Number of elastic coefficients in a biaxial nematic liquid crystal

H. Brand*
Institute for Theoretical Physics, University of California, Santa Barbara, California 93106

H. Pleiner
FB7, Universität Essen, D43 Essen, West Germany
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It is shown by explicit calculation that there are 12 bulk elastic constants and 3 surface terms in the elastic energy of biaxial nematics.

Recently the hydrodynamic description of biaxial nematic liquid crystals has attracted considerable attention.[1–6] In the following we demonstrate that there exist 12 bulk contributions and three surface terms. Throughout we will use the notation of Ref. 1. In Ref. 1 the elastic energy was derived using two director fields $\vec{n}$ and $\vec{m}$ for the description of the three spontaneously broken continuous rotational symmetries and a total of 15 coefficients has been obtained [cf. Eq. (3.15) of Ref. 1]. (In Refs. 2, 4, and 5 it has been indicated without detailed calculation that there are 12 bulk terms.) To demonstrate that there are 12 bulk contributions the anholonomity relations for the broken symmetries [Eqs. (3.3) of Ref. 1]

$$\delta_1(\vec{m}\cdot\delta_2\vec{n})-\delta_2(\vec{m}\cdot\delta_1\vec{n}) = \delta_{il}^3[(\delta_1 m_l)(\delta_2 n_i)-(\delta_2 m_l)(\delta_1 n_i)] \ , \quad (1)$$

$$\delta_1[(\vec{n}\times\vec{m})\cdot\delta_2\vec{n}]-\delta_2[(\vec{n}\times\vec{m})\cdot\delta_1\vec{n}] = m_i m_l n_j \epsilon_{ljk}[(\delta_2 n_i)(\delta_1 m_k)-(\delta_1 n_i)(\delta_2 m_k)] \ , \quad (2)$$

$$\delta_1[(\vec{m}\times\vec{n})\cdot\delta_2\vec{m}]-\delta_2[(\vec{m}\times\vec{n})\cdot\delta_1\vec{m}] = m_i n_l m_j \epsilon_{ljk}[(\delta_1 n_i)(\delta_2 n_k)-(\delta_1 n_k)(\delta_2 n_i)] \quad (3)$$

are of crucial importance. Equation (1) can be exploited as follows. We take the expression involving A_{14} and set $\delta_1 \equiv n_j\nabla_j$ and $\delta_2 \equiv m_k\nabla_k$ in Eq. (1). Then we have [using Eq. (1)]

$$\int dV\, \delta_{il}^3 n_j m_k(\nabla_k n_i)(\nabla_j m_l) = \int dV[\,\delta_{il}^3 n_j m_k(\nabla_j n_i)(\nabla_k m_l) + n_j\nabla_j(m_l m_k\nabla_k n_l) - m_k\nabla_k(m_l n_j \nabla_j n_l] \ . \quad (4)$$

The first term on the right-hand side (rhs) can be incorporated into the expression for A_{15}. The second and third contributions on the rhs can be integrated by parts leaving us with the surface contribution

$$\Sigma_1 \equiv \int dV\, \nabla_j[n_j m_k m_l(\nabla_k n_l) - n_k m_j m_l(\nabla_k n_l)] = \int d\sigma_j(\nabla_k n_l)m_l[n_j m_k - n_k m_j] \quad (5)$$

($d\sigma_j$ denotes the surface element) and the bulk contributions

$$= \int dV[(\nabla_k m_k)m_l n_j(\nabla_j n_l) - (\nabla_j n_j)m_l m_k(\nabla_k n_l)] \ , \quad (6)$$

$$= \int dV[(\delta_{kp}^3 + m_k m_p + n_k n_p)(\nabla_k m_p)m_l n_j(\nabla_j n_l) - (\delta_{jp}^3 + m_j m_p + n_j n_p)(\nabla_p n_j)m_l m_k(\nabla_k n_l)] \ , \quad (7)$$

$$= \int dV[\delta_{kp}^3(\nabla_k m_p)m_l n_j(\nabla_j n_l) - \delta_{jp}^3 m_l m_k(\nabla_p n_j) - m_j m_p m_k m_l(\nabla_p n_j)(\nabla_k n_l)] \ . \quad (8)$$

To carry out the last step [from Eq. (7) to Eq. (8)] one has to keep in mind that $\vec{m}$, $\vec{n}$, and $\vec{m}\times\vec{n}$ form a triad of unit vectors and that only three of the four deviations from the preferred directions $\vec{n}$ and $\vec{m}$ are hydrodynamic (cf. Ref. 1 for a detailed discussion of the latter point). By inspection of Eq. (8) it is checked immediately that combining Eqs. (4) and (6)–(8) yields for the bulk contributions the condition

$$A_{14} - A_{15} - A_{12} + A_2 + A_3 = 0 \quad (9)$$

in addition to the surface term [Eq. (5)]. Concerning Eq. (2) we start with the expression for A_{12} and take $\delta_1 \equiv \epsilon_{irq} n_q m_r \nabla_i$ and $\delta_2 \equiv n_j \nabla_j$ in Eq. (2) which yields

$$\int dV\, \delta_{il}^3 n_j m_k(\nabla_j n_k)(\nabla_i m_l) = \int dV[\delta_{il}^3 n_j m_k(\nabla_i n_k)(\nabla_j m_l) - \epsilon_{iqr} n_q m_r \nabla_i(\epsilon_{lmn} n_m m_n n_j \nabla_j n_l) + n_j\nabla_j(\epsilon_{lmn}\epsilon_{iqr} n_m m_n n_q m_r \nabla_i n_l)] \ . \quad (10)$$

The second and third terms in the square brackets [Eq. (10)] are integrated by parts and give the surface contribution

$$\Sigma_2 \equiv \int dV\, \nabla_j [(\nabla_i n_l)(n_j \delta_{il}^3 - n_i \delta_{jl}^3)] \tag{11}$$

and the bulk terms

$$\int dV [\epsilon_{iqr} \nabla_i (n_q m_r) \epsilon_{lmn} n_m m_n n_j (\nabla_j n_l) - (\nabla_j n_j) \epsilon_{lmn} n_m m_n \epsilon_{iqr} n_q m_r (\nabla_i n_l)] \ . \tag{12}$$

Equation (12) is rewritten as follows:

$$\begin{aligned} &= -(\nabla_p n_j) \delta_{il}^3 (\nabla_i n_l)(\delta_{pj}^3 + m_p m_j + n_p n_j) + (\nabla_i n_q)(\nabla_j n_l)(\delta_{0i}^3 + m_i m_0 + n_i n_0) \epsilon_{0qr} \epsilon_{lmn} m_r n_m m_n n_j \\ &\quad + (\nabla_i m_r)(\nabla_j n_l)[\delta_{0i}^3 + m_i m_0 + n_i n_0] \epsilon_{0qr} \epsilon_{lmn} n_q n_m m_n n_j \ , \end{aligned} \tag{13}$$

$$= -(\nabla_p n_j)(\nabla_i n_l) \delta_{il}^3 \delta_{pj}^3 - (\nabla_p n_j)(\nabla_i n_l) \delta_{il}^3 m_p m_j - (\nabla_i n_q)(\nabla_j n_l) n_i n_j \delta_{ql}^3 - (\nabla_i m_r)(\nabla_j n_l) \delta_{rl}^3 m_i n_j \ . \tag{14}$$

Equation (14) follows from Eq. (13) by taking into account that $\vec{n}$, $\vec{m}$, and $\vec{m} \times \vec{n}$ always form a triad of unit vectors and that contributions such as $\epsilon_{ijk} n_k n_j$ and $\epsilon_{ilm} m_i m_l$ vanish identically. From Eqs. (10) and (12)–(14) we have for the bulk contribution [in addition to the surface term Σ_2 (Eq. (11)]

$$A_{12} - A_{13} + A_1 + A_3 + A_7 + A_{15} = 0 \ . \tag{15}$$

The application of Eq. (3) parallels that of Eq. (2) if we start, for example, with the term involving A_3. We find for the bulk terms the additional constraint

$$A_3 - A_6 - A_9 - A_{15} - A_{11} = 0 \tag{16}$$

and the surface term Σ_3,

$$\Sigma_3 \equiv \int dV\, \nabla_k [(\nabla_l m_q)(m_l \delta_{kq}^3 - m_k \delta_{ql}^3)] \ . \tag{17}$$

Thus we have shown, by making use of the anholonomity relations [Eqs. (1)–(3)], that the number of bulk coefficients for a biaxial nematic is 12 and that there are three surface contributions [Eqs. (5), (11), and (17)]. For uniaxial nematics the corresponding expression involves three bulk and one surface term.[7] For many applications, e.g., for the normal modes, of the hydrodynamic equations the surface contributions play no role. One should keep in mind, however, that the surface terms can also become important for the macroscopic description of liquid crystals especially when situations are considered where the liquid crystal contains defects. We just mention as an example that in one of the models[8] proposed for the description of the cholesteric blue phase the surface term plays the dominant role for the existence of this phase.

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*Present address: Bell Telephone Laboratories, Murray Hill, N.J. 07974.

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