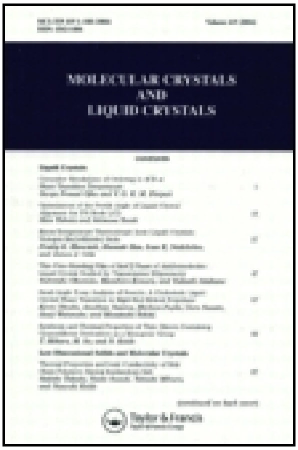

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New Theoretical Proofs for the Existence of the Three-Dimensional Solution of the K_{13} Elastic Problem in Nematics

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New Theoretical Proofs for the Existence of the Three-Dimensional Solution of the K_{13} Elastic Problem in Nematics

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The variation of bulk elastic terms of a divergent type in the energy of nematics and cholesterics is performed by direct tensor calculations. The molecular surface field of a completely free uniaxial nematic is obtained. The K_{13} elastic contribution is compared to that obtained earlier (Mol. Cryst. Liq. Cryst., **148**, 197 (1987)). The kind of the surface molecular field is checked by appropriate calculations and discussed relative to the anchoring of the liquid crystal.

Keywords: K_{13} elastic problem, 3-D variation

I. INTRODUCTION

It is well known that in the expressions of the elastic energy of uniaxial and biaxial nematics, cholesterics and some smectics there are elastic terms of a divergent type which after integration can be transformed into surface terms. Some divergent elastic terms contain only tangential space derivatives of the functions which define the orientation of the liquid crystal. Other divergent elastic terms contain also normal space derivatives. The variation of the former terms at minimization of the elastic energy is trivial while the variation of the letter terms has not been resolved in the past. First we regard the simpler case of uniaxial nematic.

The density of the elastic energy of a uniaxial nematic including divergent terms has the well known form:

$$2W = K'_{11}(\mathrm{div}\underline{n})^2 + K_{22}(\underline{n}.\mathrm{rot}\underline{n})^2 + K'_{33}(\underline{n}x\,\mathrm{rot}\underline{n})^2 - (K_{22} + K_{24})\mathrm{div}(\underline{n}\mathrm{div}\underline{n} + \underline{n}x\,\mathrm{rot}\underline{n}) + 2K_{13}\mathrm{div}(\underline{n}\mathrm{div}\underline{n}) \quad (1)$$

where K'_{11}, K_{22} and K'_{33} are elastic constants of splay, twist and bend, K_{24} and K_{13} are elastic constants of mixed bend-twist and splay-bend respectively.

The density of the $(K_{22} + K_{24})$ elastic energy of uniaxial nematic has been written in various mathematical forms since the "director" $\underline{n}$ has been defined as a unit vector.[1-8] We prefer the mathematical form which was used for the first time by Dubois-Violette and Parodi.[3] The density of the K_{13} elastic energy has been introduced in the elastic energy of nematics by Oseen,[9-11] later it has been disregarded and finally reintroduced by Nehring and Saupe.[2,12] The $(K_{22} + K_{24})$ elastic energy does not contain normal space derivatives of the "director" since they cancel between $\text{div}(\underline{n}\,\text{div}\underline{n})$ and $\text{div}(\underline{n}x\,\text{rot}\underline{n})$[1,2,6] and its variation is trivial.[13-16] The K_{13} elastic energy however, contain not only tangential space derivatives of the "director" but also normal space derivatives. The inclusion of surface terms with normal space derivatives of the "director" (the differential equations which describe the elastic behavior of the nematics are usually of a second order) leads to a novel variational task which solution is accompanied by great mathematical difficulties.

The one-dimensional solution of the K_{13} elastic problem in nematics was obtained by the author of this paper in 1977.[17] The one-dimensional case of the K_{13} elastic problem can be resolved in several different ways.[18] The similarity in these solutions is the use of inverse function $z(\theta)$, where θ is the deformational angle in the functional, which is varied with a movable boundary. This movable boundary scans the liquid crystal orientation near the real boundary while the surface torques are concentrated in the boundary. Such a minimization of the K_{13} elastic energy can be performed only with the aid of extremals, solutions of the Euler-Lagrange equations which should be satisfied at the boundary as well. This solution exists only for the case of weak anchoring of nematic. In 1984 it was criticized by some authors (see the discussion in References 18 and 19). They claimed that such a solution does not minimize the elastic energy of nematics and that the elastic problem has not a solution with continuous functions in the second-order approximation. They showed that arbitrary functions which change strongly in the boundary regions and weakly in the bulk can decrease the elastic energy for some values of the second order elastic constant K_{13}. We cannot accept their claims since they contradict first to the way of obtaining of the elastic energy of nematics which is valid for small deformations in the length scale.[1,2,9-12] Second they contradict to the divergent type of this energy and third they do not take into account the ability of the nematic to resist of the mixed splay-bend deformations at some relations between the elastic constants.[19,20] On the other hand the three-dimensional solution can aid in resolving of this dispute.

The three-dimensional solution of the K_{13} elastic problem in nematics was found in 1987 on the basis of variational arguments and calculations of Ericksen and Toupin.[18] This solution was able to distinguish between the divergent and non-divergent elastic terms included in the surface energy of nematics by Nehring and Saupe[2,12] and by Mada[21] showing that the elastic problem has a solution only for the former case. Since the problem is still discussional and the three-dimensional solution of the K_{13} elastic problem is based on general assumptions and important relations given *ad hoc* by Toupin,[22] it is necessary to recalculate this solution for the simpler case of a non-movable nematic. During the calculations we have used some important results obtained by McConnel.[23] The general kind of the surface molecular field is obtained for completely free non-polar uniaxial nematic. Part of this molecular surface field which is due to variation of the bulk divergent terms is checked by appropriate calculations. Finally, the importance of the surface molecular field is discussed relative to the anchoring of the nematic.

II. SURFACE GEOMETRY

Let us suppose that the nematic liquid crystal is completely free and fills a nonmovable volume bounded by arbitrary curved surface designated by S. In the beginning a brief summary of the geometry of surfaces is presented with notations used by Jenkins and Barratt.[24] It is convenient to employ Cartesian tensor notation, and therefore Latin subscripts on tensor quantities take the values 1, 2 and 3 and the summation convention applies to repeated indices. The comma preceding a Latin subscript denotes partial differentation with respect to the corresponding space Cartesian coordinate. The Greek indices on the surface parameters u^{α} take values 1 and 2, and a comma preceding a Greek subscript denotes partial differentation with respect to the corresponding surface parameter. Further, the summation convention applies to a repeated Greek index occurring once as a subscript and once as a superscript.

Referring to a fixed set of rectangular Cartesian coordinates, the components of the position vector $\underline{x}$ of a point on a surface have the parametric representation

$$x_i = x_i(u^{\alpha}) \tag{2}$$

and the vectors $\underline{x}_{i,\alpha}$ are tangent to the u^{α} curves in the surface.

The square of the differential element of length dl in the surface is

$$dl^2 = x_{i,\alpha}x_{i,\beta}du^{\alpha}du^{\beta} = a_{\alpha\beta}du^{\alpha}du^{\beta} \tag{3}$$

Under a change of parameters, the quantity $a_{\alpha\beta}$ transforms as a second-order covariant tensor, and is the first fundamental form of the surface. Assuming that $a \equiv \det(a_{\alpha\beta}) > 0$, the contravariant surface tensor $a^{\alpha\beta}$ associated with $a_{\alpha\beta}$ is defined by

$$a^{\alpha\gamma}a_{\gamma\beta} = \delta^{\alpha}_{\beta} \tag{4}$$

where δ^{β}_{α} is the surface Kroneker delta ($= 1$, $\alpha = \beta$; $= 0$, $\alpha \neq \beta$). The surface unit normal ν has components

$$\nu_i = \left(\frac{1}{2}\right) \varepsilon^{\alpha\beta}\varepsilon_{ijk}x_{j,\alpha}x_{k,\beta} \tag{5}$$

where ε_{ijk} is the Cartesian alternating tensor and the surface permutation tensor $\varepsilon_{\alpha\beta}$ is defined by

$$\varepsilon_{12} = -\varepsilon_{21} = a^{1/2}, \quad \varepsilon_{11} = \varepsilon_{22} = 0 \tag{6}$$

and the associated contravariant tensor $\varepsilon^{\alpha\beta}$ by

$$\varepsilon^{12} = -\varepsilon^{21} = a^{-1/2}, \quad \varepsilon^{11} = \varepsilon^{22} = 0 \tag{7}$$

Equivalently

$$\varepsilon^{\alpha\beta} = a^{\alpha\gamma}a^{\beta\lambda}\varepsilon_{\gamma\lambda} \tag{8}$$

For later use, it follows that

$$\nu_j\nu_j = 1, \quad x_jx_{j,\beta} = 0 \tag{9}$$

$$b_{\alpha\beta} = -\nu_{i,\alpha}x_{i,\beta} = -\nu_{i,\beta}x_{i,\alpha} \tag{10}$$

and $b_{\alpha\beta}$ is the second fundamental form of the surface. The expression (5) for the unit normal vector clearly shows that it is a covariant space vector and scalar in the surface. Similarly, $b_{\alpha\beta}$ is a symmetric tensor of second rank in the surface and scalar in the space.

III. ON SOME RESULTS OF McCONNEL.[23] SURFACE DIVERGENCE OF A SPACE VECTOR

During the calculations we have used also results obtained by McConnel.[23] We present these results with notations used by Jenkins and Barratt[24] as follows:

1) The *surface divergence* of the *space vector* A_i $(A_{i,i})$ defined over the surface is expressed by $g_{ij}a^{\alpha\beta}A_{i/\alpha}x_{j,\beta}$ which is scalar, where the vertical line preceding the Greek subscript denotes covariant differentation. For the case of rectangular Cartesian space coordinates, the space metric tensor is equal to the unit tensor and the covariant differentation is replaced by partial differentation.[23] Consequently, the surface divergence of the space vector A_i defined over the surface in our case is expressed by $a^{\alpha\beta}A_{i,\alpha}x_{i,\beta}$. This definition can be proved by direct tensor calculations.

2) The surface divergence of the unit normal vector ν is equal to $-2H$, where H is the mean curvature of the surface:

$$H = \left(\frac{1}{2}\right) b_{\alpha\beta}a^{\alpha\beta} \tag{11}$$

This result can be proved by direct tensor calculations.

3) Any space vector A_i defined over the surface can be expressed according to McConnel[23] in terms of tangent vectors and the unit normal by

$$A_i = D\nu_i + B^{\alpha}x_{i,\alpha} \tag{12}$$

where

$$D = (A_i\nu_i), \quad B^{\alpha} = A_i x_{i,\beta}a^{\alpha\beta} \tag{13}$$

and the surface divergence of the space vector will be

$$B^{\alpha}_{/\alpha} - 2DH = (1/a^{1/2})(\partial/\partial u^{\alpha})(a^{1/2}B^{\alpha}) - 2DH \tag{14}$$

where the vertical line preceding the Greek subscript denotes covariant differentation. This result can be proved by direct tensor calculations.

4) If we take a close curve on the surface S and integrate the surface divergence of the space vector A_i on the inner surface S bounded by the close curve C, then one obtains:

$$\int_S a^{\alpha\beta}A_{i,\alpha}x_{i,\beta}dS = \int_C B^{\alpha}(du^{\alpha}/ds)ds - 2\int_S DH\, dS \tag{15}$$

IV. ON THE VARIATION OF THE K_{13} SURFACE VOLUME-LIKE ELASTIC ENERGY OF NEMATICS

The variation of the K_{13} elastic term with respect to the director $\underline{n}$ yields:

$$\delta\left(K_{13}\int_S(\underline{n}.\nu)\mathrm{div}\underline{n}\; dS\right) = K_{13}\int_S(\delta\underline{n}.\nu)\mathrm{div}\underline{n}\; dS + K_{13}$$

$$\int_S(\underline{n}.\nu)\mathrm{div}\delta\underline{n}\; dS = K_{13}\int_S(\delta\underline{n}.\nu)\mathrm{div}\underline{n}\; dS + K_{13}$$

$$\int_S \mathrm{div}((\underline{n}.\nu)\delta\underline{n})dS - K_{13}\int_S \delta\underline{n}.\mathrm{grad}(\underline{n}.\nu)\; dS \tag{16}$$

It is convenient to express the variation $\delta\underline{n}$ as a sum of the variation of the normal component $\delta\underline{n}_{\parallel}$ and the variation of the tangential component $\delta\underline{n}_{\perp}$

$$\delta\underline{n} = \delta\underline{n}_{\parallel} + \delta\underline{n}_{\perp} \tag{17}$$

and to use the Lagrange vector identity:

$$\delta\underline{n}(\nu.\nu) = (\delta\underline{n}.\nu)\nu + \nu x(\delta\underline{n}x\nu) = (\delta\underline{n}.\nu)\nu + \delta\underline{n}_{\perp} \tag{18}$$

since $\delta\underline{n}_{\parallel}\, x\nu = 0$

Taking into account this result and that obtained by McConnel[23] (see the preceding paragraph), the integrand

$$K_{13}\int_S \mathrm{div}((\underline{n}.\nu)\delta\underline{n})dS \tag{19}$$

after some calculations is transformed into

$$K_{13}\int_S \mathrm{div}((\underline{n}.\nu)((\delta\underline{n}.\nu)\nu + \delta\underline{n}_\perp))\, dS$$

$$= -2K_{13}\int_S (\underline{n}.\nu)(\delta\underline{n}.\nu)H\, dS + K_{13}\int_C a^{\alpha\beta}\underline{x}_{,\beta}(\underline{n}.\underline{\nu})\delta\underline{n}\mu_\alpha dl \tag{20}$$

where

$$B^\alpha = \delta n_i x_{i,\beta}a^{\alpha\beta}, \quad \delta n_{\parallel i}x_{i,\beta} = 0, \quad H = \left(\frac{1}{2}\right) b_{\alpha\beta}a^{\alpha\beta} \tag{21}$$

and $\mu_\alpha = \varepsilon_{\alpha\beta}(du^\beta/dl)$ is the outward normal to C.
The linear integrand will be not taken into account further.

V. GENERAL KIND OF THE SURFACE MOLECULAR FIELD FOR COMPLETELY FREE NON-MOVABLE AND NON-POLAR NEMATIC

The surface molecular field has been introduced for the first time in the theory of nematics by de Gennes.[25] We present the general kind of this field for the case of completely free non-movable and non-polar uniaxial nematic.

The density of the elastic energy of such a nematic including the K_{13} elasticity in tensor notations has the following form[24,26–29]:

$$\begin{aligned}2U = {} & K_{22}n_{i,k}n_{i,k} + K_{24}n_{i,k}n_{k,i} + (K'_{11} - K_{22} - K_{24})n_{i,i}n_{k,k} \\ & + (K'_{33} - K_{22})n_k n_j n_{i,k}n_{i,j} + 2K_{13}n_{i,i}n_{k,k} \\ & + 2K_{13}n_k n_{i,ik} = 2U_1 + 2K_{13}n_{i,i}n_{k,k} + 2K_{13}n_k n_{i,ik}\end{aligned} \tag{22}$$

where

$$(\mathrm{div}\underline{n})^2 = n_{i,i}n_{k,k}$$

$$(\underline{n}x\mathrm{rot}\underline{n})^2 = n_k n_j n_{i,k}n_{i,j}$$

$$(\underline{n}.\mathrm{rot}\underline{n})^2 = n_{i,k}n_{i,k} - n_{i,k}n_{k,i} - n_k n_j n_{i,k}n_{i,j}$$

$$\mathrm{div}(\underline{n}\mathrm{div}\underline{n} + \underline{n}x\mathrm{rot}\underline{n}) = n_{i,i}n_{k,k} + n_{i,k}n_{k,i} \tag{23}$$

The minimization of the elastic energy of a free nematic confined in a volume V bounded by a surface S with an arbitrary form has been recently performed.[18] According to these results, the surface molecular field is expressed as follows:

$$F_i = \nu_k(\partial U_1/\partial n_{i,k}) - K_{13}\nu_i(\nu_k n_k)b_{\alpha\beta}a^{\alpha\beta} - K_{13}\nu_k D_i(n_k) + 2K_{13}\nu_i n_{k,k} \quad (24)$$

where $b_{\alpha\beta}a^{\alpha\beta} = 2H$, and H is the mean curvature of the surface, D_i are tangential gradients of the director components.

According to the results obtained in this paper, the surface molecular field has a slightly different form:

$$F_i = \nu_k(\partial U_1/\partial n_{i,k}) - K_{13}\nu_i(\nu_k n_k)b_{\alpha\beta}a^{\alpha\beta} - K_{13}(\nu_k n_k)_{,i} + 2K_{13}\nu_i n_{k,k} \quad (25)$$

The surface molecular field according to (22) and (25) can be written in the following tensor form:

$$\begin{aligned} F_i = {} & K_{22}\nu_k n_{i,k} + K_{24}\nu_k n_{k,i} + (K'_{11} - K_{22} - K_{24})\nu_i n_{k,k} \\ & + (K'_{33} - K_{22})\nu_k n_k n_j n_{i,j} + 2K_{13}\nu_i n_{k,k} - K_{13}\nu_i\nu_k n_k b_{\alpha\beta}a^{\alpha\beta} - K_{13}(n_k\nu_k)_{,i} \quad (26) \end{aligned}$$

or in the more convenient vector form:

$$\begin{aligned} \underline{F} = {} & K_{22}(\nu.\text{grad})\underline{n} + K_{24}((\nu.\text{grad})\underline{n} + (\nu x\text{rot}\underline{n})) \\ & + (K'_{11} - K_{22} - K_{24} + 2K_{13})\nu\text{div}\underline{n} \\ & + (K'_{33} - K_{22})(\nu.\underline{n})(\underline{n}x\text{rot}\underline{n}) + K_{13}\nu(\nu.\underline{n})\text{div}\nu - K_{13}\text{grad}(\underline{n}.\nu) \quad (27) \end{aligned}$$

where $\text{div}\nu = -b_{\alpha\beta}a^{\alpha\beta}$

VI. DISCUSSION OF THE OBTAINED THEORETICAL RESULTS

We can simply check the correctness of those terms in the surface molecular field which are connected with the variation of the bulk divergent elastic energy. It was mentioned that the variation of the $(K_{22} + K_{24})$ elastic energy is trivial since it contains only tangential space derivatives of the "director." However this energy can be presented as a sum of $\text{div}(\underline{n}\text{div}\underline{n})$ and $\text{div}(\underline{n}x\text{rot}\underline{n})$. Such elastic terms multiplied by different elastic constants exist in the elastic energy of biaxial nematics.[5,30-32] It is clear that the sum of the solutions obtained for a separate variation of these two divergent energies which contain also normal space derivatives of "director" should be equal to the solution obtained for variation of their sum which is trivial. In this way it is possible the simultaneously check of the correctness of the variation of the K_{13} elastic energy and $(K_{22} + K_{24})$ elastic energy.

The variation of the bulk elastic energy with a divergent term of the type $\mathrm{div}(\underline{n}x\mathrm{rot}\underline{n})$ is performed in a similar manner:

$$\delta\left(\int_S (\underline{n}x\mathrm{rot}\underline{n}).\nu\, dS\right) = \int_S [((\mathrm{rot}\underline{n}x\nu) + \mathrm{rot}(\nu x\underline{n})$$

$$- \nu(\underline{n}.\nu)\mathrm{div}\nu)\delta\underline{n}]dS = \int_S [(-2(\nu.\mathrm{grad})\underline{n} - 2(\nu x\mathrm{rot}\underline{n})$$

$$+ \mathrm{grad}(\underline{n}.\nu) + \nu\mathrm{div}\underline{n} - \nu(\underline{n}.\nu)\mathrm{div}\nu)\delta\underline{n}]dS \quad (28)$$

(During the calculations we have used a number of vector relations.) On the other hand the variation of the divergent elastic energy of the type $\mathrm{div}(\underline{n}\mathrm{div}\underline{n})$ according to our calculations performed in section IV gives:

$$\delta\left(\int_S (\underline{n}.\nu)\mathrm{div}\underline{n}\, dS\right) = \int_S [(-\mathrm{grad}(\underline{n}.\nu) + \nu\mathrm{div}\underline{n} + \nu(\underline{n}.\nu)\mathrm{div}\nu)\delta\underline{n}]dS \quad (29)$$

The sum of relations (28) and (29) yields exactly the result of variation of the $(K_{22} + K_{24})$ elastic energy (see the general kind of the surface molecular field Equation (27)). It is necessary to point out that the term $K_{22}\ \nu_k n_{k,i}$ which comes from the variation of the divergent energy cancels with the similar term obtained from the variation of the bulk twist energy. This cross check clearly shows the correctness of our calculations.

Finally we discuss the influence of the anchoring of the liquid crystal with respect to the general kind of the surface molecular field expressed by Equation (27). The surface elastic energy is written usually in the following simple form[33]:

$$\left(\frac{1}{2}\right) W_s(\nu.\underline{n})^2$$

where W_s is the strength coupling constant which takes into account the interaction of the liquid crystal with the boundary.

In the conventional cells, the liquid crystal is anchored by the walls and this anchoring can be either strong or weak. In the former case the liquid crystal orientation is nearly fixed at the wall and the surface molecular field is not significant for the orientation of the liquid crystal. For the case of weak anchoring, additional term of the kind

$$W_s(\nu.\underline{n})$$

has to be added to the surface molecular field. In general the surface energy can be a complex function of $(\nu.\underline{n})$ and the only requirement is to be an even function of $(\nu.\underline{n})$.

Our theoretical results clearly show that the coupling between the tangential and normal space derivatives of the "director" at the variation is effected by the curvature of the surface which bounds the volume containing the liquid crystal. For the one-dimensional solution,[17,18] the coupling between the deformational angle at the boundary and the normal derivative of this angle is effected with the aid of bulk behavior of the nematic and validity of the Euler—Lagrange equations at the boundary.

In conclusion, the variation of bulk divergent terms of the kind $\mathrm{div}(\underline{n}\,\mathrm{div}\underline{n})$ and $\mathrm{div}(\underline{n}\times\mathrm{rot}\underline{n})$ which are in the elastic energy of nematics is performed by direct tensor calculations. The molecular surface field of a uniaxial nematic is obtained in tensor and vector forms. Its kind is checked by appropriate calculations and discussed relative to the anchoring of the liquid crystal. The comparison of the K_{13} contribution with that obtained earlier[18] shows that the term including the curvature of the surface is the same while the gradient terms are different. The possible causes for this difference will be discussed in the near future.

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