333} - K_{1111}),$$

$$K_8 = K_{3131} + 2K_{3311} + 2K_{3113}$$

$$- \frac{1}{2}(K_{3333} + K_{1111} - K_{2222}), \quad (\text{A13})$$

$$K_9 = K_{1212} + 2K_{1122} + 2K_{1221}$$

$$- \frac{1}{2}(K_{1111} + K_{2222} - K_{3333}),$$

$$K_{10} = K_{3232} + 2K_{2233} + 2K_{2332}$$

$$- \frac{1}{2}(K_{2222} + K_{3333} - K_{1111}),$$

$$K_{11} = K_{1313} + 2K_{3311} + 2K_{3113}$$

$$- \frac{1}{2}(K_{3333} + K_{1111} - K_{2222}),$$

$$K_{12} = K_{2121} + 2K_{1122} + 2K_{1221}$$

$$- \frac{1}{2}(K_{1111} + K_{2222} - K_{3333}),$$

$$K_{13} = \frac{1}{4}(K_{2222} + K_{3333} - K_{1111}) - K_{2233},$$

$$K_{14} = \frac{1}{4}(K_{3333} + K_{1111} - K_{2222}) - K_{3311},$$

$$K_{15} = \frac{1}{4}(K_{1111} + K_{2222} - K_{3333}) - K_{1122},$$

$$K_{16} = -L_{231},$$

$$K_{17} = -L_{312},$$

$$K_{18} = -L_{123}.$$

Use the vector expressions (A9) and (A10) for the invariants and (A11) and (A12a) for the surface terms. Then it follows that the deformation free-energy density of an orientational field with orthorhombic symmetry can be expressed as

$$\begin{aligned}
f_d = & k_1 \mathbf{l} \cdot (\nabla \times \mathbf{l}) + k_2 \mathbf{m} \cdot (\nabla \times \mathbf{m}) + k_3 \mathbf{n} \cdot (\nabla \times \mathbf{n}) + \frac{1}{2} K_1 (\nabla \cdot \mathbf{l})^2 + \frac{1}{2} K_2 (\nabla \cdot \mathbf{m})^2 + \frac{1}{2} K_3 (\nabla \cdot \mathbf{n})^2 \\
& + \frac{1}{2} K_4 [\mathbf{l} \cdot (\nabla \times \mathbf{l})]^2 + \frac{1}{2} K_5 [\mathbf{m} \cdot (\nabla \times \mathbf{m})]^2 + \frac{1}{2} K_6 [\mathbf{n} \cdot (\nabla \times \mathbf{n})]^2 \\
& + \frac{1}{2} K_7 [\mathbf{n} \cdot (\nabla \times \mathbf{m})]^2 + \frac{1}{2} K_8 [\mathbf{l} \cdot (\nabla \times \mathbf{n})]^2 + \frac{1}{2} K_9 [\mathbf{m} \cdot (\nabla \times \mathbf{l})]^2 \\
& + \frac{1}{2} K_{10} [\mathbf{m} \cdot (\nabla \times \mathbf{n})]^2 + \frac{1}{2} K_{11} [\mathbf{n} \cdot (\nabla \times \mathbf{l})]^2 + \frac{1}{2} K_{12} [\mathbf{l} \cdot (\nabla \times \mathbf{m})]^2 \\
& + K_{13} \nabla \cdot [(\mathbf{l} \cdot \nabla) \mathbf{l} - \mathbf{l} (\nabla \cdot \mathbf{l})] + K_{14} \nabla \cdot [(\mathbf{m} \cdot \nabla) \mathbf{m} - \mathbf{m} (\nabla \cdot \mathbf{m})] \\
& + K_{15} \nabla \cdot [(\mathbf{n} \cdot \nabla) \mathbf{n} - \mathbf{n} (\nabla \cdot \mathbf{n})] + K_{16} \nabla \cdot \{ \mathbf{m} [\mathbf{l} \cdot (\nabla \times \mathbf{n})] + \mathbf{n} [\mathbf{l} \cdot (\nabla \times \mathbf{m})] \} \\
& + K_{17} \nabla \cdot \{ \mathbf{n} [\mathbf{m} \cdot (\nabla \times \mathbf{l})] + \mathbf{l} [\mathbf{m} \cdot (\nabla \times \mathbf{n})] \} + K_{18} \nabla \cdot \{ \mathbf{l} [\mathbf{n} \cdot (\nabla \times \mathbf{m})] + \mathbf{m} [\mathbf{n} \cdot (\nabla \times \mathbf{l})] \} . \quad (\text{A14})
\end{aligned}$$

Except for the surface terms equivalent expressions can be found in the existing literature.

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