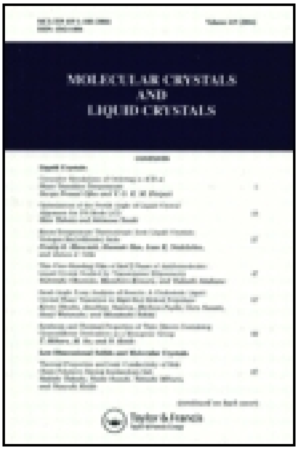

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Further Theoretical Proofs for the Existence of a Relation Between the Elastic Constants K'_{11} (K_{11}), (K'_{33})(K_{33}) and K_{13} in Nematics: Three- and One-Dimensional Cases

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Further Theoretical Proofs for the Existence of a Relation Between the Elastic Constants K'_{11} (K_{11}), $(K'_{33})(K_{33})$ and K_{13} in Nematics: Three- and One-Dimensional Cases

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The elaboration of the Ericksen's result for the inequalities in nematics has confirmed the proportionality between the second-order splay-bend elastic constant K_{13} and the difference between the elastic constants of bend K'_{33} and splay K'_{11} as well as the sign of K_{13} in accordance with the relation $2K_{13} = K'_{33} - K'_{11}$ obtained previously (Mol. Cryst. Liq. Cryst., **168**, 7, 1989). On the basis of detailed theoretical calculations for the one-dimensional case it is demonstrated that this relation follows from the requirement for a positive value of the elastic energy expressed with extremals and gradients of extremals when all possible symmetric and antisymmetric solutions are included.

Keywords: second-order splay-bend elasticity, relation between K_{13}, K'_{33} *and* K'_{11}, *extremals, inequalities in nematics*

I. INTRODUCTION

Recently I have theoretically found a relation between the elastic constants of splay K'_{11}, bend K'_{33} and second-order splay-bend K_{13} in nematics:[1]

$$2K_{13} = K'_{33} - K'_{11} \tag{1}$$

The estimations of the value and the sign of the second-order elastic constant K_{13} have been made by the researchers chiefly on the basis of the theoretical results by Nehring and Saupe who have used a simple inner field model which does not take into account any short range order effects.[2] They have obtained the following ratios for the elastic constants of a nematic liquid crystal:

$$K'_{11} : K_{22} : K'_{33} : K_{24} : K_{13} = 5 : 11 : 5 : -9 : -6 \tag{2}$$

On the other hand, Barbero and Oldano[3–5] critically have discussed my theoretical results for K_{13} elasticity (see Reference 6 and the citations therein) accepting that $K'_{11} = K'_{33}$ and K_{13} different from zero. The comparison of the relations (1) and (2) clearly shows that they are contradictory. According to relation (1), the K_{13} elastic constant must be zero when the two elastic constants of splay K'_{11} and bend

K'_{33} are equal. This requirement is equivalent to equality of the Frank elastic constants K_{11} and K_{33} due to the relations:

$$K'_{11} = K_{11} - 2K_{13}; \qquad K'_{33} = K_{33} + 2K_{13} \tag{3}$$

obtained by Nehring and Saupe.[7]

In this paper it is theoretically shown with the aid of three-dimensional calculations made in the frame of a local Cartesian coordinate system that the K_{13} elastic constant should be proportional to the difference between the elastic constants of splay K'_{11} and bend K'_{33}. This result requires a positive value of the Frank elastic constants of splay K_{11} and bend K_{33} and determines the sign of K_{13}. At this stage of the theoretical investigation, the exact ratio between K'_{11}, K'_{33} and K_{13} can be obtained only after regarding a simple example of elastic deformations as was done previously.[1] Further, the calculations are clarified and the physical importance of the obtained relation (1) is discussed. Finally, it is shown that the relation (1) is valid and for the more complicated one-dimensional case including splay-twist-bend deformations.[8]

II. THREE-DIMENSIONAL CASE: ON THE INEQUALITIES OF ERICKSEN[9] IN NEMATIC LIQUID CRYSTAL THEORY INCLUDING THE K_{13} SECOND-ORDER ELASTICITY

The three-dimensional density of the nematic elastic energy including K_{13} second-order elasticity has the well-known form:[7]

$$\begin{aligned} 2W = {} & K'_{11}(\operatorname{div}\mathbf{n})^2 + K_{22}(\mathbf{n}\cdot\operatorname{rot}\mathbf{n})^2 + K'_{33}(\mathbf{n} \times \operatorname{rot}\mathbf{n})^2 \\ & - 2(K_{22} + K_{24}) \sum_{1,i<j}^{3} (n_{i,i}n_{j,j} - n_{i,j}n_{j,i}) \\ & + 2K_{13}\operatorname{div}(\mathbf{n}\operatorname{div}\mathbf{n}) \end{aligned} \tag{4}$$

All physical and mathematical details can be found in the papers by Ericksen[9] and Nehring and Saupe.[2,7] In this paper it is adopted only the most important proposition: *for liquid crystal of nematic type, W is a minimum when* $\nabla\mathbf{n} = 0$.

The density of the nematic elastic energy according to the calculations by Ericksen[9] can be easily obtained from (4) after using the relations:

$$\mathbf{n} = (0,0,1) \tag{5}$$

$$n_{3,1} = 0 \tag{6}$$

$$n_{2,3} = 0,\ n_{1,3} > 0 \tag{7}$$

$$\nabla\mathbf{n} = \begin{vmatrix} a & b & c \\ d & e & 0 \\ 0 & 0 & 0 \end{vmatrix}, \ c > 0 \tag{8}$$

in the following form:

$$W = W_1 + W_2 + W_3 + 2K_{13}\mathrm{div}(\mathbf{n}\mathrm{div}\mathbf{n}) \tag{9}$$

where

$$2W_1 = K'_{33}\, c^2$$

$$2W_2 = K_{22}(b^2 + d^2) + 2K_{24}bd \tag{10a}$$

$$2W_3 = K'_{11}(a^2 + e^2) + 2(K'_{11} - K_{22} - K_{24})ae$$

with

$$a = \frac{\partial n_x}{\partial_x},\ b = \frac{\partial n_x}{\partial_y},\ c = \frac{\partial n_x}{\partial_z},\ d = \frac{\partial n_y}{\partial_x},\ e = \frac{\partial n_y}{\partial_y}$$

and

$$2K_{13}\mathrm{div}(\mathbf{n}\mathrm{div}\mathbf{n}) = 2K_{13}(d_1 + d_2 + (a + e)^2 - c^2) \tag{10b}$$

with

$$d_1 = \frac{\partial^2 n_x}{\partial_x \partial_z},\ d_2 = \frac{\partial^2 n_y}{\partial_y \partial_z}$$

The density of the nematic elastic energy given by Ericksen[9] and the density of the nematic elastic energy including the K_{13} second-order elasticity differ from each other by the term

$$2K_{13}(d_1 + d_2 + (a + e)^2 - c^2)$$

and the prenormalization of the elastic constants K_{11} and K_{33} by K'_{11} and K'_{33}, respectively.

In the paper by Ericksen[9] it is shown that

$$W_1 \geq 0,\ W_2 \geq 0,\ W_3 \geq 0 \tag{11}$$

when

$$K'_{11} \geq 0,\ K_{22} \geq 0,\ K'_{33} \geq 0,\ |K_{24}| \leq K_{22},\ K_{22} + K_{24} \leq 2K'_{11} \tag{12}$$

It is clear that the density of the nematic elastic energy including the K_{13} second-order elasticity will be non-negative when to the requirements expressed by relations (11) and (12) the following requirement is added:

$$2K_{13}\,(d_1 + d_2 + (a + e)^2 - c^2) \geq 0 \tag{13}$$

It is *apriori* clear that this requirement cannot be fulfilled for *arbitrary* deformations of the nematic, i.e. for arbitrary gradients of the nematic director. *Since the term K_{13} div(ndivn) influences only the boundary conditions and not the differential equation(s) of Euler-Lagrange*[10] *I shall regard the case when the nematic energy is minimal, replacing the gradients of the nematic director by gradients of EXTREMALS, solutions of the differential equation(s) of Euler-Lagrange.*

Firstly, let me note that the inequalities obtained by Ericksen[9] are valid for arbitrary functions which include also the extremals. The inclusion of the K_{13} second-order elasticity complicates very much the problem and, at this stage of the theoretical investigations, leads to the necessity to exclude the functions which cannot satisfy the Euler-Lagrange equation(s). However, this restriction is not too severe since in the equilibrium state, the gradients of the nematic director are gradients of extremals which satisfy the differential equation(s) of Euler-Lagrange. Consequently, the density of the nematic elastic energy are expressed with gradients of extremals satisfying the Euler-Lagrange equation(s). The vector differential equation of Euler-Lagrange has the well-known form:[11]

$$\mathbf{h} \times \mathbf{n} = 0 \tag{14}$$

where the vector of the bulk molecular field is expressed with the relation

$$\mathbf{h} = K'_{11}\,\mathrm{grad}(\mathrm{div}\mathbf{n}) - K_{22}\,((\mathbf{n}.\mathrm{rot}\mathbf{n})\mathrm{rot}\mathbf{n} + \mathrm{rot}(\mathbf{n}.\mathrm{rot}\mathbf{n})\mathbf{n})$$
$$+ K'_{33}\,(\mathbf{n} \times \mathrm{rot}\mathbf{n} \times \mathrm{rot}\mathbf{n} + \mathrm{rot}(\mathbf{n} \times \mathbf{n} \times \mathrm{rot}\mathbf{n})) \tag{15}$$

After some calculations, **h** can be written in a more convenient form:

$$\mathbf{h} = K'_{11}\,\mathrm{grad}(\mathrm{div}\mathbf{n}) - K_{22}(2(\mathbf{n}.\mathrm{rot}\mathbf{n})\mathrm{rot}\mathbf{n} + \mathrm{grad}(\mathbf{n}.\mathrm{rot}\mathbf{n}) \times \mathbf{n})$$
$$+ K'_{33}(2(\mathbf{n}.\mathrm{rot}\mathbf{n})\mathrm{rot}\mathbf{n} + \mathrm{grad}(\mathbf{n}.\mathrm{rot}\mathbf{n}) \times \mathbf{n} + \Delta\,\mathbf{n} - \mathrm{grad}(\mathrm{div}\mathbf{n})) \tag{16}$$

The Equation (14) is equivalent to

$$\mathbf{h}.\mathbf{n} = -\lambda \tag{17}$$

where λ is a scalar Lagrangian multiplier.
The equation (17) has the form:

$$(K'_{11} - K'_{33}\,\mathbf{n}.\mathrm{grad}(\mathrm{div}\mathbf{n}) + 2(K'_{33} - K_{22})(\mathbf{n}.\mathrm{rot}\mathbf{n})^2$$
$$- K'_{33}(\mathrm{rot}\mathbf{n})^2 + K'_{33}\,\nabla\,\mathbf{n}.\mathbf{n} = -\lambda \tag{18}$$

After some calculations Equation (18) is transformed in a more convenient form:

$$(K'_{11} - K'_{33})\mathit{div}(\mathbf{n}\mathrm{div}\mathbf{n}) + K'_{33}\mathrm{div}(\mathbf{n}\mathrm{div}\mathbf{n} + \mathbf{n} \times \mathrm{rot}\mathbf{n}) - K'_{11}(\mathrm{div}\mathbf{n})^2$$
$$- 2K_{22}(\mathbf{n}.\mathrm{rot}\mathbf{n})^2 - 2K'_{33}\,(\mathbf{n} \times \mathrm{rot}\mathbf{n})^2 = -\lambda \tag{19}$$

Write the vector Equation (19) in the local coordinate system defined by Ericksen:[9]

$$(K'_{11} - K'_{33})(d_1 + d_2 + (a + e)^2 - c^2) + 2K'_{33}(ae - db) - K'_{11}(a + e)^2 - 2K_{22}(d - b)^2 - 2K'_{33}c^2 = -\lambda \quad (20)$$

According to Frank[12] the saddle-splay deformation has a negative sign:

$$ae - db < 0 \quad (21)$$

Consider the case when the elastic constants of splay K'_{11} and bend K'_{33} are not equal. Equation (20) relates the value of div(**n**div**n**) in the local coordinate system with the gradients of the extremals and the Lagrangian multiplier λ. Use the very important suggestion by Nehring and Saupe[7] *that the second derivatives of* n *can make contribution of the same order of magnitude as quadratic terms of the first derivatives:*

$$(K'_{11} - K'_{33})(d_1 + d_2 + (a^2 + e)^2 - c^2) \sim 2K'_{33}(ae - db) \sim K'_{11}(a + e)^2 \sim 2K_{22}(d - b)^2 \sim 2K'_{33}c^2 \quad (22)$$

On the other hand, *in the equilibrium state the Lagrangian multiplier cannot be zero*. Consequently, it is possible to suggest that the first very important term in (22) containing the second spatial gradients of the director d_1 and d_2 *should be negative*:

$$(K'_{11} - K'_{33})(d_1 + d_2 + (a + e)^2 - c^2) < 0 \quad (23)$$

This inequality is equivalent to the following inequalities:

$$K'_{11} > K'_{33},\ (d_1 + d_2 + (a + e)^2 - c^2 < 0 \quad (24)$$

and

$$K'_{11} < K'_{33},\ (d_1 + d_2 + (a + e)^2 - c^2) > 0 \quad (25)$$

In the beginning of the calculations it was claimed that in the equilibrium state the term expressed by the relation (13) should be non-negative:

$$2K_{13}(d_1 + d_2 + (a + e)^2 - c^2) \geq 0 \quad (26)$$

Taking into account that in the equilibrium state $\lambda \neq 0$ and the validity of (21) and (22) one obtains finally:

$$\text{if } K'_{33} > K'_{11} \text{ then } K_{13} > 0 \quad (27)$$

$$\text{if } K'_{11} > K'_{33} \text{ then } K_{13} < 0 \quad (28)$$

Let us mention that these results coincide with those obtained previously.[1] They show also that *the second-order elastic constant* K_{13} *must be proportional to the difference between the elastic constants* K'_{11} *and* K'_{33}:

$$|K_{13}| \sim |K'_{11} - K'_{33}| \tag{29}$$

The exact value of this proportionality was obtained previously.[1] Nevertheless I clarify further the way of obtaining of the relation between K_{13}, K'_{11} and discuss further the physical reasons which lead to such relation.

III. ON THE RELATION BETWEEN K_{13}, K'_{33} AND K'_{11} PREVIOUSLY OBTAINED[1]: DISCUSSION OF THE PHYSICAL MEANING AND CLARIFICATIONS

Firstly, let me stress again that in the calculations I use only extremals and gradients of extremals. I am not interested in the complete solution of the problem which was found in our previous papers (see Reference 6 and the citations therein). I am interested only in the sign of the elastic energy when all functions and their gradients are replaced in the expression of the elastic energy by extremals and their gradients. I consider the case when all possible extremals can be included in the elastic energy. In my opinion this way of solution is correct since the $K_{13}\mathrm{div}(\mathbf{n}\mathrm{div}\mathbf{n})$ term cannot influence the behaviour of the differential equation(s) and consequently cannot influence the type of the extremals. On the other hand, all my solutions of the K_{13} elastic problem are based on a variation of a functional with a movable boundary; in this case it is well known from the literature that the minimization is performed with the aid of extremals.

Accepting that the deformation starts from initially planar orientation of the director I write the total elastic energy per unit area of a completely free nematic film in the following form:

$$I = \int_{-d/2}^{+d/2} dz \left\{ (1/2)(K'_{11}\cos^2\theta + K'_{33}\sin^2\theta)\theta'^2 + K_{13}\cos2\theta\theta'^2 + K_{13}\sin\theta\cos\theta\theta'' \right\} \tag{30}$$

where d is the thickness of the liquid crystal layer, K'_{11}, K'_{33} and K_{13} are elastic constants and θ is the deformational angle. The differential equation

$$\begin{gathered} f(\theta)\theta'' + (1/2)(d/d\theta)f(\theta) = 0 \\ \text{with } f(\theta) = K'_{11}\cos^2\theta + K'_{33}\sin^2\theta \end{gathered} \tag{31}$$

can be integrated once to obtain:[13]

$$f(\theta)(\theta')^2 = \mathrm{const} > 0 \tag{32}$$

The elastic energy expressed by (30) can be transformed in another more convenient equivalent form:

$$I = \int_{-d/2}^{+d/2} \left((1/2)f(\theta)\theta'^2 + K_{13}\cos 2\theta\theta'^2 + \left(\frac{K_{13}\sin\theta\cos\theta}{f(\theta)}\right)(\theta''f(\theta) + (1/2)(\theta'^2)(d/d\theta)f(\theta) - (1/2)(\theta'^2)(d/d\theta)f(\theta))\right) dz \tag{33}$$

Replace all functions and their gradients in (33) with solutions of the Euler-Lagrange equation (31) and their gradients:

$$I = \int_{-d/2}^{+d/2} \theta'^2\left((1/2)f(\theta) + K_{13}\cos 2\theta - \frac{K_{13}(K'_{33} - K'_{11})}{f(\theta)}\sin^2\theta\cos^2\theta\right)dz \tag{34}$$

The inequalities obtained by Ericksen[9] pointed out that the elastic constant of splay K'_{11} and bend K'_{33} must be positive (due to physical reasons the possible vanishing of these elastic constants is omitted):

$$K'_{11} > 0, K'_{33} > 0 \tag{35}$$

It is evident that the sign of the elastic energy for the case of extremals (34) is dictated by the sign of the expression in the brackets which is a function of the elastic constants and the deformation angles $\sin\theta$ and $\cos\theta$, solutions of the elastic problem under consideration.[1] The following two important cases are discussed:

a/The case of symmetric solutions expressed by cosθ(z)

It is obvious that these solutions are symmetric relative to the middle plane of the nematic layer. After a simple straightforward calculation for the numerator of the expression in the brackets one obtains a biquadratic equation for $\cos\theta(z)$:[1]

$$(K'_{11} - K'_{33})(K'_{11} - K'_{33} + 2K_{13})\cos^4\theta + 2K'_{33}(K'_{11} - K'_{33} + 2K_{13})\cos^2\theta + K'_{33}(K'_{33} - 2K_{13}) = g_1(\cos\theta(z)) \tag{36}$$

The function $g_1(\cos\theta(z))$ including all possible symmetric solutions (the isolated single solutions are not considered here) is positive when $D > 0$ and $a > 0$ and negative when $D > 0$ and $a < 0$
where

$$D = (4ac - b^2)/4a^2$$

with

$$a = (K'_{11} - K'_{33})(K'_{11} - K'_{33} + 2K_{13});\ b = 2K'_{33}(K'_{11} - K'_{33} + 2K_{13});$$
$$c = K'_{33}(K'_{33} - 2K_{13}) \tag{37}$$

These results can be summarized with the following inequalities ($K_{13} < 0$):
$g_1(\cos\theta(z)) > 0$
when

$$K'_{33} - 2K_{13} > K'_{33}$$

$$K'_{11} - K'_{33} > K'_{11} - K'_{33} + 2K_{13} > 0 \text{ when } 2K_{13} < K'_{11} - K'_{33}$$

$$K'_{11} - K'_{33} > K'_{11} - K'_{33} + 2K_{13} < 0 \quad (38)$$

and

$$g_1(\cos\theta(z)) < 0$$

when

$$-2K_{13} > K'_{11} - K'_{33} > 0 \quad (39)$$

b/The case of antisymmetric solutions expressed by sinθ(z)

The relation (36) can be transformed in the following form:

$$(K'_{33} - K'_{11})(K'_{33} - K'_{11} - 2K_{13})\sin^4\theta + 2K'_{11}(K'_{33} - K'_{11} - 2K_{13})\sin^2\theta + K'_{11}(K'_{11} + 2K_{13}) = g_2(\sin\theta(z)) \quad (40)$$

In this case the solutions are antisymmetric relative to the middle plane of the nematic layer.

The function $g_2(\sin\theta(z))$ including all possible antisymmetric solutions (the isolated single solutions are not considered here) is positive when $D > 0$ and $a > 0$ (D and a are calculated from the relation (40) and negative when $D > 0$ and $a < 0$. These results can be summarized with the following inequalities ($K_{13} > 0$):

$$g_2(\sin\theta(z)) > 0$$

when

$$K'_{11} + 2K_{13} > K'_{11}$$

$$K'_{33} - K'_{11} > K'_{33} - K'_{11} - 2K_{13} > 0 \text{ when } 2K_{13} < K'_{33} - K'_{11}$$

$$K'_{33} - K'_{11} > K'_{33} - K'_{11} - 2K_{13} < 0 \quad (41)$$

and

$$g_2(\sin\theta(z)) < 0$$

when

$$2K_{13} > K'_{33} - K'_{11} > 0 \tag{42}$$

All these results can be summarized with respect to the difference between the elastic constants of splay K'_{11} and bend K'_{33} as follows:

1/ $K'_{33} - K'_{11} > 0$

$$g_1(\cos\theta(z)) > 0 \text{ when } K_{13} < 0$$

$$g_2(\sin\theta(z)) > 0 \text{ when } 2K_{13} < K'_{33} - K'_{11},\ K_{13} > 0$$

$$g_2(\sin\theta(z)) < 0 \text{ when } 2K_{13} > K'_{33} - K'_{11},\ K_{13} > 0 \tag{43}$$

2/ $K'_{33} - K'_{11} < 0$

$$g_1(\cos\theta(z)) < 0 \text{ when } -2K_{13} > K'_{11} - K'_{33},\ K_{13} < 0$$

$$g_1(\cos\theta(z)) > 0 \text{ when } -2K_{13} < K'_{11} - K'_{33},\ K_{13} < 0$$

$$g_2(\sin\theta(z)) > 0 \text{ when } K_{13} > 0 \tag{44}$$

The inequalities (43) and (44) clearly show that *at a given sign of the second-order elastic constant* K_{13} *and at a given sign of the difference between the elastic constants of splay and bend* $K'_{11} - K'_{33}$, the expression in the brackets of the relation (34) IS POSITIVE FOR ALL POSSIBLE SOLUTIONS (symmetric or antisymmetric) when the coefficient multiplying $\cos^4\theta(z)$, respectively $\sin^4\theta(z)$ VANISHES:

$$K'_{33} - K'_{11} = 2K_{13} \tag{45}$$

With the obtaining of the relation (45) I confirm the validity of the relation between the elastic constants K'_{11}, K'_{33} and K_{13} in nematics obtained previously.[1] This relation show that the K_{13} elastic constant is a purely nonlinear (anisotropic) constant. Further, from the relations (1) and (3) one can obtain the value of the Frank elastic constants:

$$K_{11} = K'_{33} \quad \text{and } K_{33} = K'_{11} \tag{46}$$

At the first sight it is strange that elastic constants designating splay or bend are interchanged. In my opinion however, the quantities K_{11} and K_{33} being used in the notations by Nehring and Saupe[2,7] should be considered as mathematical quantities with a given value while the elastic constants of Frank K_{11} and K_{33} should be equal to the elastic constants of Oseen-Nehring-Saupe K'_{11} and K'_{33}, respectively:

$$K_{11} = K'_{11},\ K_{33} = K'_{33} \tag{47}$$

This suggestion follows from the fact that in general when the two bulk elastic constants K'_{11} and K'_{33} are not equal, the K_{13} second-order splay-bend elastic constant according to the results obtained previously[1] and those obtained in this paper cannot be zero. In other words, in the elastic energy obtained by Frank[12] the elastic constants of splay K_{11} and bend K_{33} coincide with those proposed by Oseen-Nehring-Saupe while the K_{13}div(ndivn) term has been neglected.

It is important to point out also that the relation (45) used in the expression for the elastic energy of the nematic film under consideration (34) unambigously show that the inclusion of the K_{13} elasticity leads to *decrease of the elastic deformational energy for all possible solutions even without taking into account the exact kind of the boundary conditions*:

$$I = \int_{-d/2}^{+d/2} \theta'^2((1/2)(K_{11}\cos^2\theta + K_{33}\sin^2\theta)$$

$$- (K_{13}^2/f(\theta))\sin^2\theta\cos^2\theta)\, dz \quad \text{where } f(\theta) = K'_{11}\cos^2\theta + K'_{33}\sin^2\theta > 0 \quad (48)$$

Further, it is important to point out also that the solution of the problem and the variation of θ and θ' at the boundaries are not predetermined after the use of the differential equation. The boundary conditions for the case of continuous functions have no any importance for the calculations presented previously[1] and in this paper. Finally, all solutions leading to negative value of the elastic energy are neglected since in the real experiments *spontaneous deformations* in nematics have not been observed.

IV. On the relation between K'_{11}, K'_{33} and K_{13} obtained previously[1]: discussion of the one-dimensional ease including splay-twist-bend deformations

In this part of the paper it is demonstrated that the inclusion of twist in the splay-bend deformations does not change the validity of the relation between K_{13}, K'_{33} and K'_{11}.

Consider the elastic energy of a completely free nematic film accepting that the deformation starts from initially planar orientation of the director and includes not only θ-polar elastic deformations but also ϕ-azimuthal elastic deformations.[8] The total elastic energy per unit area including the K_{13} second-order elasticity has the form:

$$I = \int_0^d (1/2)f(\theta)\theta'^2 + (1/2)g(\theta).\, \phi'^2 + K_{13}\cos 2\theta\theta'^2 + K_{13}\sin\theta\cos\theta\theta'')dz \quad (49)$$

where

$$f(\theta) = K'_{11}\cos^2\theta + K'_{33}\sin^2\theta$$

$$g(\theta) = (K_{22}\cos^2\theta + K'_{33}\sin^2\theta)\cos^2\theta$$

The differential equation of Euler-Lagrange

$$2f(\theta)\theta'' + \theta'(d/d\theta)f(\theta) - \phi'^2\,(d/d\theta)g(\theta) = 0 \tag{50}$$

and

$$g(\theta)\,\phi'' + \theta'\,\phi'\,(d/d\theta)g(\theta) = 0 \tag{51}$$

can be integrated once to obtain:[8]

$$g(\theta)\phi' = a;\ f(\theta)\theta'^2 + g(\theta)'^2 = b \tag{52}$$

In this case I follow the same way of solution. First, θ'' is determined from the differential equation (50) and used in the expression for the elastic energy (49). After simple calculations one obtains:

$$I = \int_0^d dz\theta'^2\left((1/2)f(\theta) + K_{13}\cos 2\theta - \frac{K_{13}(K'_{33} - K'_{11})\sin^2\theta\cos^2\theta}{f(\theta)}\right)$$

$$+ \frac{\phi'^2\cos^2\theta}{2f(\theta)}(K'_{11}(K_{22}\cos^2\theta + K'_{33}\sin^2\theta) + 2(K'_{33} - K'_{11})(K'_{33} - K'_{22})\sin^2\theta) \tag{53}$$

It is easy to verify that the term multiplying $(\phi'^2\cos^2\theta/2f(\theta))$ is always positive when the K_{13} elastic constant is determined from the relation (1). Consequently, the inclusion of twist in the one-dimensional splay-bend deformations does not change the relation between K_{13}, K'_{33} and K'_{11}.

CONCLUSION

From the theoretical results obtained previously[1] and elaborated in this paper it is evident that the K_{13} elastic constant is a purely nonlinear (anisotropic) elastic constant expressed with the difference between the bend elastic constant K'_{33} (or K_{33}) and splay elastic constant K'_{11} (or K_{11}).

The anisotropic character of the elastic constants K_{13} and K_{24} in nematics will be discussed on the basis of a general tensor analysis in a near future.

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