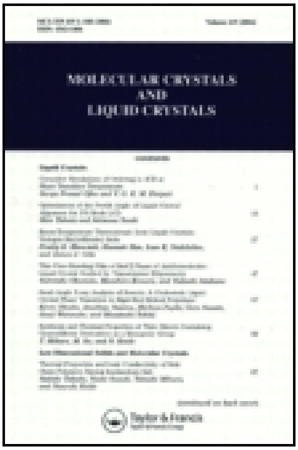

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On the Variation of the K_{13} Nematic Surface-Like Volume Energy and the Nematic Surface Energy of Mada†,‡

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Two possible ways of the one-dimensional variation of the K_{13} nematic surface-like volume energy are discussed. The first way of variation when the deformation angle θ and its derivative θ' are considered as independent functions at the boundary shows that the K_{13} problem has no solution. The second way of variation when θ and θ' are considered as dependent functions at the boundary shows that the problem can be solved by introducing of the inverse function and variation of a functional with a movable boundary. The three-dimensional solution for a variational problem including a nematic energy density containing both first and second spatial gradients has been found on the basis of *Ericksen & Toupin* variational arguments. The surface and body forces as well as the generalized surface and body forces were obtained. The surface molecular field including the K_{13} term was obtained in explicit form. This field for the one-dimensional case unambiguously confirms the validity of our boundary conditions previously obtained (J. Physique **38**, 1013, 1977). On the basis of our unpublished theoretical calculations and experimental results obtained by other researchers for some electrooptical effects, we have estimated that the value of K_{13} for the nematic MBBA at room temperature is slightly smaller than half of the splay elastic coefficient K'_{11}. In analogy with the solution of the K_{13} elastic problem and using the variational arguments of *Ericksen & Toupin* we have obtained the surface and body forces as well as the generalized surface and body forces for the case of Mada elastic energy.

Keywords: nematic, K_{13} surface-like volume energy, surface energy of Mada, one-dimensional variation, three-dimensional variation, variational arguments of Ericksen & Toupin

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‡The three-dimensional analysis was included in the revised version of the paper.[36]

I. INTRODUCTION

Recently Oldano and Barbero[1-3] critically discussed our theoretical way of the one-dimensional variation of the nematic second-order elastic energy,[4-8] derived for the first time by Oseen,[9-11] later disregarded and finally reintroduced in the elastic energy by Nehring and Saupe[12,13] (let us point out the work of Lubensky for the calculation of the splay elastic coefficient K_{11} who included also second-order elastic effects[14]). Later, a general type of the surface energy of a nematic fluid including also normal derivatives of the nematic "director" with respect to the coordinates has been obtained by Dubois-Violette and Parodi.[15]

The differential equations and boundary conditions for the energy functionals of nematic layers with a fixed boundary are clarified with the examples given by Schechter[16] in the table shown in Figure 1. Ericksen[17] and Jenkins and Barratt[18] studied in detail the variational problem for the elastic behavior of a nematic layer with a movable boundary. Their theory permits the exact solution of this problem when the type of the surface energy is known. The details in the variational problems for the case of nematics such as the conditions of Legandre, Jacobi and Weierstrass both for the one-dimensional case[19,20] and their analogs for the two- and three-dimensional cases[21] have been insufficiently studied due to the difficulties in the analysis of unstable solutions often accompanied by a hydrodynamical movement of the fluid. The inclusion of surface terms with normal 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[22] which solution is accompanied by great mathematical difficulties. The physical interpretation also raised many questions. For that reason these terms were usually disregarded by the researchers. Nevertheless, some authors dealt with this problem[1-8,23-34] due to the importance both from theoretical or practical point of view (immediately we must stress however, that after the publication of the papers of Oldano and Barbero[1-3] some authors rejected their earlier results).[3,35]

The aim of this paper is to clarify our way of the one-dimensional variation of the K_{13} surface-like volume energy and to solve the three-dimensional case based on Ericksen & Toupin variational arguments.[36]

According to Oldano and Barbero[1-3] the deformation angle θ and its derivative with respect to the coordinate, Z, θ', and consequently their variations $\delta\theta$ and $\delta\theta'$ ARE INDEPENDENT FUNCTIONS at

Функционал	Уравнения Эйлера – Лагранжа	Граничные условия
а) $I = \int_a^b F(x, w, w_x)\,dx + g_b(x, w)\|_{x=b} - g_a(x, w)\|_{x=a}$	$\frac{\partial F}{\partial w} - \frac{d}{dx}\frac{\partial F}{\partial w_x} = 0$	$\left(\frac{\partial F}{\partial w_x} + \frac{\partial g_a}{\partial w}\right)\delta w\Big\|_{x=a} = 0$ $\left(\frac{\partial F}{\partial w_x} + \frac{\partial g_b}{\partial w}\right)\delta w\Big\|_{x=b} = 0$
б) $I = \int_a^b F(x, w, w_x, w_{xx})\,dx + g_b(x, w, w_x)\|_{x=b} - g_a(x, w, w_x)\|_{x=a}$	$\frac{\partial F}{\partial w} - \frac{d}{dx}\frac{\partial F}{\partial w_x} + \frac{d^2}{dx^2}\frac{\partial F}{\partial w_{xx}} = 0$	$\left(\frac{\partial F}{\partial w_{xx}} + \frac{\partial g_a}{\partial w_x}\right)\delta w_x\Big\|_{x=a} = 0$ $\left(\frac{\partial F}{\partial w_{xx}} + \frac{\partial g_b}{\partial w_x}\right)\delta w_x\Big\|_{x=b} = 0$ $\left(\frac{\partial F}{\partial w_x} - \frac{d}{dx}\frac{\partial F}{\partial w_{xx}} + \frac{\partial g_a}{\partial w}\right)\delta w\Big\|_{x=a} = 0$ $\left(\frac{\partial F}{\partial w_x} - \frac{d}{dx}\frac{\partial F}{\partial w_{xx}} + \frac{\partial g_b}{\partial w}\right)\delta w\Big\|_{x=b} = 0$
в) $I = \int_S F(x, y, w, w_x, w_y)\,dS + \int_C [g_1(x, y, w)\,t_2 - g_2(x, y, w)\,t_1]\,ds$	$\frac{\partial F}{\partial w} - \frac{\partial}{\partial x}\frac{\partial F}{\partial w_x} - \frac{\partial}{\partial y}\frac{\partial F}{\partial w_y} = 0$	$\left[\left(\frac{\partial F}{\partial w_x} + \frac{\partial g_1}{\partial w}\right)t_2 - \left(\frac{\partial F}{\partial w_y} + \frac{\partial g_2}{\partial w}\right)t_1\right]\delta w = 0$ на кривой C
г) $I = \int_V F(x, y, z, w, w_x, w_y, w_z)\,dV + \int_S [g_1(x, y, z, w)\cos(n, x) + g_2(x, y, z, w)\cos(n, y) + g_3(x, y, z, w)\cos(n, z)]\,dS$	$\frac{\partial F}{\partial w} - \frac{\partial}{\partial x}\frac{\partial F}{\partial w_x} - \frac{\partial}{\partial y}\frac{\partial F}{\partial w_y} - \frac{\partial}{\partial z}\frac{\partial F}{\partial w_z} = 0$	$\left[\left(\frac{\partial F}{\partial w_x} + \frac{\partial g_1}{\partial w}\right)\cos(n, x) + \left(\frac{\partial F}{\partial w_y} + \frac{\partial g_2}{\partial w}\right)\cos(n, y) + \left(\frac{\partial F}{\partial w_z} + \frac{\partial g_3}{\partial w}\right)\cos(n, z)\right]\delta w = 0$ на поверхности S

FIGURE 1 A table given by Schechter[16] which shows some types of functionals, their differential equations and boundary conditions for the case of a fixed boundary.

the boundary of the liquid crystal (this possibility was rejected by me in 1979 year since I have obtained FOUR boundary conditions for TWO integral constants,[37] a result obtained independently by Oldano and Barbero[1-3] as well). According to our results[4-8] however, θ and θ', and consequently their variations $\delta\theta$ and $\delta\theta'$, can be considered as DEPENDENT FUNCTIONS at the boundary and this dependence is revealed through the BULK behavior of the liquid crystal and validity of the differential equation at the boundary (see Ref. 20, p. 64). The boundary conditions obtained by us were rigorous[4-8] whereas other authors obtained approximate boundary conditions using approximate variational methods such as those of Ritz and Galerkin, etc.[28,29] Since this problem is IMPORTANT and now DISCUSSIONAL not only for the case of the nematics, but also for the smectics A[38], smectics C,[39,40] biaxial nematics[41,42] and even for the liquid-crystalline polymers,[43] we address ourselves again to its solution.

In the first part of the paper we briefly discuss the one-dimensional solution of the K_{13} problem, obtained by us in Ref. 6 and used by a number of authors.[30-32] In the second part following the advice of the Referee of Mol. Cryst. Liq. Cryst. we present the three-dimensional calculations of the K_{13} variational problem using Ericksen & Toupin variational arguments and briefly discuss the validity of the one-dimensional solution. In the third part we estimate the value of the second-order elastic coefficient K_{13} on the basis of our unpublished theoretical calculations[37] and old experimental results obtained by other authors for the behavior of a homeotropic nematic MBBA layer under the influence of either a transversal electric field leading to a flexoelectric bending or under the influence of a normal electric field leading to a Frederiks transition. Finally we obtain and discuss the three-dimensional solution for the case of the elastic energy of nematics, proposed by Mada.[25]

II. ON THE VARIATION OF THE K_{13} SURFACE-LIKE VOLUME ENERGY WHEN θ AND θ' ARE DEPENDENT FUNCTIONS AT THE BOUNDARY

Let us first briefly discuss the solution proposed by Oldano and Barbero.[1-3] Evidently such a solution contradicts to the theorem of Ostrogradski-Gauss and consequently to the continuity of the function θ and its derivative θ'. On the other hand, such a solution shows also that the surface-like volume elastic terms with normal derivatives "are important" only in a thin boundary layer. Oldano and Barbero made the incorrect conclusion that the theory of Nehring and Saupe[12] and as a consequence all elastic theories for the smectics A, smectics C, biaxial nematics and liquid-crystalline polymers, etc. must be revised with respect to the surface interactions (we regard one completely free liquid crystal). However, it is easy to show that the change of the surface energy with inclusion of new terms *does not exhaust* the K_{13} variational problem since it *continues to exist*, now at the inner boundary $z = \rho$.[1-3] Consequently the claim of Oldano and Barbero leads to *a revision* of the elastic theories for the liquid crystals *not only in the boundary regions but also in the bulk*. If we accept for an instance that higher order elastic terms are included in the elastic energy of the nematics or the other liquid crystals, then new divergent elastic terms will appear in the energy. Evidently in these cases the variational problem will be much more complex and the same problems will be open for explanation. The acceptance that θ and θ' are independent functions at the boundary clearly shows that the variational problem *has no solution*. Mathematically this means that the variational problem has no solution in the class of the functions which are determined at the boundary by the value of the very function and its derivative. According to Mishkis[44] in such cases we must search the solution in *a wider class* of functions. This leads immediately to the assumption that θ and θ' are dependent at the boundary. This was the general idea in our works when we had obtained the rigorous boundary condition including the K_{13} term.

For the case of a deformed nematic layer we consider the functional

$$I = \int_0^d F(\theta,\theta',z)\,dz + \{(-K_{13}\sin 2\theta\theta') + (1/2)W_s(\theta - \theta_0)^2\}_{z=d} \tag{1}$$

where K_{13} and W_s are the second-order elastic coefficient and the surface coupling coefficient, respectively. Let us accept a strong homeotropic anchoring of the nematic layer at the boundary $z = 0$, i.e. $\theta(0) = 0$.

We will show first that for the case of the EXTREMALS, the variations $\delta\theta$ and $\delta\theta'$ *are dependent functions* at the boundary. For the functional (1) they satisfy the following equation of Euler & Lagrange:

$$F_\theta - (F_{\theta'})' = 0 \tag{2}$$

where the differentiation is with respect to z.

Let the curves $\theta(z)$ and $\theta = \theta(z) + \delta\theta$ are two infinitely close extremals. With the accuracy of the higher order terms the variation $\delta\theta$ must satisfy the equation of Jacobi (see Ref. 20, pp. 202, 203):

$$F_{\theta\theta}\,\delta\theta + F_{\theta\theta'}\,\delta\theta' - (F_{\theta\theta'}\,\delta\theta + F_{\theta'\theta'}\,\delta\theta')' = 0 \quad (3)$$

describing the behavior of the extremals (see Ref. 45, p. 305). Since this equation is of a second order, $\delta\theta$ and $\delta\theta'$ are DEPENDENT functions at the boundary. On the other hand, according Oldano and Barbero[1–3] the use of an arbitrary function $\theta = \theta(z) + \delta\theta$, where θ is extremal, leads to a solution with discontinuity at the boundary. Since such a solution contradicts to the divergent character of the K_{13} surface-like volume energy, to the very assumption for a continuous and relatively small value of the liquid crystal orientational gradients in the elastic free energy of the nematics[12] as well as to the lack of experimental evidence for such discontinuities[45–48] (they have not been observed even in completely free along Z nematic layers[49,50]) we shall address ourselves to the explanation of the one-dimensional solution of the K_{13} problem for the case when θ and θ' are dependent functions at the boundary. This idea was proposed in 1975 year.[51] Later we have solved the Helfrich problem for a flexoelectric bending of a homeotropic nematic layer in a transversal DC electric field.[4] Finally we derived the rigorous boundary condition for the general one-dimensional case.[6] Let us clarify the obtaining of these boundary conditions. In principle they can be calculated in two separate ways.

1) First way of solution of the K_{13} problem:

We shall minimize the functional (1) accepting that θ and θ' are dependent functions at the boundary. We write the functional in the form:

$$I = \int_0^d F(\theta,\theta',z)\,dz + \int_0^d (-K_{13}\sin 2\theta\theta')'\,dz + (1/2)W_s(\theta - \theta_0)^2_{z=d} \quad (4)$$

and change the variables $\theta(z) \rightarrow z(\theta)$ in the second integral which can be written in the following form:

$$\int_0^{\theta(d)} z'(d/d\theta)\left(\frac{-K_{13}\sin 2\theta}{z'}\right) d\theta \quad (5)$$

Regard this integral as a function of the surface deformation angle $\theta(d)$:

$$g(\theta(d)) = \int_0^{\theta(d)} z'(d/d\theta) \left(\frac{-K_{13}\sin 2\theta}{z'(\theta)} \right) d\theta \tag{6}$$

The condition $\delta I = 0$ requires the variation of the functional with respect to $\theta(d)$:

$$\delta I = \int_0^d (F_\theta - (d/dz)F_{\theta'}\ \theta\ dz$$

$$+ \left\{ F_{\theta'}\delta\theta + z'(\theta)(d/d\theta) \left(\frac{-K_{13}\sin 2\theta}{z'(\theta)} \right) \delta\theta + W_s(\theta - \theta_0)\delta\theta \right\}_{z=d} \tag{7}$$

and leads to the differential equation:

$$F_\theta - (d/dz)F_{\theta'} = 0 \tag{8}$$

and to the boundary condition:

$$F_{\theta'} - 2K_{13}\cos 2\theta\theta' + (K_{13}\sin 2\theta\ \theta''/\theta') + W_s(\theta - \theta_0) = 0_{z=d} \tag{9}$$

where

$$-(dz/d\theta)^{-2}\ (d^2z/d\theta^2) = (d^2\theta/dz^2)(d\theta/dz)^{-1}_{z=d} \tag{10}$$

The inclusion of a second order derivative in the boundary condition (9) (the differential equation is also of a second order) is a new result with a considerable physical and practical importance. For instance, the surface behavior of the nematic will include not only the surface elastic forces but also electrical and magnetical, etc. influences. This finding is a direct consequence of the divergent type of the K_{13} surface-like volume nematic energy including also normal derivatives of the "director." The second important conclusion is that the differential equation must be valid at the boundary as well, a point critized by Oldano and Barbero.[1-3] For the simplest case when the boundary angle θ is fixed, the equation of Euler & Lagrange must be valid in the open interval $(0, d)$. For the case of weak anchoring when $K_{13} = 0$, the derivative from the bulk is equalized to that from the boundary.[52–55] It is not surprising that the solution of the much more complex second-order elasticity problem requires the validity of the differential equation at the boundary. On the other hand, from the literature which deals with classical variational problems we know that the variation of the functionals is well defined in every point (see Ref. 20, p. 70). Consequently, we accepted that the differential equation is also valid at the boundary and this assumption did not contradict both for the theoretical solution of the problem and its physical interpretation.

2) Second way of solution of the K_{13} problem. Let us rewrite the functional (1) in the form:

$$I = \int_0^d F(\theta,\theta',z)\, dz + \{(-K_{13}\sin 2\theta(1/z'(\theta)) + (1/2)W_s(\theta - \theta_0)^2\}_{z=d} \quad (11)$$

where the differentiation of z is with respect to θ.

The comparison of (1) and (11) clearly shows that the equality

$$(d\theta/dz) = 1/(dz/d\theta)_{z=d} \quad (12)$$

is satisfied at the boundary $z = d$. In other words, we expressed the function θ' with the aid of the derivative of the inverse function $z(\theta)$ with respect to θ, $z'(\theta)$. Further, we regard the surfaces term including K_{13} as a function, for instance $g(\theta(d))$, of the surface deformation angle $\theta(d)$:

$$g(\theta) = -K_{13}\sin 2\theta/z'(\theta)_{z=d} \quad (13)$$

After these mathematical operations the variation of the functional (1), rewritten in the form (11), with respect of the surface deformation angle again yields the boundary condition (9).

It is not difficult to observe a similarity in the two ways of variations. In principle we introduce the inverse function and vary the functional as a functional with a movable boundary.[6] On the other hand, Mishkis also pointed out that some variational problems which are unsolvable in the usual variational way, can be solved with the aid of inverse functions.[44]

III. ON THE VARIATION OF THE K_{13} SURFACE-LIKE VOLUME ELASTIC ENERGY FOR THE THREE-DIMENSIONAL CASE WITH THE AID OF ERICKSEN & TOUPIN VARIATIONAL ARGUMENTS AND CALCULATIONS[36]

In this part of the paper following the advice of the Referee we shall present the variational calculations for the three-dimensional case by Ericksen & Toupin variational arguments.[23] Partly these calculations are based on general lows of the differential geometry presented, for instance, by Sokolnikoff[56] and by Jenkins and Barratt.[18] First we focus our attention on the variation of the free energy of a nematic liquid crystal confined in a volume V bounded by the surface S. Due to the incompressibility of the nematic and to the unit value of the nematic "director," the variation in the displacement δx and the material variation in the director Δn are subject to the constraints:[23,58]

$$\mathrm{div}\delta x = 0; n \quad \Delta n = 0 \tag{14}$$

Further we shall present the variation of the nematic energy in a convenient form postulated for the first time by Ericksen in 1961 year[57] (see the considerations of Leslie[58] as well):

$$\delta \int_V U\, dV = \int_V (F \cdot \delta x + G \cdot \Delta n)\, dV + \int_S (t \cdot \delta x + s \cdot \Delta n)\, dS \tag{15}$$

The following connection:[23,58,59]

$$\Delta n = \delta n + (\delta x \cdot \mathrm{grad})\, n \tag{16}$$

will be used also in the calculations.

During the variational calculations, according to the advice of the Referee, we shall follow the elegant way of variation proposed by Ericksen[23] for the study of the equilibrium conditions of a smectic A liquid crystal on the basis of a simpler elastic energy. We shall suppose that the nematic elastic energy consists from both first and second spatial gradients of the "director." Let us first write the general type of the variation of the free energy of a nematic liquid crystal confined in the volume V bounded by the surface S:

$$\delta \int_V U(x, \nabla n, \nabla\nabla n)\, dV = \int_V h_i \delta n_i \, dV$$

$$= \oint_S \left(\frac{\partial U}{\partial n_{i,k}} \delta n_i + \frac{\partial U}{\partial n_{i,jk}} \delta n_{i,j} + U \delta x_k \right) dS_k$$

$$= \oint_S \left(\left(\nu_k \frac{\partial U}{\partial n_{i,k}} \right) \delta n_i + \left(\nu_k \frac{\partial U}{\partial n_{i,jk}} \right) \delta n_{i,j} + U \nu_k \delta x_k \right) dS \quad (17)$$

The variations δn_i can be expressed by Δn and $(\delta x \cdot \text{grad})n$ with the aid of the relation (16):

$$\delta n = \Delta n - (\delta x \cdot \text{grad})\, n \text{ or } \delta n_i = \Delta n_i - \delta x_p \, n_{i,p} \quad (18)$$

The variations $\delta n_{i,j}$ can be expressed by the following relation:

$$\delta n_{i,j} = \Delta n_{i,j} - \delta x_{p,j} \, n_{i,p} - \delta x_p \, n_{i,jp} \quad (19)$$

obtained from the connection (16) after differentiation. Consequently for the type of the virtual work we obtain:

$$\delta \int_V U \, dV = \int_V h_i (\Delta n_i - (\delta x_p) n_{i,p}) \, dV$$

$$= \oint S \left(\left(\nu_k \frac{\partial U}{\partial n_{i,k}} \right) \left(\Delta n_i - (\delta x_p) n_{i,p} \right) + \left(\nu_k \frac{\partial U}{\partial n_{i,jk}} \right) \right.$$

$$\left. (\Delta n_{i,j} - (\delta x_{p,j}) n_{i,p} - (\delta x_p) n_{i,jp}) + U \nu_p \delta x_p \right) dS \quad (20)$$

where the volume molecular field h_i[38] is given by the relation:

$$h_i = \frac{\partial U}{\partial n_i} - \left(\frac{\partial U}{\partial n_{i,k}} \right), k + \left(\frac{\partial U}{\partial n_{i,jk}} \right), jk \quad (21)$$

Further, according to Ericksen & Toupin variational arguments we must get a linear functional of the variations which can vanish only if all the coefficients vanish, a property not exhibited by the right member of Eq. (20). Following Ericksen[23] and Toupin,[59] we now compose gradients of variations into derivatives normal and tangent to the surface, using the rules:

$$Df = \nu_i f_{,i}$$

$$D_i f = f_{,i} - \nu_i \, Df$$

where Df is the normal derivative of f, $D_i f$ are the surface gradients of f and ν_i is the unit normal to the surface. Let us stress that f is defined in the interior and on the boundary. Toupin[59] allows for some lack of smoothness, but we assume the surface and pertinent functions smooth to avoid "edge" contributions. We then have a simplified and corrected version of the integral identity which has been used by Toupin and Ericksen:

$$\oint_S D_i(f\nu_j)\, dS = \oint_S (b^k_k \nu_i \nu_j - b_{ij}) f \, dS b_{ij} = b_{ji} = -D_i \nu_j \quad (22)$$

where b is the second fundamental tensor of the surface measuring its curvature. With the indicated manipulation Eq. (21) becomes

$$\delta \int_V U \, dV = \int_V (h_i \Delta n_i - h_i n_{i,p} \delta x_p)\, dV \quad (23)$$
$$+ \oint_S \{F^1_i \Delta n_i + F^2_i \, D(\Delta n_i) + F^3_p \, \delta x_p + F^4_p \, D(\delta x_p)\}\, dS$$

where

$$F^1_i = \nu_k \frac{\partial U}{\partial n_{i,k}} + \nu_k \nu_j b^m_m \frac{\partial U}{\partial n_{i,jk}} - \nu_k D_j \left(\frac{\partial U}{\partial n_{i,jk}}\right)$$

$$F^2_i = \nu_k \nu_j \frac{\partial U}{\partial n_{i,jk}} \quad (24)$$

$$F^3_p = U\nu_p - \nu_k \frac{\partial U}{\partial n_{i,k}} n_{i,p} - \nu_k n_{i,jp} \frac{\partial U}{\partial n_{i,jk}}$$
$$- \nu_k \nu_j b^m_m n_{i,p} \frac{\partial U}{\partial n_{i,jk}} + \nu_k D_j \left(n_{i,p} \frac{\partial U}{\partial n_{i,jk}} \right)$$

$$\mathrm{F}^4_p = -\nu_k \nu_j (\mathrm{n}_{i,p}) \frac{\partial \mathrm{U}}{\partial \mathrm{n}_{i,jk}} \quad (25)$$

(the detailed calculations for $\Delta n_{i,j}$ and $\delta x_{i,j}$ are given in the Appendix I).

According to Ericksen[23] and Toupin[59] the variations $D\delta(x_p)$ and δx_p as well as $D(\Delta n_i)$ and Δn_i are independent. As Ericksen[60] has shown consideration of an arbitrary infinitesimal, rigid translation in which Δn is zero and δx = const (see also Ref. 23) leads to the vanishing of the left side of Eq. (23) because of Galilean invariance. The right-hand side yields the equation:

$$\int_V f\, dV + \oint_S F^3\, dS = 0 \tag{26}$$

where

$$f_p = h_i\, n_{i,p}$$

and normally such a condition of translational invariance is reasonably interpreted as a balance of forces.[23]

Similar consideration of an arbitrary, infinitesimal and rigid rotation in which[23]

$$\delta x = \omega \times x,\ \Delta n = \omega \times n \tag{27}$$

leads to a balance of couples

$$\oint_S (n \times F^1 + \nu \times F^2 + x \times F^3 + \nu \times F^4)\, dS + \int_V (x \times f + n \times h)\, dV = 0 \tag{28}$$

Consequently, the generalized forces are related to a body couple K and the couples of stress l^1, l^2 and l^3 through

$$K = n \times h$$

$$l^1 = n \times F^1$$

$$l^2 = \nu \times F^2$$

$$l^3 = \nu \times F^4 \tag{29}$$

It is clear that following the variational calculations of Ericksen[23] and Toupin[59] and those of Jenkins and Barratt[18] we can obtain the traction boundary conditions and the balance of the couples at the interface.

We, however, are interested only in the balance of the couple, i.e. on the expression of the surface molecular field, including the K_{13} term.[38] It is easy to show that for the case of the K_{13} surface-like volume elastic energy the following relations are valid:

$$\frac{\partial U}{\partial n_{i,jk}} = K_{13}\, n_k, \quad \nu_j = \nu_i, \quad D_j = D_i \tag{30}$$

(the term K_{13} div n is included in $\partial U/\partial n_{i,k}$).

Further from the general expression of the variation of the nematic energy given by Eq. (23) one can obtain:

$$F_i^1 = \nu_k \frac{\partial U}{\partial n_{i,k}} + K_{13}\, \nu_k\, \nu_i\, b_m^m\, n_k - \nu_k D_i (K_{13}\, n_k) \tag{31}$$

which is the final form of the surface molecular field including the K_{13} second-order surface-like volume energy.

It is important to stress that the couple of stress l^2 connected with the normal derivative of the variation Δn, $D(\Delta n)$ vanishes due to the divergent character of the K_{13} surface-like volume energy:

$$l^2 = K_{13}\, (\nu \times \nu)(n \cdot \nu) \equiv 0 \tag{32}$$

The other couple of stress l^3 connected with the normal derivative of the variation δx, $D(\delta x_p)$ must vanish:

$$l^3 = \nu \times F^4 = 0 \tag{33}$$

where

$$F_p^4 = -K_{13} \nu_k \cdot n_k\, \nu_i\, n_{i,p} \tag{34}$$

We shall not discuss here the physical meaning of this boundary condition. (Some considerations about the couple stresses being called surface distribution of couples, including the normal to the boundary S, are given by Toupin[59].)

The pseudoscalar b_m^m being in the surface molecular field given by the relation (31) can be expressed with the aid of the formula:[61]

$$b_m^m = - b_{\alpha\beta} a^{\alpha\beta} \tag{35}$$

where b is the second fundamental tensor of the surface S and a is the contravariant form of the first fundamental tensor of the surface S. For convenience we prefer to express b_m^m by the conventional spherical polar coordinate angles θ and ϕ. For this aim it is necessary to use the tensors $a_{\alpha\beta}$ and $b_{\alpha\beta}$ written in such coordinates:[62]

$$a_{\alpha\beta} = \begin{vmatrix} a_\theta \cdot a_\theta & a_\theta \cdot a_\phi \\ a_\phi \cdot a_\theta & a_\phi \cdot a_\phi \end{vmatrix} \qquad (36)$$

$$b_{\alpha\beta} = \begin{vmatrix} \nu \cdot r_{,\theta\theta} & \nu \cdot r_{,\theta\phi} \\ \nu \cdot r_{,\phi\theta} & \nu \cdot r_{,\phi\phi} \end{vmatrix} \qquad (37)$$

where r is the radius vector of the point under consideration and ν is the unit normal in this point, $a_\alpha = r_{,\alpha}$ are tangent vectors. The elements of the contravariant tensor $\alpha^{\alpha\beta}$ can be calculated, for instance from the book of Sokolnikoff[56] according to the formulae:

$$a^{11} = (a_{22}/a) \ ; \ a^{12} = a^{21} = -(a_{12}/a) \ ; \ a^{22} = (a_{11}/a) \qquad (38)$$

where

$$a = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} > 0$$

is the determinant of the first fundamental tensor of the surface S. Finally for the important pseudoscalar b_m^m we obtain:

$$b_m^m = -(1/a)(a_{22}\, b_{11} - 2\, a_{12}\, b_{21} + a_{11}\, b_{22}) \qquad (39)$$

It is clear that the value b_m^m for the one-dimensional case of the θ deformation is given by the relation:

$$b_m^m = -(d^2z/d\theta^2)(dz/d\theta)^{-2} = (d^2\theta/dz^2)(1/d\theta/dz) \qquad (40)$$

which is completely confirmed by the boundary condition obtained by us for the one-dimensional case.[9] Consequently, the boundary conditions used by us in Refs. 4–8 are correct. We should like to point out, however, that the validity of the boundary condition (9) is not occasional. During the one-dimensional calculations we have used the inverse function ($1/dz/d\theta$) which means that the variation was performed with the aid of the component of the tangential vector ($dz/d\theta$). Further, during the variational calculations of the three-dimensional case made in the frame of Ericksen & Toupin variational arguments we noted that the appearance of the pseudoscalar b^m_m was at the so-called "inner differentiation" on the surface S using the important integral indentity (22) given by Toupin.[59] For the one-dimensional case the "inner differentiation" *must be performed in a point*. In this manner it is possible to calculate directly the variation without utilizing the inverse function at the differentiation:

$$\theta\delta(d\theta/dz) = \theta\,(d^2\theta/dz^2)\,\delta z = \theta(d^2\theta/dz^2)(\delta z/\delta\theta)\delta\theta$$

$$= \theta(d^2\theta/dz^2)(1/(d\theta/dz))\,\delta\theta$$

since

$$(\delta z/\delta\theta) = (dz/d\theta)$$

as pointed out by Sokolnikoff.[56] Of course, the three-dimensional case is much more complex and the calculations would be not possible without employing Ericksen & Toupin variational arguments and calculations.

In the end of this part of the paper let us briefly discuss the physical and mathematical meaning of the important pseudoscalar b^m_m. In a number of books and handbooks, it is defined as a mean curvature H of the surface in the point under consideration:

$$(1/2)b^m_m = -H \tag{41}$$

In effect this pseudoscalar appears from the differentiation of the normal to the surface S in the point under consideration relative to the parameters u_1 and u_2 which define the surface S. As shown by McConnel[61] and by Jenkins and Barratt[18] the normal tensor differentiation of the unit vector ν to the surface S is orthogonal and consequently parallel to the surface S:

$$\nu_{i,\alpha} = -b^{\beta}_{\alpha}\,x_{i,\beta} \tag{42}$$

The second important note is that whatever to be the surface S, it must be described by the spherical coordinates θ and ϕ, peculiar for the deformations of the liquid crystal.[63,64,65] It is evident that this can be easily done with the change of the variables.[18] This must be done not only for an arbitrary curved surface but also for planar surfaces. This procedure is necessary since for the case of weak anchoring (a variation of the polar coordinates on S) the surface S parameterized by the spherical coordinate is movable[6] and the solution of the K_{13} problem is more easier. The third important note is that for some liquid crystal deformations the pseudoscalar b_m^m might be zero. This is valid for the so-called *minimal surfaces* (in our case minimal deformational surfaces).[66]

IV. POSSIBLE WAY FOR THE EXPERIMENTAL EVALUATION OF THE K_{13} ELASTIC COEFFICIENT

The rigorous boundary conditions for the one-dimensional case of the K_{13} elastic problem obtained in Ref. 6 and the theoretical calculations for the case of various one-dimensional elastic problems[4–8,30–32] clearly show several features typical for the K_{13} elastic problem only.

1. A second derivative θ'' of the deformation angle $\theta(z)$ with respect to the coordinate z presents in both the boundary condition and the differential equation. (Let us note that in the elastic theory of membranes and bars, etc. there are examples when the derivatives in both the differential equation and the boundary conditions are from one and the same order of magnitude.[67])

2. The differential equation must be valid on the boundary as well. This leads to a quadratic equation of θ' at the boundary.

3. The K_{13} surface-like volume energy is not important for the case of strong anchoring of the nematic layer. Then θ' at the boundary is determined by the differential equation, i.e. it is determined by the bulk behavior of the nematic. Consequently in this case the surface term $K_{13}\sin 2\theta\theta'$ is only an additive constant to the functional without any importance for the variation of this functional.

4. The theoretical calculations for the influence of the K_{13} elastic term on the Frederiks transition for the case of a homeotropic nematic layer, performed by me[37] and the theoretical results of Chigrinov for the elastic behavior of a hybrid nematic layer[32] clearly show that there is a thickness (minimal surface, see the preceding part), at which the influence of the K_{13} term vanishes. This is evident from the theoretical curves shown in Figure 2 and representing the threshold voltage for a homeotropic MBBA nematic layer under the action of a normal

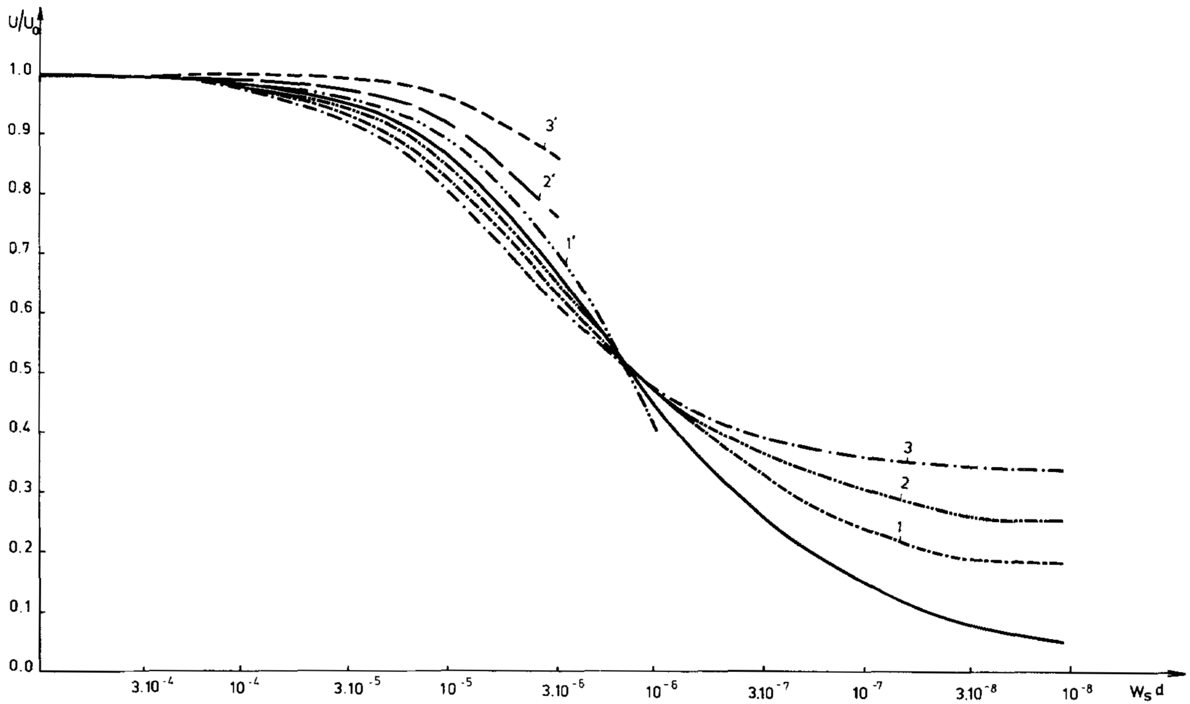

FIGURE 2 The ratio between the threshold voltage U for finite anchoring and the threshold voltage U_0 for infinite anchoring of a homeotropic MBBA nematic layers vs. the parameter $W_s d$, where W_s is the surface strength coupling coefficient and d is the thickness of the liquid crystal layer. The continuous curve corresponds to the case when $K_{13} = 0$, $K'_{33} = 8{,}6.10^{-7}$ dynes. The dashed curves 1′, 2′ and 3′ correspond to the case when $K_{13} = +2{,}1.10^{-7}$ dynes, $+4{,}3.10^{-7}$ dynes and $+6{,}4.10^{-7}$ dynes, respectively. The dashed curves 1,2 and 3 correspond to the case when $K_{13} = -1{,}6.10^{-7}$ dynes, $-3{,}2.10^{-7}$ dynes and $-4{,}8.10^{-7}$ dynes, respectively.

electric field with a different value and a different sign of the second-order elastic coefficient K_{13} as a function of the parameter $W_s d$, where W_s is the surface strength coupling coefficient and d is the thickness of the nematic layer (Ref. 37, p. 122). They were calculated from the following transendental equations:

$$tg(\pi/2)(U/U_0) = (1/2)\frac{W_s d}{(K'_{33} \pm K_{13})}(U_0/U)^2 + \left\{(1/2)\frac{W_s d}{(K'_{33} \pm K_{13})}(U_0/U)^2 \pm \frac{K_{13}}{K'_{33} \pm K_{13}}\right\}^{1/2} \qquad (43)$$

(we have used the well-known Rapini's type of the surface energy $W_s \sin^2\theta$):

where U_0 is the threshold voltage for the case of strong anchoring of the nematic layer, the upper sign corresponds for the case of negative value of K_{13} and the lower sign corresponds to the case of a positive value of K_{13}.

The numerical calculation of the threshold voltage from the relation (43) for the case of a homeotropic MBBA nematic layer at room temperature and following values of K_{13}: $+2{,}1.10^{-7}$ dynes, $+4{,}3.10^{-7}$ dynes, and $+6{,}4.10^{-7}$ dynes ($K'_{33} = 8{,}6.10^{-7}$ dynes) as well as $K_{13} = -1{,}6.10^{-7}$ dynes, $-3{,}2.10^{-7}$ dynes and $-4{,}8.10^{-7}$ dynes are shown in Figure 2, curves 1′, 2′, 3′ and 1,2,3, respectively. The curve, corresponding to the case of vanishing K_{13} : $K_{13} = 0$, is also shown. The numerical calculations unambiguously show that the Frederiks transition is of a second order for the case of a negative sign of K_{13}[12] or a first order for the case of a positive sign of K_{13} when the surface anchoring is relatively weak. In the first case ($K_{13} < 0$), the second-order elastic coefficient K_{13} may be determined from the relation:

$$tg(\pi/2)(U/U_0) = \left(\frac{K_{13}}{K'_{33} + K_{13}}\right)^{1/2} \qquad (44)$$

when the anchoring of the nematic layer is weak (Figure 2). In the second case ($K_{13} > 0$), K_{13} can be determined from the relation:

$$(1/2)\left(\frac{W_s d}{K'_{33} - K_{13}}\frac{U_0}{U}\right)^2 = \frac{K_{13}}{K'_{33} - K_{13}} \qquad (45)$$

which shows a change of the Frederiks transition from a second order to a first order.

The curves shown in Figure 2 clearly demonstrate that the K_{13} term has no influence on the threshold curves in the inflection point.

5. The influence of the K_{13} term on the elastic behavior of the nematics depends on the type of the differential equation, i.e. it depends on the bulk behavior of the liquid crystal. This influence is weak for the case of a linear deformation such as a flexoelectric bending of a homeotropic nematic layer subjected to the influence of a transversal electric field:[4]

$$\theta' = (e_{3x}E/K'_{33} - K_{13})\left(1 - \left(\frac{2(K'_{33} - K_{13})}{W_s d} - + 1\right)^{-1}\right) \tag{46}$$

where e_{3x} is the bend flexoelectric coefficient and E is the value of the applied electric field.

It is evident that in this case K_{13} only modifies the bulk elastic coefficient K'_{33}. On the other hand, the influence of the K_{13} term is significant for the case of non-linear deformations (see, for instance) the curves shown in Figure 2).

Weak or strong anchoring of a homeotropic nematic layer has been observed by Blinov and co-workers for the case either of a flexoelectric bending of the nematic layer or a Frederiks transition for two equally treated glass plates (in the latter case the surfactant layer has been coated over a semitransparent conductive layer). Blinov *et al.*[31] explained this descreapancy with the type of the surface energy (see also Refs. 68–70). This descreapancy, however, can be explained also by the theoretical curves shown in Figure 2 which are nearly independent on the thickness of the liquid crystal layer at weak anchoring. Ohtsu *et al.*[71] have found that the threshold voltage for the case of a homeotropic MBBA nematic layer is independent of the thickness of the nematic layer up to 50 microns. The maximal thickness of the penetration of the surface forces and torques via the elasticity of the liquid crystal has to be around 150–200 microns since at a larger thickness of the nematic layer, the thermal fluctuations will disturb the orientational deformations of the liquid crystal.[72,73] On the other hand, from the inflexion point which is around $W_s d \sim 10^{-6}$ dynes and a thickness of the liquid crystal layer $d \sim 200$ microns, it is easy to calculate the possible value of the surface energy which has to be in the range of $0{,}5.10^{-4}$ erg/cm^2, a value which is close to the true anchoring of one weak anchored nematic layer. Then we can immediately define the following approximate value of the

K_{13} elastic coefficient of MBBA at room temperature:[74]

$$-K_{13} \underset{\to}{\leq} (K'_{11}/2) \tag{47}$$

(see the calculations made in Appendix 2)

V. ON THE VARIATION OF THE MADA ELASTIC ENERGY

Mada[25] has proposed the following type of the elastic energy of a nematic liquid crystal:

$$F = \int_V \Lambda(n_i, n_{i,k})\, dV + \int_S \overline{\Lambda}(n_i, n_{i,k})\, dS \tag{48}$$

In analogy with the solution of the K_{13} problem and employing Ericksen & Toupin variational arguments we have obtained the following expression for the variation of this energy:

$$\delta F = \int_V (h_i \Delta n_i + f_p \delta x_p)\, dV$$

$$= \oint \{F_i^1 \Delta n_i + F_i^2 D(\Delta n_i) + F_p^3 \delta x_p + F_p^4\, D(\delta x_p)\}\, dS \tag{49}$$

where

$$h_i = \frac{\partial \Lambda}{\partial n_i} - \left(\frac{\partial \Lambda}{\partial n_{i,k}}\right)_{,k}$$

$$f_p = -n_{i,p}\, h_i$$

$$F_i^1 = \nu_k \frac{\partial \Lambda}{\partial n_{i,k}} + \frac{\partial \overline{\Lambda}}{\partial n_i} - D_k \left(\frac{\partial \overline{\Lambda}}{\partial n_{i,k}}\right)$$

$$F_i^2 = \nu_k \frac{\partial \overline{\Lambda}}{\partial n_{i,k}}$$

$$F_p^3 = D_k \left(\frac{\partial \overline{\Lambda}}{\partial n_{i,k}} n_{i,p}\right) - n_{i,p} \left(\nu_k \frac{\partial \overline{\Lambda}}{\partial n_{i,k}} + \frac{\partial \overline{\Lambda}}{\partial n_i}\right) - \frac{\partial \overline{\Lambda}}{\partial n_{i,k}} n_{i,kp}$$

$$F_p^4 = \nu_k \frac{\partial \overline{\Lambda}}{\partial n_{i,k}} n_{i,p} \tag{50}$$

(During the calculations we have applied the theorem of Green on the surface S.)

Consideration of an arbitrary infinitesimal, rigid translation in which Δn is zero and δx = const leads to the vanishing of the left-side of Eq. (49) because of Galilean invariance. The right-side of this equation yields the balance of the forces:

$$\int_V f\, dV + \oint_S F^3\, dS = 0 \tag{51}$$

Similar consideration of an arbitrary infinitesimal, rigid rotation leads to a balance of couples:

$$\int_V (x \times f + n \times h)\, dV + \oint_S (n \times F^1 + \nu \times F^2 + x \times F^3 + \nu \times F^4)\, dS = 0 \tag{52}$$

Consequently, the generalized forces are related to the body couple K and a couple stress l through

$$K = n \times h$$
$$l^1 = n \times F^1$$
$$l^2 = \nu \times F^2$$
$$l^3 = \nu \times F^4 \tag{53}$$

The equilibrium conditions for static deformations at the surface are expressed by the following two conditions:

$$n \times F^1 = 0$$
$$\nu \times F^2 = 0 \tag{54}$$

(the other couple stress l^3 is connected with the normal derivative of the displacement δx_p, $D(\delta x_p)$).

The bulk static equilibrium condition is defined by the equation:

$$n \times h = 0 \tag{55}$$

It is clear that the boundary conditions cannot be satisfied without suggestions of new connections at the boundary.

The comparison of this case with the K_{13} elastic problem clearly shows that the divergent character of the surface-like volume energy permits a solution of the problem with the aid of Ericksen & Toupin variational arguments. Evidently, the energy of Mada does not satisfy these conditions.

CONCLUSIONS

In the first part of the paper we have discussed two possible ways of one-dimensional variation of the K_{13} surface-like volume energy for the case of nematics. The first way is based on the assumption that the deformation angle θ and its derivative θ' with respect to the coordinate z and consequently their variations $\delta\theta$ and $\delta\theta'$ are independent functions at the boundary. Our analysis clearly pointed out that in this case the K_{13} problem has no solution. The second possible way of solution of the K_{13} problem is based on the assumption that θ and θ' and consequently their variations $\delta\theta$ and $\delta\theta'$ are dependent functions at the boundary. In this case we have solved the K_{13} problem by introducing of the inverse function and variating the functional as one with a movable boundary.

In the second part of the paper according to the advice of the Referee we calculated the three-dimensional case on the basis of the elegant variational procedure, proposed by Ericksen and Toupin. We have obtained all the body and surface forces as well as all the generalized surface and body forces. The variations performed unambiguously show that the K_{13} problem has really a solution which is based on general lows of the differential geometry. The surface molecular field was obtained explicitly. In its expression enters and a term involving the mean curvature H of the surface S (in our case S is parametrized by the spherical variables θ and ϕ, peculiar for the liquid crystal deformations) in the point under consideration. From the three-dimensional case one can easily obtain the one-dimensional solution for $\theta(z)$ which completely confirmed the validity of our boundary condition previously obtained.[6] The second boundary condition connected with the normal derivative of the variation δn identically vanishes due to the divergent character of the surface-like volume K_{13} energy.

On the basis of our unpublished theoretical results[37] for the threshold conditions of a homeotropic MBBA nematic layer under the action of a normal AC electric field with the inclusion of the K_{13} second-order elasticity and the experimental "controversy" evidence for *weak anchoring* of the homeotropic nematic layer under the action of a transversal DC electric field leading to a flexoelectric bending (the well-known Helfrichs' effect) and foe *strong anchoring* of the same homeotropic nematic layer under the action of an AC normal electric field leading to a Frederiks transition expressed by a thickness independence of the threshold voltage up to 150–200 microns, we concluded that the value of the K_{13} elastic coefficient for the case of the nematic MBBA at room temperature has to be slightly smaller than half of the value of the splay elastic coefficient K'_{11}. On the other hand, the theoretical calculations performed by Nehring and Saupe[13] pointed out that the ratio between K'_{11} and $-K_{13}$ must be 5/6 for the case when the long-range orientational forces are included only. Evidently the inclusion of the short-range orientational forces will lead to obtaining of the real value of the ratio of these two elastic coefficients.

On the basis of Ericksen & Toupin variational arguments we have obtained the surface and body forces as well as the generalized surface and body forces for the case of the energy proposed by Mada.[25] The equilibrium conditions for the static deformations at the surface are expressed by two vector equations whereas the derivatives in the bulk vector equation are of both first and second order. It is clear that the boundary conditions cannot be satisfied without suggestions of new connections at the boundary.

Acknowledgments

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Appendix I

Following Ericksen and Toupin we shall first calculate the term in Eq. (20) containing $\Delta n_{i,j}$:

$$\nu_k \frac{\partial U}{\partial n_{i,jk}} \Delta n_{i,j} = \nu_k \frac{\partial U}{\partial n_{i,jk}} (D_j(\Delta n_i) + \nu_j D(\Delta n_i))$$

$$= \nu_k \nu_j \frac{\partial U}{\partial n_{i,jk}} D(\Delta n_i) + \nu_k \frac{\partial U}{\partial n_{i,jk}} D_j(\Delta n_i)$$

$$+ D_j\left(\nu_k \frac{\partial U}{\partial n_{i,jk}}\right) \Delta n_i - D_j \left(\nu_k \frac{\partial U}{\partial n_{i,jk}}\right) \Delta n_i$$

$$= \nu_k \nu_j \frac{\partial U}{\partial n_{i,jk}} D(\Delta n_i) + D_j \left(\nu_k \frac{\partial U}{\partial n_{i,jk}} \Delta n_i\right) - D_j \left(\nu_k \frac{\partial U}{\partial n_{i,jk}}\right) \Delta n_i$$

$$= \nu_k \nu_j \frac{\partial U}{\partial n_{i,jk}} D(\Delta n_i) + \nu_k \nu_j b_m^m \frac{\partial U}{\partial n_{i,jk}} \Delta n_i$$

$$+ (D_j \nu_k) \frac{\partial U}{\partial n_{i,jk}} \Delta n_i - D_j \left(\nu_k \frac{\partial U}{\partial n_{i,jk}}\right) \Delta n_i$$

$$= \nu_k \nu_j \frac{\partial U}{\partial n_{i,jk}} D(\Delta n_i) + \nu_k \nu_j b_m^m \frac{\partial U}{\partial n_{i,jk}} \Delta n_i - \nu_k D_j\left(\frac{\partial U}{\partial n_{i,jk}}\right) \Delta n_i \tag{1}$$

In a similar manner we calculate the term in Eq. (20) containing $\delta x_{p,j}$:

$$\nu_k n_{i,p} \frac{\partial U}{\partial n_{i,jk}} \delta x_{p,j} = \nu_k n_{i,p} \frac{\partial U}{\partial n_{i,jk}} (D_j(\delta x_p) + \nu_j D(\delta x_p))$$

$$= \nu_k \nu_j n_{i,p} \frac{\partial U}{\partial n_{i,jk}} D(\delta x_p) + \nu_k n_{i,p} \frac{\partial U}{\partial n_{i,jk}} D_j(\delta x_p)$$

$$+ D_j\left(\nu_k n_{i,p} \frac{\partial U}{\partial n_{i,jk}}\right) \delta x_p - D_j \left(\nu_k n_{i,p} \frac{\partial U}{\partial n_{i,jk}}\right) \delta x_p$$

$$= \nu_k \nu_j n_{i,p} \frac{\partial U}{\partial n_{i,jk}} D(\delta x_p) + D_j(\nu_k n_{i,p} \frac{\partial U}{\partial n_{i,jk}} \delta x_p)$$

$$- D_j\left(\nu_k n_{i,p} \frac{\partial U}{\partial n_{i,jk}}\right) \delta x_p = \nu_k \nu_j n_{i,p} \frac{\partial U}{\partial n_{i,jk}} D(\delta x_p)$$

$$+ \nu_k \nu_j b_m^m n_{i,p} \frac{\partial U}{\partial n_{i,jk}} \delta x_p + (D_j \nu_k) n_{i,p} \frac{\partial U}{\partial n_{i,jk}} \delta x_p$$

$$- D_j\left(\nu_k\, n_{i,p} \frac{\partial U}{\partial n_{i,jk}}\right) \delta x_p = \nu_k \nu_j\, n_{i,p} \frac{\partial U}{\partial n_{i,jk}} D(\delta x_p)$$

$$+ \nu_k\, \nu_j\, b_m^m\, n_{i,p} \frac{\partial U}{\partial n_{i,jk}} \delta x_p - \nu_k D_j\left(n_{i,p} \frac{\partial U}{\partial n_{i,jk}}\right) \delta x_p \tag{2}$$

During the calculations we have used the relations (22) and the rules:

$$Df = \nu_i f_{,i}$$

$$D_i f = f_{,i} - \nu_i Df$$

in accordance with the variational arguments of Ericksen & Toupin.

Appendix II

Let us minimize the elastic energy of one completely free nematic film accepting that the deformation starts from an initially planar orientation. Write the total elastic energy per unit area in the form:

$$I = \int_0^d \{(1/2)(K'_{11}\cos^2\theta + K'_{33}\sin^2\theta)\theta'^2 + K_{13}\cos 2\theta\theta'^2 + K_{13}(\sin 2\theta/2)\theta''\} \tag{1}$$

The differential equation of Euler & Lagrange has the form:

$$f(\theta)\theta'' + (1/2)(\theta'^2)(d/d\theta)f(\theta) = 0$$

with

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

Replace θ'' from (2) into (1) and obtain the following type of the elastic energy:

$$I = \int_0^d \theta'^2 \left\{(1/2)f(\theta) + K_{13}\cos 2\theta - \frac{K_{13}(K'_{33} - K'_{11})}{f(\theta)} (\sin 2\theta/2)^2\right\} dz \tag{3}$$

It is clear that $I \geqslant 0$ when

$$(1/2)f(\theta) + K_{13}\cos 2\theta - \frac{K_{13}(K'_{33} - K'_{11})}{f(\theta)}(\sin 2\theta/2)^2 \geqslant 0 \quad (4)$$

and

$$\theta' \lesseqgtr 0$$

The acceptance that the following equality

$$(1/2)f(\theta) + K_{13}\cos 2\theta - \frac{K_{13}(K'_{33} - K'_{11})}{f(\theta)}(\sin 2\theta/2)^2 = 0 \quad (5)$$

is valid leads to a solution with a tilt of the nematic layer which contradicts to the very nature of the nematics.

Consequently from the strict inequality:

$$(1/2)f(\theta) + K_{13}\cos 2\theta - \frac{K_{13}(K'_{33} - K'_{11})}{f(\theta)}(\sin 2\theta/2) > 0 \quad (6)$$

we obtain the following inequality between $(K'_{11}/2)$ and K_{13}:

$$(K'_{11}/2) + K_{13} > 0 \quad (7)$$

which for the case of a negative value of K_{13} points out that $-K_{13}$ *must be smaller* than the half of the splay elastic coefficients K'_{11}. Analogically one can obtain that

$$(K'_{33}/2) - K_{13} > 0 \quad (8)$$

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