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G. Barbero[a]; A. Strigazzi[a]
[a] Dipartimento di Fisica, Politecnico di Torino, C.so Duca degli Abruzzi, 24, Torino, Italy

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Second order elasticity in nematics: a new anchoring source

by G. BARBERO and A. STRIGAZZI
Dipartimento di Fisica, Politecnico di Torino, C.so Duca degli Abruzzi, 24, I-10129 Torino, Italy

By considering, in the expression of the nematic free energy density, an additional term in the square of the director second derivatives, an unexpected anchoring source results, due only to surface and bulk elastic constants. As an example, the case of a planar homogeneous and of a homeotropic nematic cell, equally anchored on both walls, is discussed. In both situations the new anchoring source has a destabilizing effect.

1. Introduction

The paradoxes [1] resulting from the presence of the K_{13} surface term in the Nehring–Saupe free energy density for nematics [2] can be bypassed by introducing new terms in the square of the director second order derivatives [3]. In this paper we show that the anchoring can be partially explained as an effect of both surface and bulk elasticity. Moreover, we note that the importance of terms involving higher order derivatives has already been noted but not analysed in detail [4].

2. Theory

We consider a planar homogeneous nematic cell, with the walls normal to the z axis, at the positions $z = \pm d/2$. If the cell is subjected to a magnetic field parallel to the z axis, a Fréedericksz transition can result, involving a splay-bend distortion, dependent only on the z coordinate. For the sake of simplicity, we consider just a single principal bulk elastic constant $K = K_{11} = K_{33}$ (renormalized following [2]) and one second order bulk elastic constant K^*. Just above threshold, from symmetry considerations, the bulk free energy density of the cell is given by

$$f_B = \tfrac{1}{2}(K\theta'^2 + K^*\theta''^2 - \chi_a B^2\theta^2), \tag{1}$$

where θ is the tilt angle, measured from the wall, the prime denotes the derivative with respect to z, $\chi_a > 0$ is the magnetic susceptibility anisotropy and B is the magnetic flux density.

We suppose that there is an explicit anchoring nematic substrate, i.e. in the formalism of Rapini–Papoular the nematic substrate interaction energy is

$$f_S = \tfrac{1}{2}w\theta^2(+d/2) + \tfrac{1}{2}w\theta^2(-d/2),$$

where w is the anchoring strength due, for instance, to the equal surface treatment of both walls. If K^* is assumed to be zero, then K_{13} must also be considered zero [1], and all of the sample reorients, in the case of a magnetic flux density larger than a critical value, as is well known [5].

We now demonstrate that the presence of $K^* \neq 0$ implies some kind of anchoring, which destabilizes the preimposed homogeneous planar orientation: the critical value will become smaller than the previous one. In any case, the surface free energy density

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coming from the mixed splay-bend term is, if the undisturbed configuration is homogeneous planar,

$$f_S = K_{13}(\theta\theta')'. \tag{2}$$

Such an energy term in nematics has been criticized recently by Pleiner [6], who observed that there is no compatibility with thermodynamic stability. This is correct, since no terms involving the square of the second order derivatives were taken into account in [6].

Following our point of view, the Euler–Lagrange equation reads as a fourth order equation

$$K^*\theta^{(iv)} - K\theta'' - \chi_a B^2\theta = 0, \tag{3}$$

which, by putting $\eta = z/d$, $l = (K^*/K)^{1/2}/d$ and $\xi = (K/\chi_a)^{1/2}/(Bd)$ as a reduced coordinate, a reduced bulk elasticity, and a reduced magnetic coherence length respectively, gives

$$l^2\ddot{\theta}'' - \ddot{\theta} - \xi^{-2}\theta = 0, \tag{4}$$

where an overdot indicates a derivative with respect to η. The solution of the Euler–Lagrange equation (equation (4)) is obtained as

$$\theta(\eta) = \alpha_1 \cos(\lambda_1\eta) + \alpha_2 \cosh(\lambda_2\eta), \tag{5}$$

because of the symmetry $\theta(\eta) = \theta(-\eta)$, where

$$\lambda_1 = \xi^{-1} + O(l)$$

and

$$\lambda_2 = l^{-1} + O(l).$$

Notice that $l \ll 1$, since $K^* \ll Kd^2$, $K^*/K = \delta^2$ which is the square of a characteristic length δ, of the order of the molecular interaction. The two integration constants (α_1 and α_2) are solutions of a homogeneous system related to the boundary conditions

$$\left.\begin{aligned} l^2\ddot{\theta}_0 - (1 + R)\dot{\theta}_0 + L^{-1}\theta_0 &= 0, \\ l^2\ddot{\theta}_0 + R\theta_0 &= 0, \end{aligned}\right\} \tag{6}$$

where the index 0 corresponds to $\eta = -\frac{1}{2}$, $R = K_{13}/K$ being the surface bulk elastic ratio, and $L = K/(wd)$ is the reduced extrapolation length. The system (6) becomes

$$\left.\begin{aligned} &[(1 + R)\lambda_1 \sin(\lambda_1/2) - L^{-1}\cos(\lambda_1/2)]\alpha_1 \\ &\quad - [R\alpha_2 \sinh(\lambda_2/2) + L^{-1}\cosh(\lambda_2/2)]\alpha_2 = 0, \\ &R\alpha_1 \cos(\lambda_1/2) + (1 + R)\alpha_2 \cosh(\lambda_2/2) = 0. \end{aligned}\right\} \tag{7}$$

The coefficient determinant must be zero, giving

$$(L^{-1} - l^{-1}R^2)/(1 + R)^2 = \xi^{-1}\tan(1/2\xi), \tag{8}$$

since $\tanh(1/2\xi) \approx 1$. This is a generalization of the Rapini–Papoular equation [5]:

$$L^{-1} = \xi^{-1}\tan(1/2\xi), \tag{9}$$

valid in the case of usual anchoring, without second order elasticity.

By comparing equations (8) and (9), it appears that the ratio

$$w^* = (K/\delta)R^2 \tag{10}$$

behaves as a new kind of anchoring strength, which results only from the elastic properties of the nematic liquid crystal, destabilizing the initial homogeneous planar orientation, whereas the equivalent anchoring strength is given by

$$w' = (w - w^*)/(1 + R)^2. \tag{11}$$

Note that the second order elasticity also gives a scale factor $(1 + R)^2 > 1$, if $K_{13} > 0$ [7]. Of course, w must be greater than w^*, i.e. $|R| < (l/L)^{1/2}$ or, in other words, $|R| < (\delta w/K)^{1/2}$; otherwise the undisturbed director profile cannot have a planar homogeneous configuration, and the tilt angles at the walls are far from the easy directions. Moreover, we observe that in the strong anchoring hypothesis equation (8) gives the well-known result $\xi_c = \pi^{-1}$.

In connection with the stability of the undistorted homogeneous planar configuration, it is necessary to calculate the total free energy of the cell close to such a configuration. By substituting equation (5) into the expression for the reduced total free energy, defined as

$$G = 2Fd/K = \int_{-1/2}^{1/2} (\dot{\theta}^2 + l^2\ddot{\theta}^2 - \xi^{-2}\theta^2)\,d\eta - 4R\theta_0\dot{\theta}_0 + 2L^{-1}\theta_0^2, \tag{12}$$

we find that G is an ordinary function of α_1 and α_2. The minimum conditions imposed to equation (12) give the boundary condition (6), and the undistorted configuration is stable only if $\xi < \xi_c$, as defined in equation (8), since the hessian $H = (\partial^2 G/\partial\alpha_1^2)(\partial^2 G/\partial\alpha_2^2) - (\partial^2 G/\partial\alpha_1\partial\alpha_2)^2$ is given by

$$H = (1 + R)^2 l^{-1} \cos^2(1/2\xi)\sinh^2(1/2l) \times [(L^{-1} - l^{-1}R^2)/(1 + R)^2 - \xi^{-1}\tan(1/2\xi)] \tag{13}$$

and changes its sign for $\xi = \xi_c$; moreover, the second derivative of G with respect to α_1 is positive, for $\alpha_1 = \alpha_2 = 0$, if $|R| \lesssim (l/L)^{1/2}$, as previously pointed out.

3. Discussion

From the previous criticism [1] on the consistency of an elastic theory involving only the elastic constants K and K_{13} it follows that, if $K_{13} = 0$, then K^* also vanishes. However, no experimental values of K_{13} and K^* are yet available. This fact yields difficulties in managing the results in equations (10) and (11). Anyway, we consider the prediction of Nehring and Saupe [2], that $R = -6/5$ can be assumed. On the other hand, the characteristic length δ may be chosen between about 100 and 1000 Å: this means that w^* goes from about 10^{-2} to 10^{-1} erg cm^{-2}. Hence, the presence of both K_{13} and K^* can explain the disorder configuration, which occurs without a particular surface treatment.

The results obtained are important, since they allow us to conclude that, for a weakly anchored nematic cell, either homogeneous planar or homeotropic, it is possible to consider both $K_{13} = 0$ and $K^* = 0$ for in connection with the situation close to the threshold, under the condition that the anchoring strength is w' as defined in equation (11). In fact, instead of equation (6), just one equation will give in this case the boundary condition, viz.

$$-\dot{\theta}_0 + L'^{-1}\theta_0 = 0, \tag{14}$$

where $L' = K/w'd$. Moreover, as was demonstrated recently by Yokoyama *et al.* [8], the principal contribution w to the anchoring strength is affected by the variations of the ordinary elastic constants close to the boundary, coming, for instance, from the gradient of the order parameter.

Could, then, all anchoring be considered as an implicit anchoring, due only to the elastic behaviour of the nematic? From such a point of view all surface treatments, such as surfactants, rubbing, and so on, would just introduce impurities into the cell, changing locally the elastic properties of the sample, and determining by an indirect way the effective anchoring conditions.

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