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Order parameter dependence of the nematic liquid crystal anchoring energy: a numerical approach

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We study the influence of the surface director disorientation and of the sub-surface director distortion on the surface order parameter and on the anchoring torque of a nematic liquid crystal (NLC). The problem is treated in the framework of the Landau–de Gennes theory with an anchoring energy of the form Tr $[(Q_{ij}-Q_{0_{ij}})^2]$, where Q_{ij} is the NLC quadrupolar order parameter and $Q_{0_{ij}}$ a quadrupolar surface field. In this way both fusion mechanisms are considered: the *bulk* one consisting of the decrease of the order parameter induced by distortion and the *surface* one consisting of the decrease of the order induced by the surface disorientation. For a weak anchoring we find, analytically, that the *surface* mechanism is more important than the bulk mechanism. For a strong anchoring we find, numerically, that the maximum surface order decrease saturates at a value of $S_B/2$, where S_B is the bulk order parameter. New higher order harmonics in $a_{2n}\sin(2n\delta)$ $(n>1)$ appear in the anchoring torque (δ is the angle between the actual surface director and the easy axis).

1. Introduction

The nematic liquid crystal (NLC) can be oriented by solid substrates along well-defined directions $\mathbf{n}_0$, called *easy directions*. The surface interaction energy is described phenomenologically by a function W called *anchoring energy*. Usually the nematic scalar order parameter S is assumed uniform. In this hypothesis the anchoring energy for a monostable anchoring is written in the Rapini–Papoular (RP) form [1]

$$W_{RP}=-\frac{1}{2}\frac{K}{L}(\mathbf{n}\cdot\mathbf{n}_0)^2, \qquad (1)$$

where K is one elastic constant of the NLC and L is the anchoring extrapolation length. This form reproduces very well the anchoring measurements for weak anchoring $L\gg\xi$ (ξ is the nematic–isotropic coherence length) [2]. For stronger anchoring, deviations in $(\mathbf{n}\cdot\mathbf{n}_0)^4$ have been reported [3–5]. Recently it has been shown that these departures from the RP anchoring form could be explained by a decrease of the surface order parameter induced by the surface director disorientation [5]. In [5], the surface is supposed to orient the NLC by a surface quadrupolar field given by: $Q_{0_{ij}}=(3/2)S_0(n_{0_i}n_{0_j}-(I_{ij}/3))$, where S_0 is the preferred surface ordering when $\mathbf{n}=\mathbf{n}_0$ and I is the unity tensor. In the hypothesis of no surface biaxial order and uniform density, the anchoring energy was written as

$$W=\tfrac{1}{2}A\,\mathrm{Tr}\,[(Q_{ij}-Q_{0_{ij}})^2]. \qquad (2)$$

W in equation (2) is minimum when $Q_{ij}=Q_{0_{ij}}$ ($\mathbf{n}=\mathbf{n}_0$ and $S=S_0$), i.e. when the surface nematic quadrupolar field is along the direction of the surface quadrupolar field. When $S_0\neq S_B$ (S_B is the bulk order parameter in null external field), in the absence of surface disorientation, the surface order results from the balance between a bulk effect which tends to induce $S_S=S_B$, by continuity from the bulk, and a surface effect which tends to keep $S_S=S_0$. The surface order parameter is $S_S\neq S_B$ and an S spatial variation is present [6]. On the contrary, if $S_0=S_B$, the order parameter is uniform in the bulk in absence of any disorientation. The main result of the model in [5] is that even if $S_0=S_B$, a disorientation from the surface field direction $\mathbf{n}_0$ results in a disordering of the nematic liquid crystal at the surface, because of the competition between the surface field and the nematic ordering mean field. The surface order parameter S_S is different from the bulk order parameter S_B, and therefore there exists some region close to the surface where S varies. This *surface* source of S spatial variations is a new mechanism totally different from the *bulk* mechanism proposed in [7]. In the latter case, an S spatial variation is generated by a strong distortion close to the surface. Anyway, these two mechanisms contribute to the S spatial variations and their relative importance is so far unknown. In [5], the influence of these S spatial variations on the polar torque was not analysed.

In this paper, we treat analytically the limit of weak deviations from the RP by considering both the *surface and bulk* sources of the order parameter variations. The relative importance of these two mechanisms is analysed. Moreover, the limit of weak deviations from the RP

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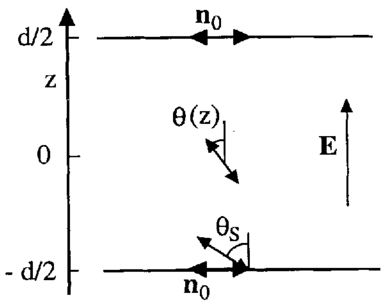


Figure 1. Schematic view of the nematic liquid crystal cell and of the NLC distortion.

anchoring form is not always experimentally true as one can see in [5]. For strong deviations from the RP, an analytical approach is not possible and the problem must be solved numerically. From the Landau–de Gennes free energy, we derive the two coupled equations of the order parameter and the director orientation angle, and solve these equations numerically.

We study the unidimensional case where all the physical quantities depend only on the distance z from the surface ($\hat{\mathbf{z}}$ is the surface normal). We call θ the angle between the director and the z axis (see figure 1). The surface is supposed to orient the NLC molecules along one easy direction $\mathbf{n}_0$ ($\theta_0 = \pi/2$) in the plane of the surface, with an anchoring energy given by equation (2). The disorienting torque is given by an electrical field $\mathbf{E}$ perpendicular to the surface that orients the NLC molecules parallel to itself because of the dielectric anisotropy $\varepsilon_a > 0$ of the NLC. At the equilibrium, a distortion $\theta(z)$ is created in the bulk and the angle θ_S on the surface is different from the easy angle θ_0. We want to remark that the angle θ_S is the macroscopic director angle at the surface and not the extrapolated surface director angle from the bulk. Due to the coupling between θ_S and S_S in the anchoring energy (2) and that of θ and S in the bulk free energy, the order parameter is not uniform in the bulk and an $S(z)$ appears. The numerical problem is to find out the solution of a system of two non-linear second order differential equations with boundary conditions for $\theta(z)$ and $S(z)$.

The plan of the paper is the following: in § 2 we derive, by using the Landau–de Gennes free energy functional, the two coupled, second order non-linear equations for $S(z)$ and $\theta(z)$ with the anchoring energy given by expression (2). In § 3 we calculate analytically the first integral of the free energy functional and discuss the relative importance of the *bulk and surface* fusion mechanisms. In the Appendix we give the detailed calculus of the first integral. In § 4 we illustrate the numerical algorithm and discuss the numerical results, and finally in § 5 we draw the conclusions.

2. Coupled $S(z)$ and $\theta(z)$ non-linear equations

First of all let us express the coefficient A in front of W in equation (2) as a function of the anchoring extrapolation length L. To do this, we compare the expression of the torque for the two anchoring energies (1) and (2) in the limit of small deviations with respect to the easy axis, under the hypothesis that the same parabolic expansion is valid for the two anchoring energies (1) and (2). The generalized anchoring energy (2) can be developed as

$$W(S_S, \theta_S) = \tfrac{3}{4}A[(S_S^2 + S_0^2 - S_S S_0(3\sin^2\theta_S - 1)]. \quad (3)$$

Along the easy direction ($\theta_S = \pi/2$), the anchoring energy (3) writes $W(S_S, \pi/2) = (3/4)\mathrm{A}(S_S - S_0)^2$ and for $A > 0$ it is a minimum when $S_S = S_0$. The general polar torque is the following

$$\frac{\partial W}{\partial \theta_S} = -\tfrac{9}{4}AS_0S_S(\theta_S)\sin(2\theta_S), \quad (4)$$

where $S_S \equiv S_S(\theta_S)$ due to the $S_S - \theta_S$ coupling in the anchoring energy (3). When θ_S is close to $\pi/2$ the polar anchoring torque can be approximated by

$$\frac{\partial W}{\partial \theta_S} \approx \tfrac{9}{2}AS_0S_S\left(\frac{\pi}{2}\right)\left(\theta_S - \frac{\pi}{2}\right). \quad (5)$$

For weak deviations of $\mathbf{n}$ from $\mathbf{n}_0$ ($\theta_S \approx \pi/2$), the RP anchoring energy (1) can be approximated as a parabola of expression

$$W_{RP} = \frac{K}{2L}\left(\theta_S - \frac{\pi}{2}\right)^2 = \tfrac{9}{2}L_1\frac{S_B^2}{2L}\left(\theta_S - \frac{\pi}{2}\right)^2, \quad (6)$$

where S_B is the bulk order parameter and K corresponds to the relationship $K = (9/2)L_1S_B^2$ [8]. The RP polar torque writes as

$$\frac{\partial W_{RP}}{\partial \theta_S} = \tfrac{9}{2}L_1\frac{S_B^2}{L}\left(\theta_S - \frac{\pi}{2}\right). \quad (7)$$

By equating the expressions (7) and (5), we find the value of the coefficient A:

$$A = \frac{S_B^2}{S_0S_S(\pi/2)}\frac{L_1}{L}. \quad (8)$$

The surface order parameter along the easy direction $S_S(\pi/2)$ is determined by the balance of the surface interactions which keep the order parameter at S_0 and the bulk interactions which keep the order parameter to S_B. When $S_0 = S_B$, the surface order parameter along $\mathbf{n}_0$ is $S_S(\pi/2) = S_B$ and the A expression (8) simplifies to

$$A = \frac{L_1}{L}. \quad (9)$$

In the following, we adopt this simplified assumption. The anchoring energy (3) and the polar torque (4) now write as

$$W(S_S, \theta_S) = \frac{3}{4}\frac{L_1}{L}\,[(S_S^2 + S_B^2 - S_S S_B(3\sin^2\theta_S - 1)], \quad (10a)$$

$$\frac{\partial W}{\partial \theta_S} = -\frac{9}{4}\frac{L_1}{L}\,S_B S_S \sin(2\theta_S). \quad (10b)$$

Let us consider a cell limited by two surfaces with the easy direction along the x axis and equal anchoring energy given by the expression (10 *a*): **z** is the normal to the surfaces and the NLC occupies the space included between $z = d/2$ and $z = -d/2$ (see figure 1), where d is the cell thickness. An electric field of displacement vector **D** along the z axis is applied to the cell. The free energy density f, in one elastic constant approximation, is given by [8]

$$f = \tfrac{9}{4} L_1 S^2 \dot{\theta}^2 + \tfrac{3}{4} L_1 \dot{S}^2 + g(S) + \frac{1}{8\pi}\frac{D^2}{\varepsilon_{zz}(S, \theta)}, \quad (11)$$

where $\dot{\theta}$ and $\dot{S}$ mean the first derivatives of θ and S with respect to z, respectively. The first term in the r.h. of (11) represents the elastic distortion energy, the second term is the energy associated with an S gradient, the third term is the homogeneous part of the Landau–de Gennes free energy density given by

$$g(S) = g(0) + \tfrac{1}{2}\alpha(T - T^*)S^2 - \tfrac{1}{3}BS^3 + \tfrac{1}{4}CS^4, \quad (12)$$

(α, B, C are all positive coefficients) and finally the last term represents the energy associated with the electric field when a constant voltage is applied over the cell. $\varepsilon_{zz}(S, \theta)$ in (11) is the zz component of the dielectric tensor given by

$$\varepsilon_{zz}(S, \theta) = \varepsilon_I - \tfrac{1}{3}\Delta\varepsilon_{\max} S(1 - 3\cos^2\theta), \quad (13)$$

where ε_I and $\Delta\varepsilon_{\max}$ are the isotropic part and the anisotropy of the dielectric constant for a perfect nematic order ($S = 1$), respectively. The functional to be minimized is the free energy density per unit of surface F given by

$$F = \int_{-(d/2)}^{d/2} f\,dz + W, \quad (14)$$

where W is the anchoring energy of the surface (10 (a)). By minimizing F in equation (14), we find the two bulk Euler–Lagrange equations

$$S^2\ddot{\theta} = -2S\dot{S}\dot{\theta} + \frac{1}{36\pi L_1}\frac{D^2}{\varepsilon_{zz}^2(S, \theta)}\Delta\varepsilon_{\max} S \sin(2\theta), \quad (15a)$$

and

$$\ddot{S} = 3S\dot{\theta}^2 + \frac{2}{3L_1}\frac{dg}{dS} + \frac{1}{36\pi L_1}\frac{D^2}{\varepsilon_{zz}^2(S, \theta)}\Delta\varepsilon_{\max}(1 - 3\cos^2\theta), \quad (15b)$$

with two boundary conditions in $z = -d/2$:

$$S_S^2\dot{\theta}\big|_{z=-(d/2)} = -\frac{1}{2L} S_S S_B \sin(2\theta_S), \quad (16a)$$

and

$$\dot{S}\big|_{z=-(d/2)} = \frac{1}{2L}\,[2S_S - S_B(3\sin^2\theta_S - 1)], \quad (16b)$$

Due to the cell symmetry, the expected solutions $S(z)$ and $\theta(z)$ are even z functions; thus the boundary conditions in $z = d/2$ can be substituted by the following conditions in $z = 0$:

$$\dot{\theta}\big|_{z=0} = 0, \quad (17a)$$

and

$$\dot{S}\big|_{z=0} = 0 \quad (17b)$$

and the bulk equations can be solved only in the half of the cell $-d/2 \le z \le 0$. The two second order differential equations (15 *a*) and (15 *b*), with the four boundary conditions (16 *a*), (16 *b*), (17 *a*) and (17 *b*), will be integrated numerically in § 4.

3. First integral of the $S(z)$ and $\theta(z)$ equations

In this section we calculate the first integral of the $S(z)$ and $\theta(z)$ equations (15 *b*) and (15 *a*). The functional f in equation (11) does not depend explicitly on z; thus it admits one first integral given by

$$\dot{S}\frac{\partial f}{\partial \dot{S}} + \dot{\theta}\frac{\partial f}{\partial \dot{\theta}} - f = C_0. \quad (18)$$

Hence, we find

$$\tfrac{3}{4} L_1 \left\{\dot{S}^2 + 3S^2\dot{\theta}^2 - \frac{4}{3L_1} g(S) - \frac{1}{6\pi L_1}\frac{D^2}{\varepsilon_{zz}(S, \theta)}\right\} = C_0. \quad (19)$$

The left hand side of equation (19) is independent of z; thus knowing the constant C_0 and by calculating the left hand side of equation (19) in $z = -d/2$, where the boundary equations (16 *a*) and (16 *b*) are valid, we find a relationship between S_S and θ_S. In this way we take into account both the *surface* and the *bulk* source of S variations and we can compare their relative importance. To make the calculus possible analytically, we adopt the hypothesis of small deviations of the order parameters all over the cell $S(z)$ from the bulk value S_B. In this limit, the homogeneous free energy density $g(S)$ in equation (12) can be approximated by a parabola centred in S_B given by

$$g(S) \approx \tfrac{3}{4} L_1 \frac{(S - S_B)^2}{\xi^2} \quad (20)$$

where the N–I coherence length ξ is given by

$$\xi = \sqrt{\left(\frac{3L_1}{\left.\dfrac{2d^2 g}{dS^2}\right|_{S=S_B}}\right)}. \quad (21)$$

By analogy with the case of a uniform order parameter, we can define an effective electric coherence length ξ_{E} as

$$\xi_{\mathrm{E}} = \sqrt{\left(\frac{4\pi K}{\Delta\varepsilon_{\mathrm{a}}}\right)}\frac{1}{E_{\mathrm{eff}}} = \sqrt{\left(\frac{18\pi L_1 S_{\mathrm{B}}}{\Delta\varepsilon_{\max}}\right)}\frac{1}{E_{\mathrm{eff}}}, \tag{22}$$

where $\varepsilon_{\mathrm{a}} = \Delta\varepsilon_{\max}S_{\mathrm{B}}$, and we have defined a sort of effective electric field E_{eff} as

$$E_{\mathrm{eff}} = \frac{D}{\varepsilon_{\parallel}} = \frac{D}{\varepsilon_{\mathrm{I}} + \frac{2}{3}\Delta\varepsilon_{\max}S_{\mathrm{B}}}. \tag{23}$$

With $g(S)$ given from equation (20) and by writing the electric displacement D in terms of ξ_{E} (22) and equation (23), the S bulk equation (15 *b*) and the first integral (19) become

$$\ddot{S} = 3S\dot{\theta}^2 + \frac{(S - S_{\mathrm{B}})}{\xi^2} + \frac{1}{2}\frac{1}{\xi_{\mathrm{E}}^2}\frac{\varepsilon_{\parallel}}{\varepsilon_{zz}(S,\theta)}S_{\mathrm{B}}(1 - 3\cos^2\theta), \tag{24}$$

and

$$\tfrac{3}{4}L_1\left\{\dot{S}^2 + 3S^2\dot{\theta}^2 - \frac{(S - S_{\mathrm{B}})^2}{\xi^2} - \frac{1}{\xi_{\mathrm{E}}^2}3S_{\mathrm{B}}\frac{\varepsilon_{\parallel}^2}{\varepsilon_{zz}(S,\theta)\Delta\varepsilon_{\max}}\right\} = C_0. \tag{25}$$

For a cell thickness d much larger than ξ_{E}, we can approximate $\ddot{S}$ and θ in the centre of the cell ($z = 0$) as $\ddot{S}(0) \approx 0$ and $\theta(0) \approx 0$, and from equation (24) we can calculate the order parameter $S(0)$ as

$$(S(0) - S_{\mathrm{B}})(\varepsilon_{\mathrm{I}} + \tfrac{2}{3}\Delta\varepsilon_{\max}S(0)) = S_{\mathrm{B}}\left(\frac{\xi}{\xi_{\mathrm{E}}}\right)^2(\varepsilon_{\mathrm{I}} + \tfrac{2}{3}\Delta\varepsilon_{\max}S_{\mathrm{B}}). \tag{26}$$

The equation (26) is of the second degree in $S(0)$. In the limit under consideration of small $S(z)$ deviations from S_{B}, $S(0)$ is given by

$$S(0) = S_{\mathrm{B}}\left(1 + \left(\frac{\xi}{\xi_{\mathrm{E}}}\right)^2\right). \tag{27}$$

The order parameter $S(0)$ far from the surface increases quadratically with the electric field amplitude ($\propto 1/\xi_{\mathrm{E}}^2$) as experimentally tested [9]. By calculating the left hand side of equation (25) for $z = 0$ with the same degree of approximation, we have for C_0 the following expression

$$C_0 = -\tfrac{3}{2}L_1\frac{S_{\mathrm{B}}}{\xi^2}\frac{\varepsilon_{\parallel}}{\Delta\varepsilon_{\max}}\left(\frac{\xi}{\xi_{\mathrm{E}}}\right)^2. \tag{28}$$

From the definition of ξ_{E} in equation (22) and the C_0 expression (28), the first integral (25) writes

$$3S^2\dot{\theta}^2 + \dot{S}^2 - \frac{(S - S_{\mathrm{B}})^2}{\xi^2} - 3S_{\mathrm{B}}\frac{1}{\xi^2}\frac{\varepsilon_{\parallel}}{\Delta\varepsilon_{\max}}\left(\frac{\xi}{\xi_{\mathrm{E}}}\right)^2\left(\frac{\varepsilon_{\parallel}}{\varepsilon_{zz}} - 1\right) = 0. \tag{29}$$

For calculating the first derivatives $\dot{\theta}$ and $\dot{S}$ in $z = -d/2$, we can exploit the relationships (16 *a*) and (16 *b*), and thus we can find an equation which links θ_{S} and S_{S} given by

$$\tfrac{3}{4}S_{\mathrm{B}}^2\left(\frac{\xi}{L}\right)^2\sin^2(2\theta_{\mathrm{S}}) + \frac{1}{4}\left(\frac{\xi}{L}\right)^2[2S_{\mathrm{S}} - S_{\mathrm{B}}(3\sin^2\theta_{\mathrm{S}} - 1)]^2$$

$$- (S_{\mathrm{S}} - S_{\mathrm{B}})^2 - 3S_{\mathrm{B}}^2\frac{\varepsilon_{\parallel}}{\varepsilon_{\mathrm{a}}}\left(\frac{\xi}{\xi_{\mathrm{E}}}\right)^2\left(\frac{\varepsilon_{\parallel}}{\varepsilon_{zz}(S_{\mathrm{S}},\theta_{\mathrm{S}})} - 1\right) = 0. \tag{30}$$

The full calculation is given in the Appendix; here we show just the final result. We find a surface order parameter $S_{\mathrm{S}}(\theta_{\mathrm{S}})$ of the first order in ξ/L given by

$$S_{\mathrm{S}}(\theta_{\mathrm{S}}) = S_{\mathrm{B}}\left(1 - \frac{3}{2}\frac{\xi}{L}\cos^2\theta_{\mathrm{S}}\right) \tag{31}$$

and a surface order decrease $\Delta S_{\mathrm{S}}(\theta_{\mathrm{S}}) = S_{\mathrm{B}} - S_{\mathrm{S}}(\theta_{\mathrm{S}})$ given by

$$\Delta S_{\mathrm{S}}(\theta_{\mathrm{S}}) = S_{\mathrm{B}}\frac{3}{2}\frac{\xi}{L}\cos^2\theta_{\mathrm{S}}. \tag{32}$$

When $\theta_{\mathrm{S}} = \pi/2$, we obtain $\Delta S_{\mathrm{S}}(\pi/2) = 0$ (i.e. $S_{\mathrm{S}} = S_{\mathrm{B}}$) as expected, due to the assumption $S_0 = S_{\mathrm{B}}$. When $\theta_{\mathrm{S}} = 0$ (i.e. the surface director is perpendicular to the easy axis), we have the maximum decrease of the surface order parameter given by $\Delta S_{\mathrm{S}}(0) = S_{\mathrm{B}}(3/2)(\xi/L)$. This result is *exactly* the same as that of [5] obtained by neglecting the order parameter decrease induced by the distortion (*bulk* 'fusion' mechanism). Thus we can conclude that in the limit of $\xi/L \ll 1$, *the bulk 'fusion' mechanism is less important than the surface fusion effect.* By substituting the S_{S} expression (31) in the anchoring polar torque (10 *b*), we find the identical expression of [5]:

$$\frac{\partial W}{\partial\theta_{\mathrm{S}}} = -\left(\frac{K}{L}\right)\left[\left(1 - \frac{\Delta s}{2}\right)\frac{\sin(2\theta_{\mathrm{S}})}{2} - \frac{\Delta s}{2}\frac{\sin(4\theta_{\mathrm{S}})}{4}\right], \tag{33}$$

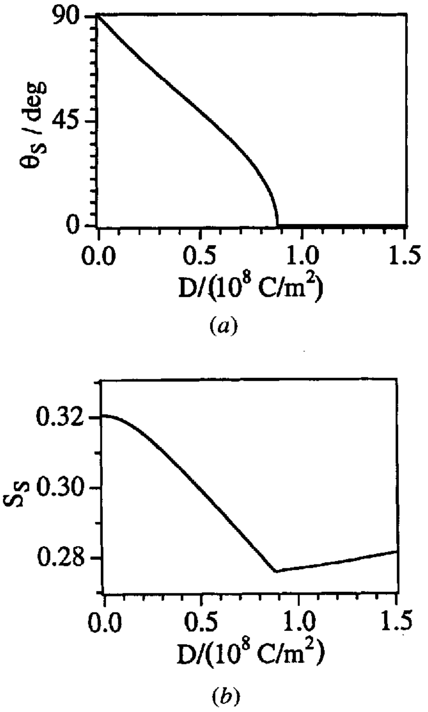
where Δs in (33) was assumed to $\Delta S_{\mathrm{S}}(0)/S_{\mathrm{B}}$.

4. Results

For strong $S(z)$ deviations from S_{B}, the problem must be solved numerically. To solve the two second order differential equations (15 *a*) and (15 *b*) with the four boundary conditions (16 *a*), (16 *b*), (17 *a*) and (17 *b*), we have used a general purpose code (COLNEW), which solves mixed order systems with multipoint boundary conditions [10]. According to [8], the numerical values of the coefficients L_1, α, B, and C used in the calculations, expressed in S.I. units, are the following: $L_1 = 1{\cdot}1 \times 10^{-11}$, $\alpha = 1{\cdot}83 \times 10^4$, $B = 3{\cdot}28 \times 10^6$ and $C = 1{\cdot}02 \times 10^7$. The dielectric constants used are given by: $\varepsilon_{\mathrm{I}} = 10{\cdot}13$ and $\Delta\varepsilon_{\max} = 33{\cdot}53$ which correspond to the nematic compound 4-pentyl-4'cyanobiphenyl (5CB) [11]. The chosen temperature and cell thickness are $T = T^*$ and $d = 10^{-4}$ m, respectively. From equations (12) and (21) we find the bulk order parameter $S_{\mathrm{B}} = 0{\cdot}32$ and the nematic–isotropic coherence length $\xi = 40$ Å.

In figures 2 (*a*) and 2 (*b*) are shown θ_{S} and S_{S} versus D for $\xi/L = 0{\cdot}1$, respectively. One can see that by increasing D above the Fréedericksz threshold $D_{\mathrm{th}} = 7{\cdot}5 \times 10^4\,\mathrm{C\,m^{-2}}$ ($D_{\mathrm{th}} = (4\pi\varepsilon_{\perp}K)^{1/2}(\pi/d)$, where $K = (9/2)L_1S_{\mathrm{B}}^2$ and $\varepsilon_{\perp} = \varepsilon_{\mathrm{I}} - (1/3)\Delta\varepsilon_{\max}S_{\mathrm{B}}$), the surface angle orients toward the electric field direction ($\theta_{\mathrm{S}} = 0$) and the surface order parameter decreases. On the contrary, the bulk order parameter increases, following equation (27). When the surface and bulk directors are oriented along the field, further increase in the field causes an increase of the bulk order parameter and, with it, of the surface order parameter ($D \approx 0{\cdot}9 \times 10^8\,\mathrm{C\,m^{-2}}$ in figure 2 (*b*)).

In figure 3 is shown the maximum surface order decrease Δs, when the applied electric field has completely disoriented the surface director (see figure 2 (*a*) and 2 (*b*)), as function of the ratio ξ/L. The straight line represents the analytical result $\Delta s = (3/2)\ (\xi/L)$. In the inset, we can observe that with $\Delta s \leq 0{\cdot}05$, the analytical expression reproduces well the numerical results. For stronger anchoring strengths, there is a saturation of the effects at a value of $\Delta s \approx 1/2$.



(*a*)

(*b*)

Figure 2. (*a*) θ_S versus D and (*b*) S_S versus D for $\xi/L = 0{\cdot}1$. The Fréedericksz threshold $D_{\mathrm{th}} = 7{\cdot}5 \times 10^4\,\mathrm{C\,m^{-2}}$ is not visible in (*a*) due to the scale used for D.

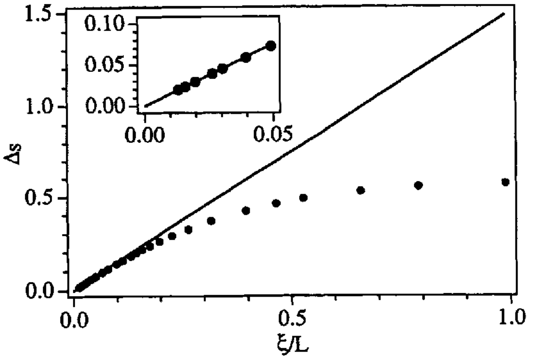
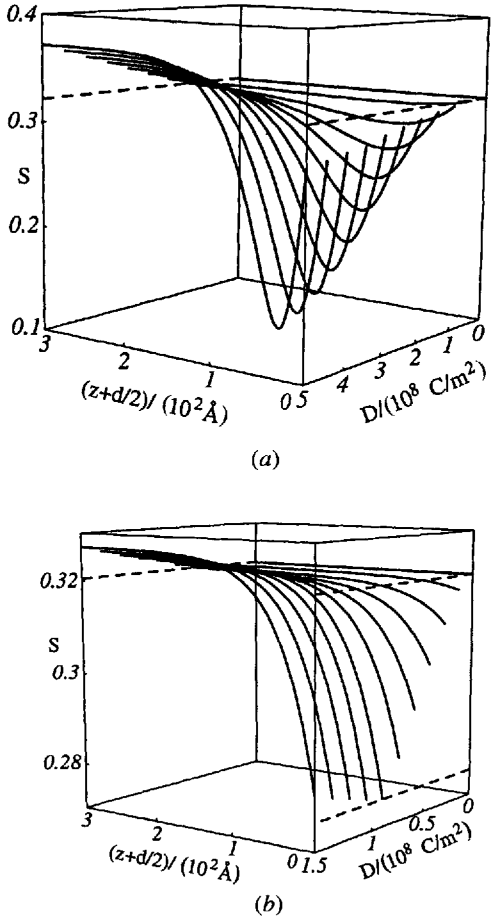


Figure 3. Maximum decrease of the surface order normalized to the bulk order parameter $\Delta s = \Delta S(0)/S_{\mathrm{B}}$ versus the ratio ξ/L. In the inset is represented a magnification of the lower left hand corner of the main figure.

In figure 4 (*a*) and 4 (*b*), the 3D plots of the order parameter $S(z)$ as a function of z and D for $\xi/L = 10$ (strong anchoring) and $\xi/L = 0{\cdot}1$ (weak anchoring) are shown, respectively. One can see that the characteristic variation in length of $S(z)$ is about $4\xi = 160$ Å for both curves. In figure 4 (*a*), by increasing D, S goes to the bulk values non-monotonically, first decreasing near the surface, and then increasing to the bulk value. The solid line in figure 5 represents the spatial derivative of θ and the dashed line the order parameter $S(z)$. The distortion behaves as a source of the order parameter decrease, and the surface order minimum is reached a little after the maximum distortion (in modulus). This behaviour is due



(*a*)

(*b*)

Figure 4. 3D plot of the order parameter S as function of $z + d/2$ and D for (*a*) $\xi/L = 10$ and (*b*) $\xi/L = 0{\cdot}1$. The dashed lines have been added to help the reader: in (*a*) they represent the function $S(0, D) = S_{\mathrm{B}}$ and $S(3 \times 10^2\,\text{Å}, D) = S_{\mathrm{B}}$, in (*b*) the values of $S(0, D) = S_{\mathrm{B}}$, $S(0, D) = S(\theta_S = 0)$ and $S(3 \times 10^2\,\text{Å}, D) = S_{\mathrm{B}}$.

to the *bulk* fusion mechanism [7]. In figure 4(*b*), $S(z)$ monotonically goes from the surface value S_S, which is lower than S_B (dashed line) due to the *surface* 'fusion' mechanism, to the bulk value larger than S_B (dashed line) due to the ordering effect of the electric field. As estimated in § 3 for small ξ/L, the *bulk* fusion mechanism is weaker than the corresponding *surface* mechanism.

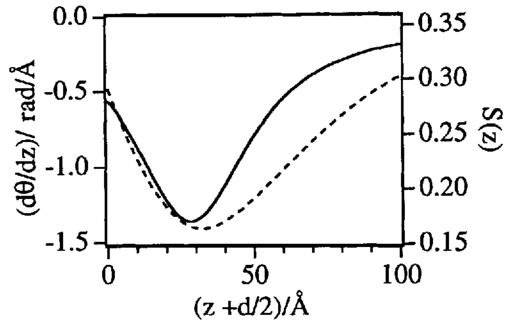


Figure 5. $d\theta/dz$ (——) and $S(z)$ (– – –) versus $z + d/2$ for $\xi/L = 10$ and $D = 4 \times 10^{10}\,\mathrm{C\,m^{-2}}$.

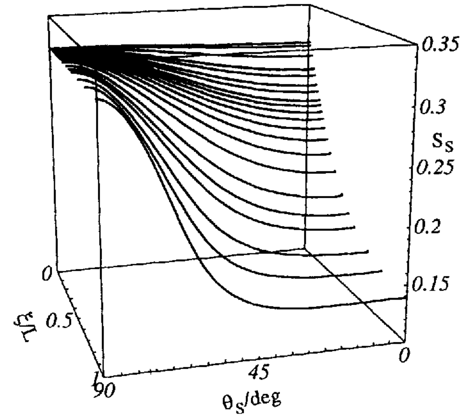


Figure 6. 3D plot of S_S versus ξ/L and θ_S.

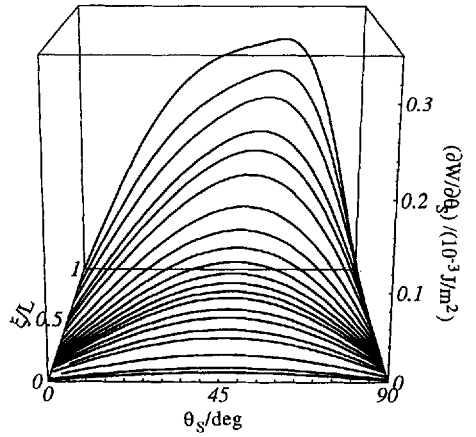
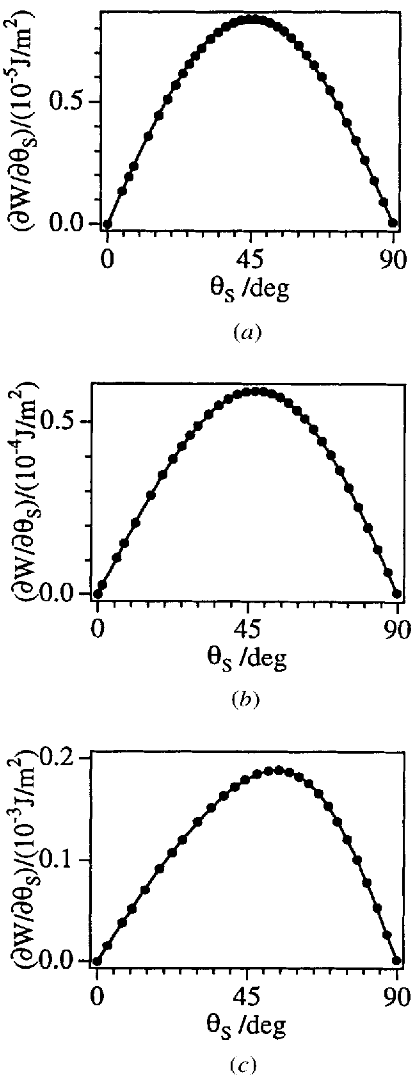


Figure 7. 3D plot of the polar torque $\partial W/\partial\theta_S$ versus ξ/L and θ_S.

In figure 6, the 3D plot of the surface order parameter S_S versus the surface polar angle θ_S and the ratio ξ/L is reported. Along the easy axis $\theta_S = 90°$, the order parameter is $S_B = 0{\cdot}32$. The $S_S(\theta_S)$ curve for $\xi/L \approx 1$ does not follow the equation (32), but saturates just after 45°, at the value in $\theta_S = 0$.

Figure 7 shows a 3D plot of the polar torque versus θ_S and ξ/L. The polar torque is of the RP form for $\xi/L \ll 1$. By increasing the anchoring force, i.e. the ratio ξ/L, higher and higher harmonics are included, as one can see on the curve for $\xi/L = 1$.

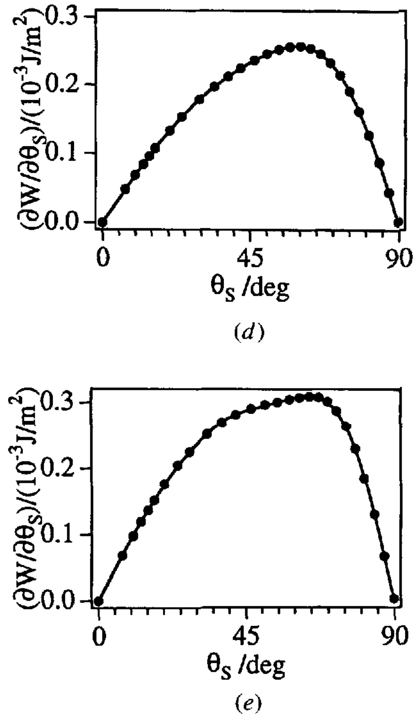
In figure 8(*a–d*), the polar torque versus the polar angle for four values of the extrapolation length from $\xi/L = 0{\cdot}013$ to $\xi/L = 1$ are shown. The solid line represents the best fit with the expression $a_2 \sin(2\theta_S) + a_4 \sin(4\theta_S) + a_6 \sin(6\theta_S) + a_8(8\theta_S) + a_{10} \sin(10\theta_S)$.



(*a*)

(*b*)

(*c*)



(*d*)

(*e*)

Figure 8. $\partial W/\partial\theta_S$ versus θ_S for (*a*) $\xi/L = 0{\cdot}013$, (*b*) $\xi/L = 0{\cdot}1$, (*c*) $\xi/L = 0{\cdot}4$, (*d*) $\xi/L = 0{\cdot}66$, (*e*) $\xi/L = 1$. The solid lines represent the best fit with $\partial W/\partial\theta_S = a_2 \sin(2\theta_S) + a_4 \sin(4\theta_S) + a_6 \sin(6\theta_S) + a_8 \sin(8\theta_S) + a_{10} \sin(10\theta_S)$.

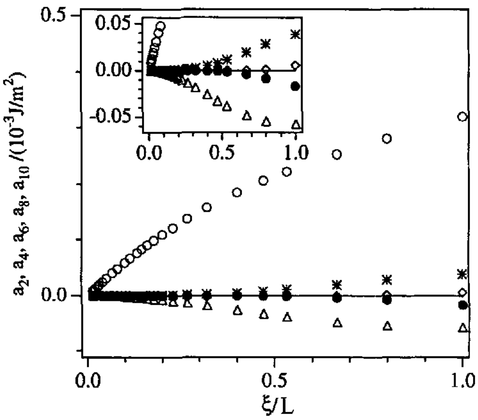


Figure 9. The amplitudes a_2 (○), a_4 (△), a_6 (★), a_8 (●), a_{10} (◇) versus ξ/L. In the inset is represented a magnification of part of the principal figure.

Figure 9 shows the amplitudes a_2, a_4, a_6, a_8, a_{10} versus the ratio ξ/L. The amplitudes a_2, a_6, a_{10} are all positive, whereas the amplitudes a_4, a_8 are negative.

5. Conclusions

We have studied the influence of surface director disorientation and of sub-surface director distortion on the order parameter and on the anchoring torque, as recently proposed in [5]. The surface disorientation is due to the disorienting effect of an external field. The problem is treated in the framework of the Landau–de Gennes theory with an anchoring energy of the form $\mathrm{Tr}\,[(Q_{ij} - Q_{0_{ij}})^2]$, where Q_{ij} is the NLC quadrupolar order parameter and $Q_{0_{ij}}$ a quadrupolar surface field. In this way both 'fusion' mechanisms are considered the *bulk* mechanism consisting of the decrease of the order parameter induced by distortion [7] and *surface* mechanism consisting of the decrease of the order induced by the surface disorientation [5].

For weak anchoring, $\xi/L \ll 1$ (ξ is the nematic–isotropic coherence length, and L is the anchoring extrapolation length), by calculating analytically the first integral of the Landau–de Gennes free energy we find that *the surface mechanism is more important than the bulk mechanism.* We find a maximum surface order decrease $\Delta s = (S_B - S_S(0))/S_B$ which follows a linear law in ξ/L. The anchoring torque includes, besides the Rapini–Papoular term in $\sin(2\theta_S)$, a new term in $\sin(4\theta_S)$.

For strong anchoring, $\xi/L \approx 1$, the problem must be solved numerically. The numerical results confirm that a sub-surface order parameter decrease is produced by a strong sub-surface distortion. Δs no longer follows a linear law, but saturates at a value of $\Delta s \approx 1/2$. By increasing the ratio ξ/L, new higher order harmonics in $a_{2n} \sin(2n\theta_S)$ with $n > 2$ appear in the anchoring torque. The amplitudes a_4 and a_8 are negative, whereas a_2, a_6 and a_{10} are positive.

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Appendix

In § 3, we have obtained the expression (30) for the first integral of the free energy density functional (11). In this appendix, we show the detailed calculations that lead to the expression (32) for the surface order parameter decrease starting from equation (30).

In the limit of $S_S \approx S_B$, the expression $(\varepsilon_\parallel/\varepsilon_{zz}(S_S, \theta_S) - 1)$ in the last term of equation (30) writes

$$\begin{aligned}\left(\frac{\varepsilon_\parallel}{\varepsilon_{zz}(S_S, \theta_S)} - 1\right) &= \left(\frac{\varepsilon_\parallel}{\varepsilon_{zz}(S_B, \theta_S)} - 1\right) - \frac{\varepsilon_\parallel}{\varepsilon_{zz}(S_B, \theta_S)^2}\,\frac{\Delta\varepsilon_{\max}}{3} \\ &\quad \times (3\cos^2\theta_S - 1)(S_S - S_B) \\ &\quad + \frac{\varepsilon_\parallel}{\varepsilon_{zz}(S_B, \theta_S)^3}\,\frac{\Delta\varepsilon^2_{\max}}{9} \\ &\quad \times (3\cos^2\theta_S - 1)^2(S_S - S_B)^2 \\ &\quad + O((S_S - S_B)^2). \qquad \text{(A 1)}\end{aligned}$$

By substituting this term in (30) we find

$$\frac{1}{4}\left(\frac{\xi}{L}\right)^2[2(S_S - S_B) + 3\cos^2\theta_S]^2 - (S_S - S_B)^2$$
$$+ \tfrac{3}{4}S_B^2\left(\frac{\varepsilon}{L}\right)^2 \sin^2(2\theta_S) - 3S_B^2\frac{\varepsilon_\parallel}{\varepsilon_a}\left(\frac{\xi}{\xi_E}\right)^2$$
$$\times\left[\left(\frac{\varepsilon_\parallel}{\varepsilon_{zz}(S_B,\theta_S)} - 1\right) - \frac{\varepsilon_\parallel}{\varepsilon_{zz}(S_B,\theta_S)^2}\frac{\Delta\varepsilon_{\max}}{3}\right.$$
$$\times(3\cos^2\theta_S - 1)(S_S - S_B) + \frac{\varepsilon_\parallel}{\varepsilon_{zz}(S_B,\theta_S)^3}\frac{\Delta\varepsilon_{\max}^2}{9}$$
$$\left.\times(3\cos^2\theta_S - 1)^2(S_S - S_B)^2\right] = 0. \qquad (\mathrm{A\,2})$$

The expression (A 2) can be developed as a function of the small parameter $\beta = \xi/L$. On the hypothesis that

$$\frac{S_S - S_B}{S_B} = q\frac{\xi}{L} = q\beta, \qquad (\mathrm{A\,3})$$

where q is a function to be determined and

$$\xi/\xi_E = (\xi/L)(L/\varepsilon_E) = (L/\varepsilon_E)\beta,$$

we obtain

$$\tfrac{9}{4}\beta^2\cos^4\theta_S - q^2\beta^2 + \tfrac{3}{4}\beta^2\sin^2 2\theta_S$$
$$-3\frac{\varepsilon_\parallel}{\varepsilon_a}\beta^2\left(\frac{L}{\varepsilon_E}\right)^2\left[\frac{\varepsilon_\parallel}{\varepsilon_{zz}(S_B,\theta_S)} - 1\right]^2 = 0. \qquad (\mathrm{A\,4})$$

The last term in (A 4) is of the same order in β as the other terms only if the ratio L/ε_E is developed at zero order in β. From (A 3), zero order in β implies $S(z) = S_B$; thus the ratio L/ε_E is the same as that in the problem of splay-bend deformation with uniform $S(z) = S_B$ and isotropic elastic constants. From the definition of ξ_E in equation (22) and E_{eff} in equation (23) we obtain

$$\frac{L}{\xi_E} = \cos\theta_S\sqrt{\left(\frac{\varepsilon_{zz}(S_B,\theta_S)}{\varepsilon_\parallel}\right)}. \qquad (\mathrm{A\,5})$$

By substituting L/ξ_E (A 5) in (A 4) we find

$$q = -\tfrac{3}{2}\cos^2\theta_S \qquad (\mathrm{A\,6})$$

and the correction, at the first order in L/ξ, to the surface order parameter writes

$$\Delta S_S(\theta_S) = S_B\frac{3}{2}\frac{\xi}{L}\cos^2\theta_S. \qquad (\mathrm{A\,7})$$

as in equation (32).

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