
**Liquid Crystals**
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713926090

# On a theoretical analysis on the influence of non-uniformity of the order parameter on the surface energy in nematics

G. Barbero[a]; N. V. Madhusudana[b]
[a] Dipartimento di Fisica, Politecnico, Torino, Italy [b] Raman Research Institute, Bangalore, India

**To cite this Article** Barbero, G. and Madhusudana, N. V.(1990) 'On a theoretical analysis on the influence of non-uniformity of the order parameter on the surface energy in nematics', Liquid Crystals, 7: 2, 299 — 301
**To link to this Article: DOI:** 10.1080/02678299008029218
**URL:** http://dx.doi.org/10.1080/02678299008029218

Liquid Crystals, 1990, Vol. 7, No. 2, 299–301

# On a theoretical analysis on the influence of non-uniformity of the order parameter on the surface energy in nematics

by G. BARBERO† and N. V. MADHUSUDANA‡

† Dipartimento di Fisica, Politecnico, C. Duca Abruzzi 24, 10129 Torino, Italy

‡ Raman Research Institute, Bangalore 560080, India

(*Received 9 October 1989; accepted 28 November 1989*)

Recently Pikin and Terent'ev have analysed the influence of the non-uniformity of the order parameter on the measured value of the surface cohesion energy in nematic liquid crystals (1988, *Sov. Phys. Crystallogr.*, **33**, 641). We argue that since the mathematical problem is ill-posed, the analysis has to be revised. In particular, quadratic terms in the second derivatives of the deformation angle and the order parameter should be taken into account.



In a recent paper Pikin and Terent'ev [1] have analysed the influence of the spatial variation of the scalar order parameter on the surface anchoring energy at the nematic–substrate interface. The importance of this influence was recognized by Mada [2] some years ago. This approach is very interesting; however, as we shall discuss, due to some mathematical difficulties, the problem requires a careful reconsideration.

The geometry considered in [1] is as follows: a nematic liquid crystal with positive diamagnetic anisotropy is aligned homogeneously between two glass plates located at $z = 0$ and $z = d$. The anchoring at the surfaces is supposed to be weak. A magnetic field of strength $B$ acts along the $z$ axis. The angle between the distorted director $\mathbf{n}$ and its undistorted orientation is denoted by $\theta(z)$. The scalar order parameter is denoted by the usual symbol $S$. The total free energy of the system is assumed to be a sum of the usual Landau expansion in powers of $S$ and the distortion energy arising from both the gradients in $S$ and $\theta$. We consider equation (2) of [1]. After integration of the divergent terms, the free energy of the nematic layers can be written as

$$F = \int_0^d f(S, S', \theta, \theta')\,dz + G_0(S, S', \theta, \theta') + G_d(S, S', \theta, \theta'), \qquad (1)$$

where

$$f(S, S', \theta, \theta') = (2/3)aS^2 + (2/9)bS^3 + (4/9)cS^4 + (2/3)PS'^2 + (1/6)PSS'\theta' + PS^2\theta'^2,$$

and

$$G_i(S, S', \theta, \theta') = \mp \{(2/3)D_0SS' + (1/6)D\sin(2\theta)\theta'S^2 + (1/3)D[SS'(\sin^2\theta + 1/3)]\} + WS(\sin^2\theta - 1/3),$$

where the symbols have the same meaning as in [1]. In $G_i(S, S', \theta, \theta')$, $i = 0$ corresponds to a negative sign and $i = d$ corresponds to a positive sign.

As is well-known [3] the functions $S(z)$ and $\theta(z)$ minimizing $F$ given by equation (1) are not continuous, but possess surface discontinuities, whose magnitude can be estimated by using different techniques [4, 5]. In fact by minimizing $F$ given by equation (1) we obtain

$$\begin{aligned}\delta F = & \int_0^d \left\{\left(\frac{\partial f}{\partial S} - \frac{d}{\partial z}\frac{\partial f}{\partial S'}\right)\delta S + \left(\frac{\partial f}{\partial \theta} - \frac{d}{dz}\frac{\partial f}{\partial \theta'}\right)\delta\theta\right\} dz \\ & + \left\{\left(-\frac{\partial f}{\partial S'} + \frac{\partial G_0}{\partial S}\right)\delta S + \frac{\partial G_0}{\partial S'}\delta S' + \left(-\frac{\partial f}{\partial \theta'} + \frac{\partial G_0}{\partial \theta}\right)\delta\theta + \frac{\partial G_0}{\partial \theta'}\delta\theta'\right\}_0 \\ & + \left\{\left(\frac{\partial f}{\partial S'} + \frac{\partial G_d}{\partial S}\right)\delta S + \frac{\partial G_d}{\partial S'}\delta S' + \left(\frac{\partial f}{\partial \theta'} + \frac{\partial G_d}{\partial \theta}\right)\delta\theta + \frac{\partial G_d}{\partial \theta'}\delta\theta'\right\}_d . \quad (2)\end{aligned}$$

This equation holds for any arbitrary functions $\delta S(z)$ and $\delta\theta(z)$, where $\delta S(z)$ and $\delta\theta(z)$ have their usual meaning (see, e.g., [6]). In [1] the equilibrium configurations were obtained by using the Euler–Lagrange equations, viz.

$$\frac{\partial f}{\partial S} - \frac{d}{dz}\frac{\partial f}{\partial S'} = 0,$$

and

$$\frac{\partial f}{\partial \theta} - \frac{d}{dz}\frac{\partial f}{\partial \theta'} = 0$$

(see equations (3) and (4) of [1]). As these are differential equations of second order, we can find a total of four integration constants from them. In general, relations of the kind

$$(\partial S')_i = \mu_i(\delta S)_i, \quad i = 0, d \quad (3)$$

and

$$(\delta\theta')_i = \lambda_i(\delta\theta)_{i'} \quad i = 0, d, \quad (4)$$

do not exist, here $\mu_i$ and $\lambda_i$ are four quantities depending on $S$, $S'$, $\theta$ and $\theta'$. Equations (3) and (4) are true only for exponential functions, but as is well known, $\delta S(z)$ and $\delta\theta(z)$ in equation (2) are, in fact, arbitrary functions. Hence, in general, for any arbitrary $\delta S(z)$ and $\delta\theta(z)$, we deduce eight boundary conditions from equation (2); the problem is then mathematically ill-posed [7]. As discussed elsewhere [3] this implies that $S(z)$ and $\theta(z)$ minimizing equation (1) are discontinuous functions. It follows that the analysis reported in [1] holds only if $G_i(S, S', \theta, \theta')$ reduces to $G_i(S, \theta)$, i.e. if $D_0 = D = 0$. But in this case equation (11) of [1] becomes simply

$$\Phi = 2(\bar{W}/K)(1 + 1/24) \approx 2(\bar{W}/K),$$

and we regain the well-known equation (see, e.g., [4])

$$B^* \approx (\pi/d)\surd(K/\chi_a)[1 - (K/\bar{W})/d].$$

(Note that $K/\bar{W} = 2L$, where $L$ is the usual extrapolation length.)

The same objections hold for the analysis made in [1], of the influence of $S$ variations on the experimental method used to measure the flexoelectric coefficients.

In this case, for the analysis to be correct, we have to substitute in equation (18) of [1], $K_0 = K_{13} = 0$. We then obtain $\tilde{K} = K$, $\tilde{W} = \bar{W}(1 + 1/24) \approx \bar{W}$ and

$$\tilde{f}_3 = f_3\{1 - (3/48)[d^2E^2f_3(f_1 + f_3)/(K + \bar{W}d)^2]\}. \quad (5)$$

By observing that $f_3\,(f_1 + f_3) \lesssim K$ [8], and that usually $d \gg K/\bar{W}$ the second term in the brackets of equation (5) is equivalent to $(3/48)E^2L^2/K \ll 1$, for the usual fields and the usual anchoring energies [8]. Consequently $\tilde{f}_3 \approx f_3$, i.e. the corrections are found to be negligible.

Of course the surface-like elastic constants can contribute to the effective anchoring energy as discussed recently [9–12]. Assuming that an elastic description is still valid and that the uniaxial symmetry of the nematic is maintained near the surface, the analysis has to be performed in a manner different from that proposed in [1]. More precisely, it is necessary to take into account quadratic terms in second order derivatives in the total free energy density. With the inclusion of these terms, surface variations of $S(z)$ and $\theta(z)$, localized over quasi-microscopic lengths appear in the problem. Consequently $S'(0)$ and $S'(d)$ are no longer small quantities and the perturbation technique presented in [1] must be modified. The self-energies associated with order electricity and flexoelectricity can become important in this case, since the Debye screening length is usually larger than the penetration depth near the surface.

In conclusion, we may note that the symmetry of the nematic cannot be expected to be uniaxial near the surface, and hence the description should be quite complicated with several phenomenological constants.



## References


[1] Pikin, S. A., and Terent'ev, E. M., 1988, *Sov. Phys. Crystallogr.*, **33**, 641; 1989, American Institute of Physics (1988, *Kristallografiya*, **33**, 1084).

[2] Mada, H., 1984, *Molec. Crystals liq. Crystals*, **108**, 317.

[3] Oldano, C., and Barbero, G., 1985, *Physics Lett.* A, **110**, 213.

[4] Barbero, G., and Meuti, M., 1985, *Nuovo Cim.* D, **11**, 213.

[5] Barbero, G., and Oldano, C., 1989, *Molec. Crystals liq. Crystals*, **170**, 99.

[6] Smirnov, V. I., 1986, *Course des Mathematiques Superieures* (MIR), Tome 4, 2nd partie.

[7] From our discussion it follows that equations (5) and (6) as well as the fundamental equation (6′) of [1] are not obtained by minimizing $F$ given by equation (2) of the same reference, and hence they must be considered incorrect.

[8] Madhusudana, N. V., and Durand, G., 1985, *J. Phys. Lett., Paris*, **46**, 195.

[9] Yokoyama, H., Kamei, H., and Kobayashi, S., 1987, *J. appl. Phys.*, **61**, 4501.

[10] Barbero, G., Madhusudana, N. V., and Oldano, C., 1989, *J. Phys., Paris*, **50**, 2263.

[11] Barbero, G., and Strigazzi, A., 1989, *Liq. Crystals*, **5**, 693.

[12] Yokoyama, H., 1988, *Molec. Crystals liq. Crystals*, **165**, 265.