Surface defects and forces in nematic liquid crystal samples

F. C. Cardoso and L. R. Evangelista
Departamento de Física, Universidade Estadual de Maringá, Avenida Colombo, 5790, 87020-900 Maringá Paraná, Brazil
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The existence of surface defects resulting from the inhomogeneity of the surface treatment in a nematic liquid crystal sample of definite thickness is investigated. We consider two significant experimental arrangements for the flat surfaces, in the hypothesis of strong anchoring. By means of a theoretical model, the force between the surface defects is analytically determined. The forces are shown to have a nonlinear dependence on the relative displacement between the defects.

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The physical properties of a nematic liquid crystal (NLC) sample depend on the spatial distribution of the director field $\vec{n}$. This field coincides with the average molecular orientation of the molecules forming the phase. When the director $\vec{n}$ is everywhere parallel to a plane, it may be written in terms of one angle (twist or tilt angle, according to the experimental situation considered) [1,2]. The evaluation of the director field or of, say, the tilt angle is performed in the frame of the elastic continuum theory [3]. This elastic theory has been formulated long ago by Ericksen [4] and Leslie [5] and it is mainly applied to the study of one-dimensional problems, in which all the physical quantities depend on one coordinate [6].

It is well known that in the absence of external fields, the director $\vec{n}$ depends on the surface treatment. According to the treatment it is possible to characterize surface nonhomogeneities influencing the NLC orientation. Recently, this influence was analyzed by means of a complete analytical model [7] in the situations of strong and weak anchoring at the surfaces. The analysis was proposed in order to improve the definition of the surface energy [8] in a continuum description, and in order to connect the anchoring energy experimentally detected with the random distribution of the easy axes. The same analysis [7] was extended in order to describe walls of orientation induced by sharp variations of the surface treatment [9]. These discontinuities in the surface molecular orientation are responsible for the presence of surface defects and forces between them. Previous elastic models were applied to analyze two-dimensional systems by Lonberg and Meyer [10] and Kléman [11], among others [1,2]. The analysis of Ref. [10] dealt with periodic patterns induced by external field in samples characterized by uniform surface treatment. On the other hand, the fundamental work of Kléman [11] was mainly devoted to the analysis of surface defects in the absence of external fields. More recently, an experiment was performed in which a topological (bulk) line defect is forced to move with constant speed under the action of an applied voltage [12]. This kind of experiment can be used to study viscous effects near the highly strained core region, and is very useful for the understanding of nonlinear dynamics in liquid crystalline systems.

In this paper, the model proposed and applied in Refs. [7] and [9] is used to determine the forces between defects in a NLC sample characterized by nonhomogeneous surfaces, in the absence of external field. We are dealing here with a kind of surface defects resulting from the inhomogeneities in the treatment of the flat surfaces limiting a NLC sample. A force appears between these surface defects and is analytically determined.

Let us consider a nematic slab of thickness d. The Cartesian reference frame is chosen with the z axis normal to the bounding plates, located at $z = \pm d/2$. The x axis is parallel to the direction along which the surface tilt angle is expected to change, and the tilt angle θ made by the nematic director with the z axis, is supposed to be y independent. In the one constant approximation, $K_{11} = K_{22} = K_{33} = K$, the bulk free energy density due to elastic distortions is given by [1]

$$f_b = \tfrac{1}{2}K(\vec{\nabla}\theta)^2, \tag{1}$$

where $\vec{\nabla}\theta = \mathbf{i}(\partial\theta/\partial x) + \mathbf{k}(\partial\theta/\partial z)$, with $\mathbf{i}$ and $\mathbf{k}$ being the unit vectors parallel to the x and z axes, respectively. Thus, the total bulk elastic free energy per unit length along y will be

$$F[\theta(x,z)] = \int_{-\infty}^{\infty} dx \int_{-d/2}^{d/2} dz \frac{1}{2}K(\vec{\nabla}\theta)^2. \tag{2}$$

The principle of the continuum theory states that the actual director profile, or $\theta(x,z)$, is deduced by minimizing the total free energy given by (2). Usual calculations give

$$\frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial z^2} = 0, \quad -\infty < x < \infty, \quad -\frac{d}{2} \le z \le \frac{d}{2}. \tag{3}$$

The solution is a harmonic function $\theta(x,z)$, which needs to satisfy appropriated boundary conditions. Let us initially analyze the general situation of strong anchoring in both surfaces, namely,

$$\theta(x, \pm d/2) = \Theta_\pm(x), \tag{4}$$

where $\Theta_\pm(x)$ accounts for the surface orientation imposed by the surface treatment, i.e., the easy axes on the upper and lower surfaces, respectively.

It is possible to show [7,9] that the solution of Eq. (3), satisfying boundary conditions (4), can be expressed in terms of propagators as

$$\theta(x,z) = \int_{-\infty}^{\infty} [G_+(x'-x,z)\Theta_+(x') + G_-(x'-x,z)\Theta_-(x')]dx', \tag{5}$$

where

$$G_\pm(x'-x,z) = \frac{\pi}{2d}\frac{\cos(\pi z/d)}{\cosh[\pi(x'-x)/d] \mp \sin(\pi z/d)}. \tag{6}$$

Equations (5) and (6) give the complete solution of the problem in the strong anchoring hypothesis. The same analysis can be carried out for the case of weak anchoring at the surfaces. For completeness, we present also the general equations for the case of weak anchoring. This situation can be analyzed by taking into account the existence of a finite surface energy, which we will assume to be of the kind proposed by Rapini and Papoular [13], i.e., $f_s = (W/2)(\theta - \Theta)^2$, where W is the anchoring strength. The strong anchoring case corresponds to the limit $W \to \infty$. The total elastic free energy of the nematic sample, per unit length along the y axis is given by Eq. (2) plus the surface terms, namely,

$$F[\theta(x,z)] = \int_{-\infty}^{\infty} dx \int_{-d/2}^{d/2} dz \frac{1}{2}K(\vec{\nabla}\theta)^2 + \int_{-\infty}^{\infty}\frac{1}{2}\Big[W_-[\theta_-(x)-\Theta_-(x)]^2 + W_-[\theta_+(x)-\Theta_+(x)]^2\Big]dx, \tag{7}$$

where $\theta_\pm(x)$ is the actual value of the surface tilt angle and W_- and W_+ refer to the lower and upper surface, respectively. For simplicity's sake, we present only the case of symmetric surfaces, i.e., $W_- = W_+ = W$. In this case of weak anchoring, in order to determine the profile of the tilt angle we need to solve Eq. (3), but now subject to the boundary conditions [14]:

$$\pm L\left[\frac{\partial\theta}{\partial z}\right]_{z=\pm d/2} + \theta_\pm(x) - \Theta_\pm(x) = 0. \tag{8}$$

In Eq. (8), $L = K/W$ is the extrapolation length [11]. The general solution for the weak anchoring situation can be written in the form

$$\theta_W(x,z) = \int_{-\infty}^{\infty} [G_+(x'-x,z)\theta_+(x') + G_-(x'-x,z)\theta_-(x')]dx'. \tag{9}$$

By substituting the general solution into the boundary conditions (8), we obtain

$$\theta_\pm = \Theta_\pm \pm L\int_{-\infty}^{\infty} dx'\left[\theta_+(x)\frac{\partial G_+(x-x',z)}{\partial z} + \theta_-(x)\frac{\partial G_-(x-x',z)}{\partial z}\right]_{z=\pm d/2}. \tag{10}$$

This completes the mathematical tool to determine the profile of the tilt angle in the slab.

Within the framework of the general equations we have presented it is possible to investigate the presence of surface defects and the formation of walls of orientation in the nematic medium, as a consequence of the surface inhomogeneities [9]. With this aim in mind we will consider in detail two particular but experimentally relevant situations, characterized by different arrangements of the surfaces in the slab. From now on, we will consider only the strong anchoring situation, which is closer to the experimental one when we are dealing with treated surfaces.

Let us exemplify by considering the arrangement for which

$$\Theta_+(x) = \begin{cases}\Theta_1, & x<0\\ \Theta_2, & x>0,\end{cases} \qquad \Theta_-(x) = \begin{cases}\Theta_3, & x<\Lambda\\ \Theta_4, & x>\Lambda.\end{cases} \tag{11}$$

In this case, we have initially four distinct surfaces, characterized by four different easy directions. There are two points in which the nematic orientation can change abruptly on the surfaces. These points are horizontally displaced by a quantity Λ. Taking into account the boundary conditions (11) and applying Eqs. (5) and (6) we obtain for the tilt angle

$$\theta(x,z) = \Theta_1\int_{-\infty}^{0} G_+(x'-x,z)dx' + \Theta_2\int_{0}^{\infty} G_+(x'-x,z)dx' + \Theta_3\int_{-\infty}^{\Lambda} G_-(x'-x,z)dx' + \Theta_4\int_{\Lambda}^{\infty} G_-(x'-x,z)dx'.$$

The integrations are performed easily, giving

$$\theta(x,z) = (\Theta_1+\Theta_2)\,t_1 + (\Theta_1-\Theta_2)\,t_2 + (\Theta_3+\Theta_4)\,t_3 + (\Theta_3-\Theta_4)\,t_4, \tag{12}$$

where the quantities t_i, $i = 1,...,4$ have been introduced to save space. They are defined in the following way:

$$t_1 = \arctan[\Delta(z)], \tag{13}$$

$$t_2 = \arctan\left[\Delta(z)\tanh\left(\frac{\pi x}{2d}\right)\right], \tag{14}$$

$$t_3 = \arctan\left[\frac{1}{\Delta(z)}\right], \tag{15}$$

$$t_4 = \arctan\left[[\Delta(z)]^{-1}\tanh\left(\frac{\pi(\Lambda-x)}{2d}\right)\right], \tag{16}$$

where

$$\Delta(z) = \sqrt{\frac{1+\sin(\pi z/d)}{1-\sin(\pi z/d)}}. \quad (17)$$

For the case of two surfaces whose easy axes are such that $\Theta_1 = \Theta_4$ and $\Theta_2 = \Theta_3$ (case I), the solution (12), by taking into account Eqs. (13)–(17), becomes

$$\theta(x,z) = \frac{(\Theta_1+\Theta_2)}{2} + \frac{(\Theta_2-\Theta_1)}{\pi}\arctan\left[\frac{[1+\sin(\pi z/d)]\tanh[\pi x/2d]+[1-\sin(\pi z/d)]\tanh[\pi(\Lambda-x)/2d]}{\cos(\pi z/d)(1+\tanh[\pi x/2d]\,\tanh[\pi(\Lambda-x)/2d])}\right]. \quad (18)$$

A similar structure arises when we consider the case corresponding to two surfaces whose easy axes are such that $\Theta_1 = \Theta_3$ and $\Theta_2 = \Theta_4$ (case II). The $\theta(x,z)$ profile is given by

$$\theta(x,z) = \frac{(\Theta_1+\Theta_2)}{2} - \frac{(\Theta_2-\Theta_1)}{\pi}\arctan\left[\frac{[1+\sin(\pi z/d)]\tanh[\pi x/2d]-[1-\sin(\pi z/d)]\tanh[\pi(\Lambda-x)/2d]}{\cos(\pi z/d)(1-\tanh[\pi x/2d]\,\tanh[\pi(\Lambda-x)/2d])}\right], \quad (19)$$

which can be obtained from (18) by changing $\Theta_1 \rightleftharpoons \Theta_2$ and $\Lambda - x \to -(\Lambda - x)$. These solutions (18) and (19) describe walls of orientation, which are induced in the nematic medium by the inhomogeneity of the surface treatment [9]. In both situations we have a slab of thickness d with two disclinations localized at $x = 0, z = d/2$ and $x = \Lambda, z = -d/2$.

The total elastic energy F of our system can be calculated from Eq. (2) for the strong anchoring situation. We observe that, due to the presence of a relative horizontal displacement Λ between the disclinations at the surfaces, these quantities are now explicit functions of Λ. If we assume as a normal configuration the one for which $\Lambda = 0$, it is possible to define an excess of elastic energy, relatively to this configuration, whose origin is directly connected with the presence of the quantity Λ. We obtain through Eq. (2) the following results:

$$E(\Lambda) = F(\Lambda) - F(\Lambda=0) = \mp\frac{K}{\pi}(\Theta_2-\Theta_1)^2\ln\left(\cosh\left[\frac{\pi\Lambda}{2d}\right]\right), \quad (20)$$

where $(-)$ and $(+)$ refer, respectively, to cases I and II.

On dimensional grounds, it is possible to define a force per unit length along y, between the surface defects, whose component in the x direction is given by

$$f(\Lambda) = -\frac{\partial E(\Lambda)}{\partial\Lambda}. \quad (21)$$

According to the boundary conditions, we are able to show that this force can be attractive or repulsive. In fact, from (20) and (21) we obtain for the force, the following expression

$$f(\Lambda) = \pm K\frac{(\Theta_2-\Theta_1)^2}{2d}\tanh\left(\frac{\pi\Lambda}{2d}\right), \quad (22)$$

which is repulsive for the first arrangement (case I) and attractive for the second one (case II). A linear behavior is found when $\Lambda \ll d$, because $f(\Lambda) \propto \pm\Lambda$. On the contrary, for high values of Λ, the force tends to a constant value $f \simeq \pm K(\Theta_2-\Theta_1)^2/2d$. We can observe that for case II, E, as given by Eq. (20), is a positive quantity, whereas for case I, E is negative, for any value of Λ. This indicates that the configuration for which $\Lambda = 0$ is the stable one only for case II. The other arrangement (case I), for which $E < 0$ when $\Lambda \neq 0$, indicates that the situation $\Lambda = 0$ is unstable. The order of magnitude of this force can be estimated by assuming $\Lambda \simeq d$, and $\Theta_2 - \Theta_1 = \pi/2$. For a sample of thickness $d = 10\,\mu$m and $K \simeq 10^{-6}$ dyn, we obtain $f \simeq 10^{-3}$ dyn/cm.

In this paper we have analyzed the effect of surface inhomogeneities on the nematic orientation. We have considered two possibly relevant experimental arrangements where the surfaces of a slab of thickness d, characterized by different easy directions, are horizontally displaced by a quantity Λ. These arrangements are responsible for the appearence of walls of orientation in the nematic sample. In particular, we have explicitly determined the forces between surface defects in the slab for the situation of strong anchoring at the surfaces. This force is found to be a nonlinear function of the relative horizontal displacement between the defects. A possible experimental set-up can be built in order to explore this interesting nonlinear behavior of the force since it can be connected to the effective viscosity of the system [12]. However, for this kind of experiment it could be more convenient to analyze the behavior of the entire system under the action of an external field. This general analysis is presently in progress.

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