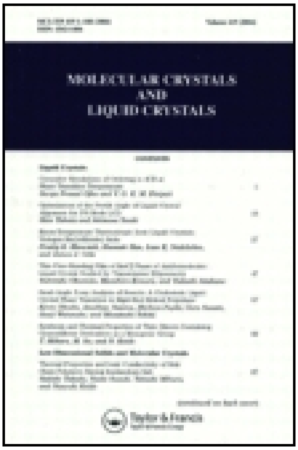

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Some Considerations on the Elastic Theory for Nematic Liquid Crystals

G. Barbero [a] [b]

[a] Dipartimento di Fisica, Politecnico, Corso Duca degli Abruzzi, 24, 70729, Torino, Italia

[b] Laboratoire de Physique dés Solides, Băt. S 10, 91405, Orsay, France

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Some Considerations on the Elastic Theory for Nematic Liquid Crystals

G. BARBERO

Dipartimento di Fisica, Politecnico, Corso Duca degli Abruzzi, 24, 10129 Torino, Italia
and
Laboratoire de Physique dès Solides, Bât. S10, 91405 Orsay, France

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The elastic theory for nematic liquid crystals is critically analysed. After a review on the variational calculus formalism, the range of applicability of the Lagrangian method for the solution of practical problems is discussed. It is underlined that only a limited number of problems can be solved by means of a variational approach. The role at the Jacobi equation is also discussed. The importance of the non linear character of the K_{13}-problem is analyzed in the framework of a simple molecular model. Finally, the principle of virtual work is applied to the elastic theory of nematic liquid crystals. Our analysis shows that the K_{13} elastic problem is an ill-posed one, since this problem can only be solved by means of a variational, or virtual work, approach by modifying the bulk elastic free energy and taking into account new terms quadratic in the second order deviatives. However it is necessary to remember that, in the proximity of a surface, a spatial variation of the density and of the scalar order parameter of the liquid crystal are expected, and hence a true elastic description is no longer possible.

1. INTRODUCTION

Since most physical processes in nature may be formulated in terms of a variational principle, provided they can be expressed as a set of mathematically simple differential equations, it is not surprising that an unwarranted place within the law of nature has been reserved for such a "least" theorem.[1] Thus, Planck claimed the action principle "to come nearest to the ideal final aim of theoretical research."

Purpose of the present investigation is to show that in some cases the variational principle does not work in the elastic theory of liquid crystals.[2] In particular, we show that some unclear aspects of this theory are probably due to an uncritical adoption of the variational approach.[3] The range of application of the Lagrange formalism is considered in sect. 2. In sect. 3, the usual variational procedure is recalled, and the role of the Jacobi equation reconsidered.[4] In sect. 4, the relevance of some non-linear terms on the elastic theory of liquid crystals are discussed.[5] Finally in sect. 5 the principle of virtual work is applied to the elastic theory of liquid crystals.

2. VARIATIONAL PRINCIPLES

It is well known that in many branches of physics the solution of a variety of problems can be greatly simplified if the basic equations can be expressed in the form of a variational principle. Fermat's principle in optics and Hamilton's principle in mechanics are two well-known examples.[6] Classical non relativistic mechanics is based on Newton's equations of motion, which hold *without any restriction* on the nature of the forces $\underline{F}$ and their dependence on the coordinate $\underline{r}$, their derivative and time

$$\underline{F} = m\ddot{\underline{r}}, \tag{1}$$

where the dot means a derivative with respect to t.

An alternative formulation was given by Lagrange.[7,8] His equations

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\underline{r}}} - \frac{\partial L}{\partial \underline{r}} = 0, \tag{2}$$

are a consequence of Hamilton's variational principle

$$\delta \int L(\underline{r},\dot{\underline{r}},t)dt = 0. \tag{3}$$

However, Newton's equations (1) can ordinarily be brought into the form (2) only if the forces are derivable from a potential energy V, which is a function of $\underline{r}$ and t alone, but not of $\dot{\underline{r}}$. In this case the Lagrangian L equals the difference of kinetic and potential energy. The Lagrange method can be extended to cover velocity and acceleration dependent forces $\underline{F}$ for which one can find a function U such that

$$\underline{F} = \frac{d}{dt}\frac{\partial U}{\partial \dot{\underline{r}}} - \frac{\partial U}{\partial \dot{\underline{r}}}. \tag{4}$$

A well known example of such a force is the Lorentz force of electrodynamics. In such a case L no longer represents the difference of kinetic and potential energy.[9]

A similar extension of the formalism is possible for certain forces depending on higher-order derivatives of $\underline{r}$. The formalism can also be extended to continuous systems of fields,[10,11] in which case the Euler-Lagrange equations (2) of the variational principle become partial differential equations.

Variational principles have been applied also to thermodynamics. Historically, the application of minimal principles to thermodynamics was first undertaken by Helmoltz,[12] who showed that the Lagrangian function for a reversible process is analogous to the negative Helmoltz free energy. The use of the Lagrangian formalism, when possible, allows one to obtain all the conservation laws by simply analysing the invariance properties of the Lagrangian. This is a consequence of the Noether's theorem.[13] It should be, however, pointed out that deriving the equilibrium equation by a variational principle is not always possible, as discussed by several authors.[14–16] Furthermore, as discussed for the Lorentz's force, the Lagrangian of the system is not always the kinetic energy minus the potential energy. More precisely, L must be built through a knowledge of the Newton equations, and can be used subsequently for further investigations. Another well known example of the Lagrangian formalism applied to field theory is represented by the electromagnetic field. By starting from the Maxwell equations, the Lagrangian density is built, and used, e.g., for the quantization of the field.[17]

The last two examples show clearly that variational theorems, and this includes any principle of minimum, are no less and no more than means of summarizing existing results.

In particular, if minimization of some Lagrangian function leads to absurd results, this does not mean that the problem has not a solution, but that this solution cannot be deduced through a variational principle. In this case, it is necessary to solve the problem starting from Newton's equations.

3. STATIC THEORY FOR NEMATIC LIQUID CRYSTALS

3.1 Variational Approach

There are several approaches to the formulation of a static theory for nematic liquid crystals, but the majority begin by assuming a local elastic energy density f depending on the molecular average orientation $\underline{n}$ (the so-called nematic director) and its first spatial derivatives $n_{i,j} = \partial n_i/\partial x_j$, i.e.

$$f = f_F(n_i, n_{i,j}). \tag{5}$$

Usually f_F is expanded in power of $n_{i,j}$ as

$$f_F = L_{ik} n_{i,k} + L_{ijkn} n_{i,k} n_{j,n}$$

where L_{ik} and L_{ijkn} play the role of "elastic constants," as we will show in sect. 4. In the nematic phase the undistorted configuration corresponds, in the bulk, to a minimum of f_F. Consequently, in the bulk, $L_{ik} = 0$. In the following we limit ourselves to consider nematic liquid crystals, and hence we neglect L_{ik}. By decomposing L_{ijkn} in terms of the elements of symmetry of the nematic phase, routine calculations allow to write f_F in the form

$$f_F = (1/2)k_{11}(div\underline{n})^2 + (1/2)k_{22}(\underline{n}\cdot curl\underline{n})^2 + (1/2)k_{33}(\underline{n}xcurl\underline{n})^2$$
$$+ (k_{22} + k_{24})div(\underline{n}div\underline{n} + \underline{n}xcurl\underline{n}). \tag{5'}$$

k_{11}, k_{22}, k_{33}, and k_{24} are known as Frank's elastic constants of splay, twist, bend and saddle-splay respectively. We point out that Equation (5′) contains only terms biquadratic in the first derivatives of $\underline{n}$.

In the simplest formulation the actual vectorial field $\underline{n}(\underline{r})$ is deduced by means of a variational principle. More precisely the basic principle involved in this formulation is that the equilibrium state of the director $\underline{n}(\underline{r})$ is always given by that director configuration that minimizes the total elastic energy of the system, defined as

$$G = \int_V \int \int f_F(n_i, n_{i,j}) dV. \tag{6}$$

in the strong anchoring case, i.e. for fixed $\underline{n}$ on the boundary S of the volume V, or

$$G = \int_V \int \int f_F(n_i,n_{i,j})dV + \int \int_S f_S(n_i)dS, \qquad (6')$$

if the surface anchoring energy $f_s(n_i)$ is finite.

This procedure was followed by Oseen[18] and Frank,[19] and it is reported in many books on liquid crystals.[20,21] Hence, in this case, $\underline{n}(\underline{r})$ is obtained by imposing that

$$\delta G = \delta \int_V \int \int f_F(n_i,n_{i,j})dV = 0.$$

in the strong anchoring case, or

$$\delta G = \delta \int_V \int \int f_F(n_i,n_{i,j})dV + \delta \int \int_S f_S(n_i)dS = 0,$$

in the event of weak anchoring energy $f_s(n_i)$.

In a broader mechanical framework, one can invoke a principle of virtual work, as done in the pioneering paper of Ericksen.[22] More completely static theory can be derived as a special case of general dynamic theory, as shown by Ericksen[23] and Leslie.[24]

With the above elastic density all approaches essentially yield the same equations, as it can be easily shown.[22]

Some years ago Nehring and Saupe,[25] following Oseen,[18] proposed a generalization of the above elastic energy density (5), in which

$$f_{NS} = f(n_i,n_{i,j},n_{i,jk}) \qquad (7)$$

By expanding f_{NS} in terms of $n_{i,j}$ and $n_{i,jk}$ in the hypothesis that $n_{i,jk}$ is of the order of $n_{i,j}n_{k,e}$, one obtains now

$$f_{NS} = L_{ik}n_{i,k} + L_{ikn}n_{i,kn} + L_{ijkn}n_{i,k}n_{j,n},$$

as it will be discussed in sect. 4. As in the case of the f_F, in the bulk L_{ik} is zero for nematic liquid crystals. By decomposing again L_{ikn} and L_{ijkn} in terms of the elements of symmetry of the nematic phase, f_{NS} can be written as

$$f_{NS} = (1/2)K_{11}(div\underline{n})^2 + (1/2)K_{22}(\underline{n}\cdot curl\underline{n})^2 + (1/2)K_{33}(\underline{n}xcurl\underline{n})^2$$
$$+ (K_{22} + K_{24})div(\underline{n}div\underline{n} + \underline{n}xcurl\underline{n}) + K_{13}div(\underline{n}div\underline{n}).$$

K_{11}, K_{22}, K_{33} and K_{24} are now the elastic constants of splay twist, bend and saddle-splay respectively. They are connected to Frank's elastic constants by simple equations of renormalization involving K_{13}, as discussed in Reference 25. We point out that now the previous expression of f_{NS} contains terms which are linear in second order derivatives of $\underline{n}$. By indicating again the first four terms in the above expression for f_{NS} by f_F we can rewrite f_{NS} as

$$f_{NS}(n_i,n_{i,j},n_{i,jk}) = f_F(n_i,n_{i,j}) + K_{13}div(\underline{n}div\underline{n}). \tag{7'}$$

This elastic energy density gives a surface contribution depending on the normal first derivatives of the director.

The elastic theory concerning f_{NS} is based up to now only on the variational approach.[26,27]

In some previous papers[28] we have analysed the influence of the K_{13} on the nematic orientation induced by surface treatments or external fields. Our analysis shows that some published results, relative to this subject, must be revised since the variational problem is ill-posed. In particular Hinov's boundary conditions[29] are not deduced by minimizing the total elastic energy.

In recent papers[30–31] Hinov reanalyses the problem, in order to show that his analysis is consistent, by invoking Jacobi's equation and the non linear character of the K_{13}-term.

Let us now consider Reference 30, in order to discuss the role played by Jacobi's equation in a variational problem. In particular we wish to show that the boundary conditions of the problem connected to the K_{13}-term cannot be deduced by a variational principle without to generalize the elastic free energy.[32] The importance of the non-linear character of the K_{13}-term on the elastic problem will be discussed in the next section by using a simple molecular model.

3.2 First and second order variation of a functional

As in Reference 30 let $\underline{n}$ be the nematic director and θ the tilt angle between $\underline{n}$ and the surface normal. We limit ourselves to consider a planar problem in which $\underline{n}$ and θ, depend only on the distance z from the considered point to the limiting surfaces. We choose a Cartesian reference frame having the z-axis normal to the boundaries, placed in $z_1 = 0$ and $z_2 = d$; d is the sample thickness. Furthermore, by analysing the problem with the variational method, we indicate with $\delta\theta(z)$ an arbitrary function, such that, if $\theta^*(z)$ is the function minimizing a given functional, $\theta(z) = \theta^*(z) + \delta\theta(z)$ is another function close to the $\theta^*(z)$ in the variational sense.[31]

Let us consider now the usual well known functional.

$$J[\theta(z)] = \int_{z_2}^{z_1} f(\theta,\theta')dz, \tag{8}$$

for fixed values of θ at the boundaries, which implies $\delta\theta(z_1) = \delta\theta(z_2) = 0$. In Equation 8 the prime means derivation with respect to z. In the elastic problem relative to nematic liquid crystals, $J(\theta,\theta')$ represents the total energy of the nematic sample in the strong anchoring case. $f(\theta,\theta')$ is then the bulk elastic energy. By taking into account expressions (7′) and (5′), $f(\theta,\theta')$ is found to be

$$f = (1/2)(K_{11}\sin^2\theta + K_{33}\cos^2\theta)\theta'^2, \tag{7''}$$

coming from f_F, whereas the K_{13}-term is

$$f_{13} = K_{13}\frac{d}{dz}\left[\frac{1}{2}\sin(2\theta)\theta'\right], \tag{7'''}$$

whose effect will be analysed later.

By putting in (8) $\theta(z) = \theta^*(z) + \delta\theta(z)$ and expanding J in power series of $\delta\theta(z)$ up to the second order, one easily obtains

$$\Delta J = \int_{z_2}^{z_1}[f(\theta^* + \delta\theta,\theta^{*\prime} + \delta\theta') - f(\theta^*,\theta^{*\prime})]dz = (\delta J)_1 + (\delta J)_2 + \ldots . \tag{9}$$

where

$$(\delta J)_1 = \int_{z_2}^{z_1}\left[\frac{\partial f}{\partial\theta} - \frac{d}{dz}\frac{\partial f}{\partial\theta'}\right]_{\theta=\theta^*}\delta\theta dz, \tag{10}$$

and

$$(\delta J)_2 = \int_{z_1}^{z_2}\left[\frac{\partial^2 f}{\partial\theta^2}(\delta\theta)^2 + 2\frac{\partial^2 f}{\partial\theta\partial\theta'}\delta\theta\delta\theta' + \frac{\partial^2 f}{\partial\theta'^2}(\delta\theta')^2\right]_{\theta=\theta^*}dz. \tag{11}$$

The derivation of $(\delta J)_1$ from Equation 9, as well known, requires and integration by parts of $(\partial f/\partial\theta')\delta\theta'$, leading to surface terms. This implies that in Equation 10 are present two other terms of the kind

$$\left[\frac{\partial f}{\partial\theta'}\delta\theta\right]_{z_2} - \left[\frac{\partial f}{\partial\theta'}\delta\theta\right]_{z_1}$$

that in our case are identically zero, as follows from the strong anchoring hypothesis.

$(\delta J)_1$ is usually called the first variation and $(\delta J)_2$ the second variation of J respectively, since $(\delta J)_1$ is of the order of $\delta\theta$, whereas $(\delta J)_2$ of the order of $(\delta\theta)^2$. The extremizing function $\theta^*(z)$ is deduced by putting

$$(\delta J)_1 = 0, \text{ for any } \delta\theta(z)\epsilon C_1, \tag{12}$$

where C_1 is the class of continuous functions with their continuous first derivative. Condition (12) gives the well known Euler Lagrange equation. Therefore the sign of the increment ΔJ coincides with the sign of $(\delta J)_2$. It is then important to know if there exists some condition ensuring constancy of sign of the second variation $(\delta J)_2$, and thus also constancy of sign of the increment ΔJ in the problem involving an extremum. In fact, in this case one can deduce easily if the extremum corresponds to a maximum or a minimum. This condition is known as Jacobi (Legendre) condition.

3.3 Jacobi's Equation

For the reader who is not familiar with the variational calculus we recall below how it is possible to deduce this condition in the case considered. Since in our hypotheses $\delta\theta(z_1) = \delta\theta(z_2) = 0$, as follows from the fact that $\theta(z)$ takes fixed values at the boundaries, for every $w(z)$ function we have

$$\int_{z_1}^{z_2} [w'(\delta\theta)^2 + 2w\delta\theta\delta\theta']dz = \int_{z_1}^{z_2} d[w(\delta\theta)^2]$$

$$= [w(\delta\theta)^2](z_2) - [w(\delta\theta)^2](z_1) = 0. \quad (13)$$

Adding the integral (13) to (11) the second variation of J can be written as

$$(\delta J)_2 = \int_{z_1}^{z_2} \left\{\left[w' + \frac{\partial^2 f}{\partial\theta^2}\right](\delta\theta)^2 + 2\left[w + \frac{\partial^2 f}{\partial\theta\partial\theta'}\right]\delta\theta\delta\theta' + \frac{\partial^2 f}{\partial\theta'^2}(\delta\theta')^2\right\}dz. \quad (14)$$

If it is possible to choose $w(z)$, in such a way that the brace parenthesis appearing in Equation 14 is transformed into a perfect square, within a multiplying factor, we can easily analyse the sign of ΔJ. This is possible if the non linear differential equation, known as Jacobi equation,

$$\left[w' + \frac{\partial^2 f}{\partial\theta^2}\right]\frac{\partial^2 f}{\partial\theta'^2} = \left[\frac{\partial^2 f}{\partial\theta\partial\theta'} + w\right]^2, \quad (15)$$

has a differential solution $w(z)$ in the range (z_1,z_2). In this case $(\delta J)_2$ can be put in the form

$$(\delta J)_2 = \int_{z_1}^{z_2} \frac{\partial^2 f}{\partial\theta'^2}\left\{\delta\theta' + \delta\theta\,\frac{(\partial^2 f/\partial\theta\partial\theta') + w}{\partial^2 f/\partial\theta'^2}\right\}^2 dz, \quad (16)$$

and consequently the sign of $(\delta J)_2$ coincides with the one of $\delta^2 f/\partial\theta'^2$.

Note that Jacobi's equation does not fix the functional class of the arbitrary functions of $\delta\theta(z)$, since $\delta\theta(z)$ is absent in Equation 15, but it permits to write $(\delta J)_2$ in the form (16).

3.4 Variational approach to the K_{13}-elastic problem

Let us consider now our problem involving K_{13}. In this case by substituting f and f_{13} given by (7″) and (7‴) in (8) we obtain that the new functional to consider is

$$J[\theta(z)] = \int_{z_1}^{z_2} f(\theta,\theta')dz + (1/2)K_{13}\{\sin[2\theta(z_1)\theta'(z_1) - \sin[2\theta(z_2)]\theta'(z_2)\}, \quad (17)$$

in the strong anchoring case. In the opposite case of weak anchoring in (17) it is present also the surface anchoring energy coming from the nematic-substrate interaction.[3] The first variation of (17), after a straightforward calculation, is found to be

$$(\delta J)_1 = \int_{z_1}^{z_2} \left[\frac{\partial f}{\partial \theta} - \frac{d}{dz}\frac{\partial f}{\partial \theta'}\right]\delta\theta dz + (1/2)K_{13}\{\sin[2\theta(z_1)]\delta\theta'(z_1) - \sin[2\theta(z_2)]\delta\theta'(z_2)\}. \quad (18)$$

The requirement that $(\delta J)_1$ be identically zero for any function $\delta\theta(z)$ gives the Euler-Lagrange equation

$$\frac{\partial f}{\partial \theta} - \frac{d}{dz}\frac{\partial f}{\partial \theta'} = 0, \quad (19)$$

which must be solved with the boundary conditions

$$\theta(z_1) = \theta_1, \theta(z_2) = \theta_2 \quad (20)$$

Equation 20 follow from the strong anchoring hypotheses (which imply $\delta\theta(z_1) = \delta\theta(z_2) = 0$). Furthermore the condition $(\delta J)_1 = 0$ implies also

$$\sin[2\theta(z_1)] = \sin\theta(z_2)] = 0. \quad (21)$$

since $\delta\theta'(z_1)$ and $\delta\theta'(z_2)$ take arbitrary values, independent of $\delta\theta(z_1)$ or $\delta\theta(z_2)$, on the boundary. By observing that Equations 21 are satisfied only for particular values of $\theta(z_1)$ and $\theta(z_2)$, we deduce that Equation 19, which is a second order differential equation, cannot be solved in general taking into account boundary conditions (20) and (21). Consequently starting from (17) we cannot deduce the equilibrium equation by means of a variational principle. This implies that the equilibirum equations of the problem must be searched in a different way, or that the elastic energy must be modified in order to have a well posed problem.[32]

In recent papers a relation of the kind

$$\delta\theta'(z_i) = Q_i\, \delta\theta(z_i), \quad (22)$$

where Q_i is independent of $\delta\theta(z_i)$, between $\delta\theta'(z)$ and $\delta\theta(z)$ has been suggested.[29] This is a consequence, according to Reference 29 of the Jacobi equation. But, as shown above, Jacobi's equation does not fix the functional form of the arbitrary functions $\delta\theta(z)$; it only tells us when it is possible to determine a $w(z)$ such that $(\delta J)_2$ can be written in the form (16).

A simple example shows clearly that a relation of the kind (22) cannot exist. In fact if we are analysing a problem in the strong anchoring hypothesis, the arbitrary functions

$$\delta\theta_1(z) = p(z - z_1)(z - z_2)^2,$$

$$\delta\theta_2(z) = q \sin[(z - z_1)/d]\ \mathrm{tg}[(z - z_2)/d], \quad (23)$$

where $z_2 - z_1 = d$, and p and q are two small parameters, represent two possible variations of $\theta^*(z)$. It is easy to verify that

$$\delta\theta_1(z_1) = \delta\theta_1(z_2) = \delta\theta_2(z_1) = \delta\theta_2(z_2) = 0, \tag{24}$$

in agreement with the fact that $\theta(z_1)$ and $\theta(z_2)$ are imposed by the strong boundary conditions, but

$$\begin{aligned} \delta\theta_1'(z_1) &= pd^2,\ \delta\theta_1'(z_2) = 0 \\ \delta\theta_2'(z_1) &= -(q/d)\mathrm{tg}1, \\ \delta\theta_2'(z_2) &= (q/d)(\mathrm{tg}1)/(\cos 1) \end{aligned} \tag{25}$$

Equations 25 show that, in general, a relation of the kind (22), does not exist. Consequently the boundary conditions proposed by Hinov are not deduced by using a variational approach. In the above analysis we have considered the strong anchoring case. This problem is important if $\theta \neq 0$ or $\theta \neq \pi/2$ on the boundaries, since in this case the K_{13}-contribution is non zero. In the general case the problem is more complicated, but $\delta\theta(z)$ remains a true arbitrary function of the same class of the searched minimizing function. Finally, we note that the presence of the K_{13} in the elastic energy of nematics introduces some difficulties in the solution of the problem, if a variational approach is used. These difficulties can be removed if the elastic energy is modified as discussed recently.[32]

4. IMPORTANCE OF THE NON LINEAR CHARACTER OF THE K$_{13}$-ELASTIC PROBLEM

4.1 The K_{13} elastic problem and the one constant approximation

Recent papers[30,31] on the K_{13}-effect on the nematic orientation induced by external fields or surface treatments, have underlined the importance of the non linear character of the elastic problem. More precisely in these papers[30,31] it is claimed that, if the elastic density energy of the nematic, given by Equation 7″, valid for a planar and unidimensional problem, reduces to

$$f_F = (1/2)K\theta'^2, \tag{26}$$

where

$$K = K_{11}' = K_{33}, \tag{27}$$

is the common value of the splay and bend elastic constants, then $K_{13} = 0$. According to this point of view, to solve a problem in the one constant approximation for the bulk, in order to obtain information on the K_{13} effect, is meaningless.[30,31] In this section, following Vertogen's approach[34–36] we will obtain some expressions for the elastic constants, which show the importance of the different contributions of the molecular interaction law on the elastic parameters. In particular, we will show that it is possible to have equal splay and bend elastic constants and in the same time a K_{13} different from zero. This is a well known result, obtained in a special case twenty years ago by Nehring and Saupe.[37]

4.2 Molecular interaction energy and elastic energy

Let us consider a generical two-body interaction law $g(\underline{n},\underline{n}',\underline{r})$ between two molecules, where $\underline{n}$ and $\underline{n}'$ are the directors at points $\underline{R}$ and $\underline{R}'$ respectively and $\underline{r} = \underline{R}' - \underline{R}$. For the sake of simplicitly the system is assumed to possess perfect order ($S = 1$, where S is the scalar order parameter), i.e. we assume that the molecular long axis at a generical point $\underline{R}$ is in the direction of $\underline{n}(\underline{R})$. We are interested only in small distortions: $\underline{n}'(R') = \underline{n}(R) + \Delta\underline{n}(\underline{R},\underline{r})$, with $|\Delta\underline{n}| << 1$. By expanding g in terms of $\Delta\underline{n}$, we have

$$\begin{aligned} g(\underline{n},\underline{n}',\underline{r}) &= g[\underline{n}(\underline{R}),\underline{n}(\underline{R}) + \Delta\underline{n}(\underline{R},\underline{r}),\underline{r}] \\ &= g(\underline{n},\underline{n},\underline{r}) + q_i(\underline{R},\underline{r})\Delta n_i(\underline{R},\underline{r}) \\ &\quad + (1/2)q_{ij}(\underline{R},\underline{r})\Delta n_i(\underline{R},\underline{r})\Delta n_i(\underline{R},\underline{r}) + 0(3), \qquad (28) \end{aligned}$$

where

$$q_i(\underline{R},\underline{r}) = \left[\frac{\partial g}{\partial n_i'}\right]_{\Delta n = 0}, \text{ and } q_{ij}(\underline{R},\underline{r}) = \left[\frac{\partial^2 g}{\partial n_i'\partial n_j'}\right]_{\Delta n = 0} = q_{ji}(\underline{R},\underline{r}). \qquad (29)$$

If we suppose that the molecular interaction force goes rapidly to zero when $|\underline{r}|$ grows, we can write

$$\Delta n_i(\underline{R},\underline{r}) = n_{i,k}(\underline{R})r_k + (1/2)n_{i,jk}(\underline{R})r_j r_k + 0(3). \qquad (30)$$

This gives

$$\Delta n_i(\underline{R},\underline{r})\Delta n_j(\underline{R},\underline{r}) = n_{i,k}(\underline{R})n_{j,n}(\underline{R})r_k r_n + 0(3). \qquad (31)$$

By substituting Equations 30 and 31 in Equation 28, we obtain

$$\begin{aligned} g(\underline{n},\underline{n}',\underline{r}) &= g(\underline{n},\underline{n},\underline{r}) + q_i(\underline{R},\underline{r})n_{i,k}(\underline{R})u_k r + (1/2)[q_i(\underline{R},\underline{r})n_{i,km}(\underline{R}) \\ &\quad + q_{ij}(\underline{R},\underline{r})n_{i,k}(\underline{R})n_{j,m}(\underline{R})]u_k u_m r^2 + 0(3), \qquad (32) \end{aligned}$$

where $\underline{u} = \underline{r}/|\underline{r}|$. The free energy density f is calculated by integrating the above expression of g over the volume V_N, defined by the interaction range r_N of the interaction law and by the molecular dimension r_o. The volume V_N has not a simple shape, but it depends on the anisotropy of the molecules and the interaction law.

For the sake of mathematical simplicity, however, we consider it, in a first approximation, spherical. Hence

$$f(\underline{R}) = (1/2)\int\int_{V_N}\int g(\underline{n},\underline{n}',\underline{r})dV. \tag{33}$$

Using (32), the above expression can be written as

$$f(\underline{R}) = f_0(\underline{R}) + L_{ik}(\underline{R})n_{i,k}(\underline{R}) + L_{ikn}(\underline{R})n_{i,kn}(\underline{R}) + L_{ijkn}(\underline{R})n_{i,k}(\underline{R})n_{j,n}(\underline{R}) + 0(3), \tag{34}$$

where

$$L_{ik}(\underline{R}) = (1/2)\int\int\int_{V_N} q_i(\underline{R},\underline{r})u_k r dV, \tag{35}$$

$$L_{ikm}(\underline{R}) = (1/4)\int\int\int_{V_N} q_i(\underline{R},\underline{r})u_k u_m r^2 dV = L_{imk}(\underline{R}), \tag{36}$$

$$L_{ijkm}(\underline{R}) = (1/4)\int\int\int_{V_N} q_{ij}(\underline{R},\underline{r})u_k u_m r^2 dV. \tag{37}$$

The tensor $L_{ijkm}(\underline{R})$, defined in (37), is symmetric with respect to the first and the second pairs of indexes

$$L_{ijkm}(\underline{R}) = L_{jikm}(\underline{R}) = L_{jimk}(\underline{R}) = L_{ijmk}(\underline{R}). \tag{38}$$

In (34) the term

$$f_0(\underline{R}) = (1/2)\int\int\int_{V_N} g(\underline{n},\underline{n},\underline{r})dV, \tag{39}$$

represents the free energy density of the undistorted state.

g depends only on the three rotational invariants made using $\underline{n}$, $\underline{n}'$ and $\underline{u}$, i.e.

$$g(\underline{n},\underline{n}',\underline{r}) = g[(\underline{n}\cdot\underline{u}),(\underline{n}'\cdot\underline{u}),(\underline{n}\cdot\underline{n}'),r]. \tag{40}$$

Consequently we can expand g in a Taylor's series in the following way

$$g(\underline{n},\underline{n}',\underline{r}) = -\sum_{abc} J_{a,b,c}(r)(\underline{n}\cdot\underline{u})^a(\underline{n}'\cdot\underline{u})^b(\underline{n}\cdot\underline{n}')^c. \tag{41}$$

In this expansion, the coupling constants $J_{a,b,c}$ depend only on the modulus of $\underline{r}$ and not on its direction, since the described interaction g must be invariant with respect to rotations. By taking into account that the states $\underline{n}$ and $-\underline{n}$ are equivalent, we deduce

$$g(\underline{n},\underline{n}',\underline{r}) = g(-\underline{n},\underline{n}',\underline{r}) = g(\underline{n},-\underline{n}',\underline{r}), \tag{42}$$

and consequently $(a + c)$, $(b + c)$ and $(a + b)$ are even number. Using the expansion (41), the quantities $q_i(\underline{R},\underline{r})$ and $q_{ij}(\underline{R},\underline{r})$ defined in (29) become

$$q_i(\underline{R},\underline{r}) = -\sum_{abc} J_{a,b,c}(r)(\underline{n}\cdot\underline{u})^a[bu_i(\underline{n}\cdot\underline{u})^{b-1} + cn_i(\underline{n}\cdot\underline{u})^b], \tag{43}$$

$$q_{ij}(\underline{R},\underline{r}) = -\sum_{abc} J_{a,b,c}(r)(\underline{n}\cdot\underline{u})^a[b(b-1)u_iu_j(\underline{n}\cdot\underline{u})^{b-2} + bc(u_in_j + u_jn_i)(\underline{n}\cdot\underline{u})^{b-1} + c(c-1)n_in_j(\underline{n}\cdot\underline{u})^b]. \tag{44}$$

Let us calculate now the second order terms of the free energy density (Equation 34). Since $n_in_i = 1$, one obtains

$$n_in_{i,j} = 0. \tag{45}$$

Using this relation and Equations 43 and 44, the free energy density given by Equation 34 can be written

$$f = A_{ikm}n_{i,km} + B_{km}n_jn_{j,km} + C_{ijkm}n_{i,k}n_{j,m}, \tag{46}$$

where (in the bulk, the volume integration is performed over a spherical volume V_N)

$$A_{ikm} = -(1/16\pi)\sum_{abc} J(a,b,c)b \int\int_{4\pi} (\underline{n}\cdot\underline{u})^{a+b-1}u_iu_ku_m d\Omega, \tag{47}$$

$$B_{km} = -(1/16\pi)\sum_{abc} J(a,b,c)c \int\int_{4\pi} (n\cdot u)^{a+b}u_ku_m d\Omega, \tag{48}$$

$$C_{ijkm} = -(1/16\pi)\sum_{abc} J(a,b,c)b(b-1) \int\int_{4\pi} (\underline{n}\cdot\underline{u})^{a+b-2}u_iu_ju_ku_m d\Omega, \tag{49}$$

$$J(a,b,c) = 4\pi \int J_{a,b,c}(r)r^4 dr, \tag{50}$$

and $d\Omega$ is the element of solid angle, when $\underline{n}$ is the polar axis. Expression 46 coincides with expression 34. Equation 46 gives the elastic energy in terms of $n_{i,j}$ and $n_{i,jk}$. The coefficients A_{ikm}, B_{km} and C_{ijkm} can then be considered as elastic coefficients.

4.3 Elastic coefficients and molecular interaction law

The tensors $\underline{\underline{A}}$, $\underline{\underline{B}}$ and $\underline{\underline{C}}$, defined in 47, 48 and 49 are symmetric with respect to all their indexes. These tensors can be expanded, as usual, in terms of the unit tensor $\underline{\underline{\delta}}$ and $\underline{n}$, obtaining

$$A_{ikm} = A_1 n_i n_k n_m + A_2(n_i \delta_{km} + n_k \delta_{im} + n_m \delta_{ik}), \tag{51}$$

$$B_{km} = B_1 n_k n_m + B_2 \delta_{km}, \tag{52}$$

$$\begin{aligned} C_{kmij} = {} & C_1 n_k n_m n_i n_j + C_3(\delta_{km}\delta_{ij} + \delta_{ki}\delta_{mj} + \delta_{kj}\delta_{mi}) + C_2(n_k n_m \delta_{ij} \\ & + n_i n_j \delta_{km} + n_k n_i \delta_{mj} + n_k n_j \delta_{mi} + n_m n_j \delta_{ki} + n_m n_i \delta_{kj}), \end{aligned} \tag{53}$$

From 51 it follows that

$$\begin{aligned} A_1 &= (1/2)(5 n_i n_k n_m A_{ikm} - 3 n_i A_{ikk}), \\ A_2 &= (1/2)(n_i A_{ikk} - n_i n_k n_m A_{ikm}). \end{aligned} \tag{54}$$

By operating the same way, from 52

$$\begin{aligned} B_1 &= (1/2)(3 n_k n_m B_{km} - B_{kk}), \\ B_2 &= (1/2)(B_{kk} - n_k n_m B_{km}), \end{aligned} \tag{55}$$

and finally, from 53

$$\begin{aligned} C_2 &= (1/2)(6 n_i n_j C_{kkij} - 5 n_k n_m n_i n_j C_{kmij} - C_{kkii}), \\ C_3 &= (1/8)(n_k n_m n_i n_j C_{kmij} + C_{kkii} - 2 n_i n_j C_{kkij}). \end{aligned} \tag{56}$$

It is not necessary to evaluate the term C_1 because it gives no contributions to the elastic energy (see Equation 45). By Equation 47, we can write

$$\begin{aligned} n_i A_{ikk} &= -(1/4) \sum_{a,b,c} J(a,b,c) \frac{b}{a+b+1}, \\ n_i n_k n_m A_{ikm} &= -(1/4) \sum_{a,b,c} J(a,b,c) \frac{b}{a+b+3}. \end{aligned} \tag{57}$$

Then, Equations 54 give

$$\begin{aligned} A_1 &= -(1/4) \sum_{a,b,c} J(a,b,c) \frac{b(a+b+2)}{(a+b+3)(a+b+1)}, \\ A_2 &= -(1/4) \sum_{a,b,c} J(a,b,c) \frac{b}{(a+b+1)(a+b+3)}. \end{aligned} \tag{58}$$

From 48, we obtain

$$B_{kk} = -(1/4)\sum_{a,b,c} J(a,b,c)\frac{c}{a+b+1},$$

$$n_k n_m B_{km} = -(1/4)\sum_{a,b,c} J(a,b,c)\frac{c}{a+b+3}, \qquad (59)$$

and substituting B_{kk} and $n_k n_j B_{kj}$ in 55:

$$B_1 = -(1/4)\sum_{a,b,c} J(a,b,c)\frac{c(a+b)}{(a+b+3)(a+b+1)},$$

$$B_2 = -(1/4)\sum_{a,b,c} J(a,b,c)\frac{c}{(a+b+3)(a+b+1)}. \qquad (60)$$

From 49, we deduce furthermore

$$C_{kkii} = -(1/4)\sum_{a,b,c} J(a,b,c)\frac{b(b-1)}{a+b-1},$$

$$n_i n_j C_{kkij} = -(1/4)\sum_{a,b,c} J(a,b,c)\frac{b(b-1)}{a+b+1},$$

$$n_k n_m n_i n_j C_{kmij} = -(1/4)\sum_{a,b,c} J(a,b,c)\frac{b(b-1)}{a+b+3}, \qquad (61)$$

and, from 56, we have

$$C_2 = -(1/4)\sum_{a,b,c} J(a,b,c)\frac{b(b-1)(a+b-2)}{(a+b+3)(a+b+1)(a+b-1)},$$

$$C_3 = -(1/4)\sum_{a,b,c} J(a,b,c)\frac{b(b-1)}{(a+b+3)(a+b+1)(a+b-1)}. \qquad (62)$$

Now, using Equation 51, it follows that

$$A_{ikm}n_{i,km} = -3A_2(div\underline{n})^2 - A_2(\underline{n}\cdot curl\underline{n})^2 - (A_1 + A_2)(\underline{n}xcurl\underline{n})^2$$
$$+ A_2 div(\underline{n}div\underline{n} + \underline{n}xcurl\underline{n}) + 2A_2 div(\underline{n}div\underline{n}). \qquad (63)$$

and, by Equation 52, we can write

$$B_{km}n_i n_{i,km} = -B_2(div\underline{n})^2 - B_2(\underline{n}\cdot curl\underline{n})^2$$
$$-(B_1 + B_2)(\underline{n}xcurl\underline{n})^2 + B_2 div(\underline{n}div\underline{n} + \underline{n}xcurl\underline{n}) \qquad (64)$$

Finally, from 53, we obtain

$$C_{kmij}n_{i,k}n_{j,m} = 3C_3(div\underline{n})^2 + C_3(\underline{n}\cdot curl\underline{n})^2 + (C_2 + C_3)(\underline{n}xcurl\underline{n})^2 - 2C_3 div(\underline{n}div\underline{n} + \underline{n}xcurl\underline{n}). \qquad (65)$$

4.4 Nehring–Saupe elastic energy density

We can now rewrite the elastic energy given by Equation 46 in the standard form, in which only *div$\underline{n}$*, *$\underline{n}\cdot curl\underline{n}$* and *$\underline{n}xcurl\underline{n}$* appear. By adding Equations 63, 64 and 65, we have

$$f = (1/2)\,\{K_{11}(div\underline{n})^2 + K_{22}(\underline{n}\cdot curl\underline{n})^2 + K_{33}(\underline{n}xcurl\underline{n})^2\} + K_{13}div(\underline{n}div\underline{n}) + (K_{22} + K_{24})div(\underline{n}div\underline{n} + \underline{n}xcurl\underline{n}), \qquad (66)$$

where

$$K_{11} = 2(-3A_2 - B_2 + 3C_3),$$

$$K_{22} = 2(-A_2 - B_2 + C_3),$$

$$K_{33} = 2(-A_1 - A_2 - B_1 - B_2 + C_2 + C_3),$$

$$K_{13} = 2A_2,\ K_{22} + K_{24} = -A_2 + B_2 - 2C_3. \qquad (67)$$

From Equation 67, using Equation 58, 60 and 62, we can derive the usual nematic elastic constants:

$$K_{11} = (1/2)\sum_{a,b,c} \frac{J(a,b,c)}{(a + b + 1)(a + b + 3)} \left\{3\frac{ab}{a + b + 1} + c\right\}$$

$$K_{22} = (1/2)\sum_{a,b,c} \frac{J(a,b,c)}{(a + b + a + 1)(a + b + 3)} \left\{\frac{ab}{a + b - 1} + c\right\}$$

$$K_{33} = (1/2)\sum_{a,b,c} \frac{J(a,b,c)}{a + b + 3} \left\{\frac{ab}{a + b + 1} + c\right\} \qquad (68)$$

for the bulk, firstly given by Vertogen,[34] and

$$K_{13} = -(1/2)\sum_{a,b,c} J(a,b,c)\frac{b}{(a + b + 1)(a + b + 3)} \qquad (69)$$

$$K_{22} + K_{24} = (1/4)\sum_{a,b,c} J(a,b,c)\frac{3b + c}{(a + b + 1)(a + b + 3)} \qquad (70)$$

for the divergence terms.

Therefore if the molecular interaction law is known, we are able, by means of Equations 50, 68, 69 and 70, to calculate immediately all the relevant elastic constants.

The obtained relations show that K_{13} is different from zero, whenever that the interaction law depends on $(\underline{n}\cdot\underline{u})$, as discussed in a separate paper.[38]

In the case of the induced-dipole induced-dipole interaction analysed by Nehring and Saupe, $g(\underline{n},\underline{n}',\underline{r})$ is

$$g = J(r)[3(\underline{n}\cdot\underline{u})(\underline{n}'\cdot\underline{u}) - (\underline{n}\cdot\underline{n}')]^2,$$

where $J(r) = C/r$.[6] By writing g in the form

$$g = J(r)[(\underline{n}\cdot\underline{n}')^2 - 6(\underline{n}\cdot\underline{u})(\underline{n}'\cdot\underline{u})(\underline{n}\cdot\underline{n}') + 9(\underline{n}\cdot\underline{u})^2(\underline{n}'\cdot\underline{u})^2],$$

we have[34]

$$J(a,b,c) = J[\delta_{a0}\delta_{b0}\delta_{c2} - 6\delta_{a1}\delta_{b1}\delta_{c1} + 9\delta_{a2}\delta_{b2}\delta_{c0}],$$

where

$$J = 4\pi\int_0^\infty J(r)r^4dr.$$

We can now easily evaluate the sum appearing in Equations 68, 69, and 70 to obtain

$$K_{11} = K_{33} = (1/21)J,\ K_{22} = (11/105)J,\ K_{13} = -(2/35)J.$$

These equations show that, in this case splay and bend elastic constants are equal, and K_{13} is different from zero.[37] Hence the non linear character of the energy density is not a fundamental characteristic of the K_{13}-elastic problem. It follows that the variational problem, when the K_{13} energy term is present and the energy density is the usual one, is ill posed. Consequently the proposed boundary conditions relative to this variational problem[26,27] are not correct and must be revised, even if Hinov claims that they work well.

5. ON THE VIRTUAL WORK PRINCIPLE

5.1 Basic Ipotheses

In this section the virtual work principle is recalled, and later applied to the K_{13}-elastic problem.

Let us consider a nematic sample of volume V, bounded by a surface S. Let $f_F = f_F(n_i,n_{i,j})$ be the usual volume elastic energy density, and $f_s = f_s(n_i)$ the surface elastic energy density. The total elastic energy of the sample is given by Equation 6′, which we rewrite as

$$G = \int\int_V\int f_F dV + \int\int_S f_s ds = G_v + G_s.$$

Let us suppose now that by means of some external forces or torques the following deformations are induced on the sample

$$1)\ x_i \to x_i' = x_i + \delta x_i,$$

$$2)\ n_i(\underline{x}) \to n_i'(\underline{x}') = n_i(\underline{x}) + \delta n_i(\underline{x},\underline{x}')$$

$$3)\ n_{i,j}(\underline{x}) \to (n_{i,j})' = n_{i,j}(\underline{x}) + \delta(n_{i,j})(\underline{x},\underline{x}'). \tag{71}$$

Consequently the bulk and surface elastic energy densities become, at the first order in the deformations,

$$f_F \to f_F' = f_F[n_i + \delta n_i, n_{i,j} + \delta(n_{i,j})] = f_F + Y_i\delta n_i + Z_{ij}\delta(n_{i,j}), \tag{72}$$

$$f_s \to f_s' = f_s(n_i + \delta n_i) = f_s + y_i\delta n_i, \tag{73}$$

where

$$Y_i = \partial f_F/\partial n_i, Z_{ij} = \partial f_F/\partial(n_{i,j}),\ y_i = \partial f_s/\partial n_i. \tag{74}$$

It follows that after application of the external forces and torques G is

$$G' = \int\int_{V'}\int f_F' dV' + \int\int_{S'} f_s' ds' = (G_V)' + (G_S)', \tag{75}$$

where V' and S' are the volume and surface of the sample in the deformed state.

5.2 Bulk and surface variations of the elastic energy

Let us consider first the volume term appearing in Equation 75. By taking into account Equation 72 routine calculations give

$$(G_V)' = \int\int_{V'}\int f_F' dV' = \int\int_V\int [f_F + Y_i\delta n_i + Z_{ij}\delta(n_{i,j})]J(\underline{x}'/\underline{x})dV, \tag{76}$$

where

$$J(\underline{x}'/\underline{x}) = det(\partial x_j'/\partial x_k) = det(x_{j,k}'), \tag{77}$$

is the Jacobian of the transformation (71-1).[39] Since, as follows from (71-1), $x'_{j,k} = \delta_{ik} + (\delta x_j)'_k$, at the first order in the variations, $J(\underline{x}'/\underline{x})$ is found to be

$$J(\underline{x}'/\underline{x}) = 1 + (\delta x_i)_{,i}. \tag{78}$$

Hence

$$\delta G_V = (G_V)' - G_V = \int\int_V\int [Y_i \delta n_i + Z_{ij}\delta(n_{i,j}) + f_F(\delta x_i)_{,i}]dV. \tag{79}$$

Note that $\delta(n_{i,j}) \neq (\delta n_i)_{,j}$, i.e. δ and $\partial/\partial x_j$ do not commute: $[\delta,\partial/\partial x_j] \neq 0$. In fact, as it is easy to verify,

$$\delta(n_{i,j}) = (\delta n_i)_{,j} - n_{i,k}(\delta x_k)_{,j}. \tag{80}$$

Equation 80 shows that only if $\delta x_k \equiv 0$, it is possible to interchange the operators δ and $\partial/\partial x_j$. For this reason it is useful to introduce another variation operator δ^* of the parameter characterizing the elastic deformation in the following way:

$$\delta n_i(\underline{x},\underline{x}') = n'_i(\underline{x}') - n_i(\underline{x}) = n_{i,j}\delta x_j + \delta^* n_i. \tag{81}$$

The quantity

$$n'_i(\underline{x}') - n'_i(\underline{x}) \sim n_{i,j}\delta x_j, \tag{82}$$

takes into account the director variation coming only from the spatial displacement ($\underline{x}' = \underline{x} + \delta\underline{x}$), whereas

$$n'_i(\underline{x}) - n_i(\underline{x}) = \delta^* n_i(\underline{x}), \tag{83}$$

takes into account only the rotation of $\underline{n}$, at a fixed spatial position. By operating in the same way it is also possible to write

$$\delta(n_{i,j}) = n_{i,jk}\delta x_k + \delta^*(n_{i,j}), \tag{84}$$

where now

$$\delta^*(n_{i,j}) = (\delta^* n_i)_{,j}, \tag{85}$$

i.e. δ^* and $\partial/\partial x_j$ commute, as it is easy to verify.

By taking into account 81 and 84, a straightforward calculation gives

$$\delta G_V = -\int\int_V\int [(Z_{ij,j} - Y_i)\delta n_i - (X_{kj,j} - f_{F,k})\delta x_k]dV$$
$$+ \int\int_S [Z_{ij}\delta n_i - (X_{kj} - f_F\delta_{kj})\delta x_k]N_j dS, \tag{86}$$

where

$$X_{kj} = Z_{ij}n_{i,k}, \tag{87}$$

and $\underline{N}$ is the unit vector normal to S in a given point. Let us consider now the surface contribution to the total elastic energy, G_S. In the deformed situation $(G_S)'$ is found to be[39]

$$(G_S)' = \int\int_{S'} f'_s dS' = \int\int_S [f_s + y_i\delta n_i]J(x'/x)(x_{e,i}N_e x_{k,i}N_k)^{1/2}dS, \tag{88}$$

where Equation 73 has been taken into account and furthermore the dS' has been transformed in the usual way in order to have an integration over the old surface S. Routine calculations give for $\delta G_s = (G_s)' - G_s$ the expression

$$\delta G_S = \int\int_S [y_i\delta n_i + f_s(\delta_{ij} - N_iN_j)(\delta x_j)_{,i}]dS. \tag{89}$$

5.3 Bulk equilibrium equations, and boundary conditions

The total variation of the elastic energy is found by adding Equations 86 and 89. In this way δG is found to be

$$\delta G = \delta G_V + \delta G_S = -\int\int_V\int [(Z_{ij,j} - Y_i)\delta n_i - (X_{kj,j} - f_{F,k})\delta x_k]dV$$

$$+ \int\int_s [(Z_{ij}N_j + y_i)\delta n_i - (X_{kj} - f_F\delta_{kj})\delta x_k + f_s(\delta_{ij} - N_iN_j)(\delta x_j)_{,i}]dS. \tag{90}$$

Starting by Equation 90 it is possible to assume a principle of virtual work of the form

$$\delta G = \int\int_V\int (c_i\delta x_i + d_i\delta n_i)dV + \int\int_S [a_i\delta x_i + b_i\delta n_i + e_{ij}(\delta x_j)_{,i}]dS, \tag{91}$$

which is equivalent to assume the differntial equations of equilibrium

$$1)\ d_i + Z_{ij,j} - Y_i = 0,$$

$$2)\ -(X_{kj,j} - f_{F,k}) + c_i = 0, \tag{92}$$

with the boundary conditions

$$1)\ b_i = Z_{ij}N_j + y_i,$$

$$2)\ a_j = -(X_{kj} - f_F\delta_{kj})N_k,$$

$$3)\ e_{ij} = f_s(\delta_{ij} - N_iN_j). \tag{93}$$

In the event that $\delta x_i = 0$ and $\delta n_i = \varepsilon_{iml}\omega_m n_l = \delta^* n_i$, δG given by Equation 90 reduces to the one that it is possible to deduce by means of the variational analysis. In this case d_i coincide with the torque bulk density and b_i with the surface torque density connected to external fields. In this subcase Equations 92-2 and 93-2, 93-3 are not important, and the basic equation of the elastic problem are Equations 92-1 and 93-1, as well known.

In the unidimensional case, 92-1 reduces to a second order differential equation in the angle characterizing the director orientation. The boundary conditions 93-1 reduce to two conditions on the above mentioned angle on the planes limiting the sample. The problem is then well posed and admits continuous solution.

5.4 Virtual work principle and K_{13}-elastic program

Let us consider now, in the general frame of Equation 71, the presence of the K_{13}-term. In this case the surface contribution of G contains the usual G_s and furthermore the term $G_{13} = \int\int K_{13}(n_{j,j})n_k N_k dS$, obtained by means of Gauss' theorem. Routine calculations give now for the δG the expression

$$\begin{aligned}\delta G &= \delta G_v + \delta G_s + \delta G_{13}\\ &= -\int\int_V\int [(Z_{ij,j} - Y_i)\delta n_i - (X_{kj,j} - f_{F,k})\delta x_k]dV + \int\int_S \{(Z_{ij}N_j\\ &\quad + y_i + K_{13}n_{j,j}N_i)\delta n_i + K_{13}n_i N_i \delta(n_{j,j}) - (X_{kj} - f_F\delta_{kj})\delta x_k\\ &\quad + [f_s(\delta_{ij} - N_i N_j) + K_{13}n_{k,k}(n_r N_r \delta_{ij} - n_i N_j)](\delta x_j)_{,i}\}dS, \qquad (94)\end{aligned}$$

instead of Equation 90.

Since in Equation 94 is present, in the surface contribution, a term in $\delta(n_{j,j})$ it is no longer possible to assume a principle of virtual work of the form Equation 91. Equation 91 must be modified in the form

$$\delta G = \int\int_V\int (c_i\delta x_i + d_i\delta n_i)dV + \int\int_S [a_i\delta x_i + b_i\delta n_i + e_{ij}(\delta x_j)_{,i} + t\delta(n_{j,j})]dS. \qquad (95)$$

It follows that the bulk equations (92) do not change, whereas the boundary conditions (93) contain another equation of the kind

$$t = K_{13}n_i N_i. \qquad (96)$$

The existence of Equation 96 implies that the problem is now ill-posed. In fact since in the previous case (where the K_{13} was not considered) the problem has a well defined solution, the boundary conditions (93) allow one to solve the bulk equations (92). On the contrary when the K_{13}-term is considered the supplementary boundary condition (96) must be satisfied: consequently either Equation 96 is identically satisfied, or the problem is impossible. In the first case t must be identically equal to $K_{13}n_iN_i$, i.e. it is not connected to external forces or torques, and this is not consistent with our hypothesis, that t be due only to external actions. Hence the K_{13} problem is not a well posed problem, even if the principle of virtual work is invoked.

6. CONCLUSIONS

In this paper a review of the variational calculus formalism has been given. The range of applicability of the Lagrangian formalism to solve practical problems has been discussed, underlining in particular that only some problems can be solved by means of a variational approach. If some absurd results obtained by solving a given problem with a variational technique are obtained, this only means that the approach used does not work in this case. The well known K_{13}-problem is of this kind since, by solving the Euler-Lagrange equation, which is a differential second order equation, it is necessary to satisfy four boundary conditions, since $\delta\theta$ and $\delta\theta'$ are undependent quantities at the boundary.

Consequently, if one wishes to apply the variational approach, the elastic energy density must be modified, as recently discussed.[32] In this case a sharp variation of the tilt angle near to the boundary is expected. This "surface variation" is independent of the new terms which are introduced in the elastic energy in order to have a well posed variational problem.[32] This fact suggests that alternative procedure may yield similar results.

The role of the Jacobi equation has also been discussed, pointing out that it is not an equation for the arbitrary function $\delta\theta$, but a condition to write in a particular manner the second variation of a given functional. Finally the importance of the non linear character of the K_{13}-problem is discussed by using a simple molecular model. In this way we have shown that it is possible to have the splay elastic constant equal to the bend one, and in the same time a $K_{13} \neq 0$. This fact shows that recent results must be completely revised. Furthermore the principle of virtual work has been applied to the elastic theory of nematic liquid crystals. In this way we have shown that the K_{13}-elastic problem cannot be solved even in this framework, if the bulk energy density is not modified.

References

1. W. Yourgran and S. Mandelstam, "Variational Principles in Dynamics and Quantum Theory", London 1956.
2. P. G. de Gennes, "The Physics of Liquid Crystals", Clarendon Press 1974.
3. C. Oldano and G. Barbero, *Phys. Lett. A*, **110A**, 213 (1985).
4. L. Elsogts, "Differential Equations and the Calculus of Variations" MIR, Moscow (1980).
5. H. Hinov and A. I. Derzhanski, *J. de Phys.*, **40**, C3-105 (1979).
6. R. B. Feynman and M. Sands Leighton, *The Feynman Lectures on Physics sect. 19*, **2**, Addison Wesley 1963.
7. J. L. Lagrange, *Mécanique analytique*, Paris 1788.
8. L. Landau and I. M. Lifshictz, "Mécanique", MIR (Moscow) (1976).
9. H. Goldstein, "Classical Méchanics", Cambridge, Mass, (1950).

10. L. Landau and I. M. Lifshictz, "Theorie des champs", MIR (Moscw) (1976).
11. N. N. Bogolioubov and D. V. Chirov, "Introduction à la theorie quantique des champs" Dunod (Paris) (1960).
12. H. Helmoltz, *Crelle's Journ.*, **100**, 137 (1886).
13. E. Noether, *Nachr. Akad. Wiss. Gottingen, Math. Phys. Kl*, 235 (1918) and R. S. Akopyan and B. Ya. Zel'dovich, *JETP* **56**, 1239 (1983) for the application of this theorem to liquid crystals.
14. P. Havas, *Phys. Rev.*, **83**, 224 (1951).
15. H. Helmoltz, *Journ. f.d. reine u angew. Math.* **100**, 137 (1887).
16. E. Gerjoury, A. R. P. Rau and L. Spruch, *Rev. of Modern Physics*, **55**, 725 (1983).
17. C. Cohen-Tannoudji, J. Dupont-Roc and G. Grynberg, "Photons et atomes" Inter Editions (Paris), (1987).
18. C. W. Oseen, *Trans. Faraday Soc.*, **29**, 883 (1933).
19. F. C. Frank, *Disc. Faraday Soc.*, **25**, 19 (1958).
20. G. Vertogen and W. H. de Jeu, "Thermotropic Liquid Crystals, Fundamentals", Springer-Verlag (1988).
21. E. B. Priestley, P. G. Wojtowicz and Ping Sheng, "Introduction to Liquid Crystals", New York, Plenum Press (1975).
22. J. L. Ericksen, *Trans. of the Society of Reology*, **V**, 23 (1961).
23. J. L. Ericksen, *Archs. ration. Mech. Analysis*, **9**, 371 (1962).
24. F. M. Leslie, *Archs. ration. Mech. Analysis*, **28**, 265 (1968); *J. Phys. D: Appl. Phys.*, **3**, 889 (1970); *Phil. Trans. R. Soc. Lond. A*, **309**, 955 (1983).
25. J. Nehring and A. Saupe, *J. Chem. Phys.*, **54**, 337 (1971).
26. A. I. Derzhanski and H. P. Hinov, *Phys. Lett.* **56A**, 465 (1976).
27. H. P. Hinov, *J. Physique Lett.*, **38**, 215 (1977).
28. G. Barbero, C. Oldano, *Il Nuovo Cimento*, **6D**, 479 (1985); C. Oldano and G. Barbero, *J. Phys. Lett.*, **46**, 451 (1985); G. Barbero and C. Oldano, *Mol. Cryst. Liq. Cryst.*, **168**, 1 (1989).
29. H. P. Hinov, *Mol. Cryst. Liq. Cryst.*, **148**, 197 (1987).
30. H. P. Hinov, *Mol. Cryst. Liq. Cryst.*, **168**, 7 (1989).
31. H. P. Hinov, *Mol. Cryst. Liq. Cryst.*, **178**, 53 (1990).
32. G. Barbero, N. V Madhusudana and C. Oldano, *J. de Phys.*, **50**, 2263 (1989).
33. V. Smirnov, "Course de Mathematiques superieures", Tome IV, Premiére partie p. 211, MIR (Moscow) (1975).
34. G. Vertogen, *Physica*, **117A**, 227 (1983), and *Phys. Lett.*, **89A**, 448 (1983).
35. G. Vertogen, S. D. Flapper and C. Dullemond, *J. Chem. Phys.*, **76**, 616 (1982).
36. G. Gover and G. Vertogen, *Phys. Rev.*, **A30**, 1398 (1984) and *Liq. Cryst.* **2**, 31 (1987).
37. J. Nehring and A. Saupe, *J. Chem. Phys.*, **56**, 5527 (1972).
38. G. Barbero and C. Oldano, *Mol. Cryst. Liq. Cryst.*, **170**, 99 (1989).
39. D. F. Nelson, "Electric, Optic and Acoustic Interactions in Dielectrics", John Wiley and Sons (1979), p. 38.