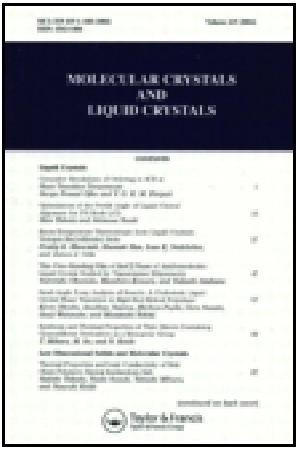

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Comment on the Criticism of the One-Dimensional Solution of the K_{13} Elastic Problem in Nematics

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Comment on the Criticism of the One-Dimensional Solution of the K_{13} Elastic Problem in Nematics

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On the basis of a simple one-dimensional theoretical analysis made in the frame of the Euler-Lagrange formalism it is shown that the K_{13} elastic problem is a purely nonlinear elastic problem. This result completely invalidates the criticism of the one-dimensional solution of the K_{13} elastic problem in nematics based on linear functions and constants. It is found the magnitude and the sign of the second-order elastic constant K_{13} and it is shown that the Frank elastic constants of splay K_{11} and bend K_{33} must be positive. These results clearly show that the K_{13} elastic problem can be successfully resolved only in the frame of the Euler-Lagrange formalism and that the elastic theory of Nehring and Saupe for the case of the nematics has been obtained under correct assumptions.

In several papers[1–3] Barbero and Oldano using linear functions or constants, on the basis of elastic functionals of the type:

$$F(\theta(z)) = 2\left\{\int_0^d (k/2)\theta'^2\,dz + (w/2)(\theta - \theta_e)^2 - K_{13}\theta\theta'\right\} \tag{1}$$

critically have discussed my way of the variation of the K_{13} elastic surface-like volume energy in nematics (see Reference 4 and the citations therein). Something more, contrary to my theoretical results, Barbero and Oldano claim that when the functional contains a term which depends linearly on θ'' and is integrable, this functional has not any solution in the class of the continuous functions.[1] According to them the distorting effects of the various terms containing the K_{13} second-order elasticity cancel each other in the bulk, but not in a boundary layer of a thickness r.[1] On the basis of these assumptions Barbero and Oldano have concluded that the solution of the K_{13} elastic problem obtained by me cannot minimize the elastic energy of the nematics and that the elastic theory of Nehring and Saupe[5] must be reconsidered.

First, let me note that in the last paper[1] Barbero and Oldano have completely disregarded the three-dimensional solution of the problem obtained by me[4] which unambiguously confirms the validity of the theoretical results for the one-dimensional case. Nevertheless, on the basis of a simple one-dimensional analysis made in the frame of Euler-Lagrange formalism I shall prove that the K_{13} elastic problem in nematics is a purely nonlinear elastic problem. This result as I shall demonstrate below completely invalidates the criticism of Oldano and Barbero. First, I shall show that using extremals the functional containing the K_{13} elastic terms can be easily transformed into a function of θ and θ' only and that the K_{13} elastic terms are important in every point in the nematic layer. Something more, I shall theoretically find the magnitude and the sign of the second-order elastic constant K_{13} and shall show that the divergent term in (1) disappears. I shall demonstrate that the K_{13} elastic problem is essential when there are nonlinear elastic deformations in the nematic layer due to an eventual competition between the surface and bulk elastic torques and influence of external electric or magnetic, etc. forces.

Let me minimize the elastic energy of a completely free nematic film accepting that the deformation starts from an initially planar orientation of the nematic layer. The total elastic energy per unit area has the form:

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

where d is the thickness of the liquid crystal layer, K'_{11}, K'_{33} and K_{13} are elastic constants and θ is the deformation angle. The differential equation of Euler-Lagrange has the form:

$$f(\theta)\theta'' + (1/2)(\theta'^2)(d/d\theta)f(\theta) = 0 \qquad (3)$$

with

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

It is possible to integrate this differential equation once to obtain[6]:

$$f(\theta)(\theta')^2 = \text{constant} \qquad (4)$$

Let me remember from the papers of Nehring and Saupe[5,7] that there is a relation between the elastic constants of Frank K_{11} and K_{33} and the elastic constants of Oseen-Nehring-Saupe K'_{11} and K'_{33} as follows:

$$K'_{11} = K_{11} - 2K_{13},\quad K'_{33} = K_{33} + 2K_{13} \qquad (5)$$

It is easy to show that for linear solutions or constants, i.e. linear extremals or constants for the case of the Euler-Lagrange formalism, the divergent elastic term in the expression for the elastic energy used by Oldano and Barbero (1) disappears *if and only if* the second-order elastic constant K_{13} is zero and the Frank elastic constants of splay K_{11} and bend K_{33} are both positive and equal (from physical considerations it seems unreasonable to accept that one of these two elastic constants is zero[8]):

$$K_{13} = 0 \text{ when } K_{11} = K_{33} = K > 0 \tag{6}$$

Let me now replace θ'' from the differential equation (3) in the expression for the elastic energy of the nematic layer given by (2):

$$I = \int_0^d \theta'^2 \left\{ (1/2)f(\theta) + K_{13}\cos 2\theta - \frac{K_{13}(K'_{33} - K'_{11})}{f(\theta)}\sin^2\theta \cos^2\theta \right\} dz \tag{7}$$

where

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

It is clear that the replacement of θ'' with an extremal transforms the functional I into a function of θ'^2, θ and the elastic constants. Further, from this expression it is evident that the K_{13} elasticity is important in every point in the nematic layer which is in the bulk or near to the boundary. It is clear also that for any kind of the extremal including the linear or nonlinear solution, the sign of the elastic energy in (7) will be dectated by the sign of the expression in the brackets which is a function of the elastic constants and the deformational angles $\sin\theta$ and $\cos\theta$ only.

It is evident that the function

$$f(\theta) = K'_{11}\cos^2\theta + K'_{33}\sin^2\theta \tag{8}$$

must be positive. Consequently, the bulk elastic constants of Oseen-Nehring-Saupe K'_{11} and K'_{33} must be also positive:

$$K'_{11} > 0,\ K'_{33} > 0 \tag{9}$$

After a simple straightforward calculation, for the numerator of the expression in the brackets I have obtained a biquadratic expression for $\cos\theta$ which must have a minimal positive value for any linear or nonlinear solution of the problem when $\theta' \neq 0$ (the trivial case when the solution is represented by constants will be discussed below):

$$\begin{aligned}(K'_{11} - K'_{33})(K'_{11} - K'_{33} + 2K_{13})\cos^4\theta + 2K'_{33}(K'_{11} - K'_{33} \\ + 2K_{13})\cos^2\theta + K'_{33}(K'_{33} - 2K_{13}) > 0\end{aligned} \tag{10}$$

It is obvious that this remarkable expression has a minimal positive value when the following relations are valid:

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

Similarly, the minimization of the elastic energy of a completely free nematic film accepting that the deformation starts from an initially homeotropic orientation of the nematic layer leads to the following relations between the elastic constants:

$$K_{11} = (K'_{11} + 2K_{13}) > 0,\ -2K_{13} = K'_{11} - K'_{33},\ K'_{11} > K'_{33} - K_{13} > 0 \quad (12)$$

The relations (11) and (12) clearly show first, that the K_{13} elastic problem is connected with the nonlinear elastic behavior of the nematics when the two bulk elastic constants of splay K'_{11} and bend K'_{33} are not equal: $K'_{11} \neq K'_{33}$; second, the elastic constant K_{13} is zero ($K_{13} = 0$) when the bulk elastic constants of Oseen-Nehring-Saupe K'_{11} and K'_{33} are equal. This requirement is equivalent to the case when the two elastic constants of Frank K_{11} and K_{33} are equal. In other words, the divergent term in the expression of the elastic energy used by Barbero and Oldano (1) must ultimately disappear. The third important conclusion which can be drawn from these results is that the Frank elastic constants K_{11} and K_{33} must be positive:

$$K_{11} > 0,\ K_{33} > 0 \quad (13)$$

The fourth very important conclusion is that the K_{13} elastic problem can be successfully resolved only in the frame of the Euler-Lagrange formalism (let me stress that in the calculations I have used only the expression for the elastic energy (2) and the differential equation (3)).

As far as the nondeformed state of the nematics is concerned, i.e. when the solution of the variational problem is θ = constant, $\theta' = 0$, the value of the elastic energy must be ultimately zero for any value of the deformation angle, i.e. for any inclination of the nematic molecules. Let me stress that contrary to the claim of Barbero and Oldano[1] these angles do not contain the second-order elastic constant K_{13}.

It is evident that the theoretical results obtained above are valid and for the case of an arbitrary anchoring of the nematic layer.

Let me now demonstrate that the boundary condition discussed by me in Reference 4 (see Equation (9) in Reference 4 where there is a small error with a coefficient of 1/2):

$$F_{\theta'} - K_{13}\cos 2\theta\theta' + (K_{13}\sin\theta \cos\theta\theta''/\theta') + W_s(\theta - \theta_0) = 0 \quad (14)$$

is valid for any kind of a solution in the frame of the Euler-Lagrange formalism.

For instance, the expression $K_{13}\sin\theta\cos\theta\theta''/\theta'$ can be transformed according to (4) in the following more convenient form:

$$(K_{13}\sin\theta\cos\theta\theta''/\theta') = K_{13}\sin\theta\cos\theta\,(-1/2)\theta'^2(d/d\theta)f(\theta)/f(\theta)\theta'$$

$$= (-K_{13}\sin\theta\cos\theta(d/d\theta)f(\theta))\,\theta'/2f(\theta) \quad (15)$$

which for the case of a constant solution when θ = constant, $\theta' = 0$ apparently is zero.

Let me finally discuss the boundary condition:

$$(f(\theta) - K_{13}\cos 2\theta)\theta' + W_s(\theta - \theta_0) = 0 \quad (16)$$

which is obtained from (2), (14) and (15).

The surface deformational angle $\theta(d)$ will be different from the surface equilibrium angle θ_0 *if and only if* $\theta' \neq 0$ (see the results obtained above). Consequently for a constant solution $\theta = \theta_0$ and contrary to the calculations of Barbero and Oldano[1] which are wrong, there is no relation between the equilibrium deformational angle θ_0, the second-order elastic constant K_{13} and the surface strength coupling constant W_s.

In conclusion, I have shown that the K_{13} elastic problem is a purely nonlinear elastic problem which cannot be critically discussed with the use of linear functions or constants. I have theoretically found the magnitude and the sign of the second-order elastic constant K_{13} and have shown that the Frank elastic constants of splay K_{11} and bend K_{33} must be positive. It is evident that the elastic theory of Nehring and Saupe[5] has been obtained under correct assumptions contrary to the conclusion of Barbero and Oldano[1-3] that it must be reconsidered.

The simple theoretical example of Nehring and Saupe[7] however, is very approximate since the calculations show that the splay elastic constant of Frank K_{11} must be negative. Such a result gives the impression that the K_{13} elastic constant is important only in the cases when one of the two elastic constants of Frank is negative. The results obtained in this paper however, unambiguously demonstrate the importance of the K_{13} elastic problem for all the mesomorphic liquid crystalline systems when the anchoring is weak. The importance of such a surface volume-like elastic energy will increase with the increase of the difference between the two bulk elastic constants K'_{11} and K'_{33} and for the case of the nematic liquid crystalline polymers this elasticity will be crucial for their elastic behavior. Finally, the results obtained in this paper clearly show that for the case of weak anchoring it is unreasonable to disregard the influence of the divergent surface terms in the elastic energy not only for the case of the nematics but also for all the mesomorphic liquid crystalline systems.

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