Flexoelectricity in Nematics Confined to Cylindrical Geometry

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Abstract

Abstract: External fields act on the order parameter, the tensor which is describing the local order of molecules, driving the liquid crystal cells to their final configuration. The external actions can be an applied magnetic or electric field or the confinement created by the walls of the cell. Here we consider a nematic liquid crystal confined in a cylindrical cell. Besides elasticity, electric field and confinement, we consider the flexoelectricity too. Given the free energy density of the nematic, the corresponding Euler-Lagrange equation is solved numerically. A phase diagram of the director configuration according to the flexoelectricity of the material is obtained.

Keywords: Liquid Crystals, Nematics, Confined nematics.

Introduction

The free energy density of a liquid crystal is depending on the distortion of the local order parameter from its uniformly aligned configuration. This quantity contains terms describing the coupling of elastic strains and external fields. In some circumstances, the director field can exhibit a spatial undulated distortion too. In fact, we see helicoidally periodic alignments in liquid crystal materials which are cholesteric or ferroelectric [1]. In nematics, a periodic structure can appear spontaneously too, with period that can be controlled by external factors such as applied fields, saddle-splay elasticity and asymmetric anchoring conditions [2-4]. The electric field controls the instability produced by the flexoelectric effect too [5-7].

In this paper we will consider a nematic liquid crystal confined in a cylindrical cell. Let us assume as order parameter the director field **n**, describing the local mean orientation of molecules. The flexoelectric contribution to the bulk free energy is given by $f_{Flexo} = -\mathbf{P}\cdot\mathbf{E}$. Flexoelectricity is a property of liquid crystals similar to the piezoelectric effect. In certain anisotropic materials, which contain molecular asymmetry or quadrupolar ordering with permanent molecular dipoles, an applied electric field may induce an orientational distortion. Conversely any distortion will induce a macroscopic polarization within the material. The polarization vector **P** in the flexoelectric term is then described with a distortion in the nematic director field:

$$\vec{P} = e_S \vec{n}(\vec{\nabla} \cdot \vec{n}) - e_B (\vec{n} \cdot \vec{\nabla})\vec{n} = e_S \, \vec{n} \, div \vec{n} + e_B \vec{n} \times rot \, \vec{n} \qquad (1)$$

The two terms in the polarization vector are due to the splay and the bend contribution. The coupling of the polarization **P** with an external electric field results in the appearance of a periodic distortion. In fact, Meyer showed that the infinite liquid crystal must be disturbed, the perturbation is periodic along the director orientation and the period is inversely proportional to electric field strength [5]. The nematic planar cell was studied in [7]. Here we will discuss the role of flexoelectricity in a confined geometry with cylindrical symmetry. The problem of a cylindrical confinements had been addressed by the author in previous papers [8,9].

Cylindrical cell

Here we are giving a reduced version of the theory proposed in [9]. Let us consider a cylinder with radius R. In this cylindrical cell, we can imagine to have a nematic liquid crystal. We use the frame as in Figure 1 and solve the Euler-Lagrange equation in cylindrical coordinates.

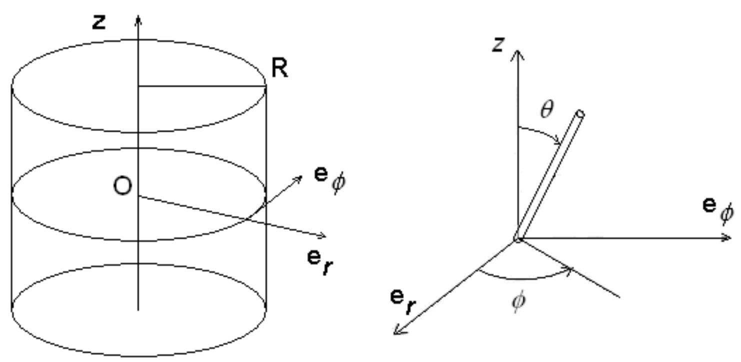

Figure 1: Cylindrical cell and frame of references on the left and on the right the angles of director chosen for calculations

The bulk free energy density in the one elastic constant approximation, with an electric field applied parallel to the z-axis, is given by:

$$f = \frac{1}{2} K \left[(div \, \vec{n})^2 + (rot \, \vec{n})^2 \right] - \frac{\varepsilon_o \Delta\varepsilon}{2} (\vec{E} \cdot \vec{n})^2$$

In a simplified approach, we assume θ=θ(r), only depending on the radial distance, and moreover, φ=0. The Euler-Lagrange equation and the bulk free energy density are [9]:

$$\frac{\partial f}{\partial \theta} = \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial f}{\partial (\partial\theta/\partial r)} \right) \tag{2}$$

$$f = \frac{K}{2}\left[\left(\frac{\partial\theta}{\partial r}\right)^2 + \frac{\sin^2\theta}{r^2} + 2\frac{\sin\theta\cos\theta}{r}\left(\frac{\partial\theta}{\partial r}\right)\right] - \frac{\varepsilon_o \Delta\varepsilon}{2}(E\cos\theta)^2 \tag{3}$$

The Euler-Lagrange equation turns out to be:

$$\frac{\sin\theta\cos\theta}{r^2} + \xi^2 \sin\theta\cos\theta = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\theta}{\partial r}\right) \quad ; \quad \xi^2 = \varepsilon_o \Delta\varepsilon E^2 / K \tag{4}$$

Let us note the presence of the dielectric anisotropy in the term which is coupling electric field and director. Moreover, let us write the surface energy density as:

$$f_{Surf} = -W_H \sin^2\theta_R + W_P \sin^2\theta_R \quad \text{where} \quad W_H > 0; W_P < 0 \tag{5}$$

For an anchoring that is favouring an homeotropic alignment of the nematic perpendicular at the wall of the cylinder, we use:

$$f_{Surf} = -W_H \sin^2\theta_R \tag{6}$$

If we want to avoid the presence of a defect at the axis of cylinder (z-axis), the director must escape in the z-direction. The solution, if the applied electric field is zero, is given by an inverse tangent:

$$\theta^o(r) = 2\tan^{-1}\left(\beta\frac{r}{R}\right) \quad \text{where } \beta = 1 \text{ means strong anchoring} \tag{7}$$

This is a well-known solution obtained by Belavin and Polyakov [10]. To solve the equation in the case of electric field different from zero, we choose a solution as:

$$\theta(r) = \theta^o(r) + \theta'(r) \qquad (8)$$

Using (8), we have two equations to solve:

$$\frac{\sin\theta^o \cos\theta^o}{r^2} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\theta^o}{\partial r}\right)$$
$$\xi^2 \sin\theta^o \cos\theta^o = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\theta'}{\partial r}\right) \qquad (9)$$

The second equation can be solved iteratively. In the numerical solution, it is observed that at the fourth step of iteration the solution is within 0.1%. So we have:

$$\xi^2 \sin\tilde{\theta}^j \cos\tilde{\theta}^j = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\theta^{j+1}}{\partial r}\right) \quad ; \quad \tilde{\theta}^j = \theta^o + \theta^j \qquad (10)$$

Actually, we arrive at the following solutions:

$$\theta^o(r) = 2\tan^{-1}\left(\beta\frac{r}{R}\right); \quad \theta^{j+1}(r) = \xi^2 \int_0^r \frac{dr''}{r''} \int_0^{r''} \sin\tilde{\theta}^j(r')\cos\tilde{\theta}^j(r')\,r'dr' \qquad (11)$$

and then at final solution:

$$\theta(r) = \theta^o(r) + \theta^{j+1}(r) \qquad (12)$$

To determine the value of parameter β we determine the solution minimizing the reduced total free energy:

$$\frac{F}{2\pi RL} = \int_0^d f\,r\,dr + f_{Surf} \qquad (13)$$

where L is an arbitrary length of the cylindrical cell.

Flexoelectricity

Let us consider the contribution of flexoelectricity to Euler-Lagrange equation. After calculation, we see that this contribution depends on the difference between the splay and bend flexoelectric coefficients:

$$\frac{\partial f}{\partial \theta} - \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial f}{\partial (\partial \theta / \partial r)} \right) = (e_S - e_B) E \frac{\sin^2 \theta}{r} \qquad (14)$$

Defining two parameters, the equation to solve is the following:

$$\xi^2 \sin \tilde{\theta}^j \cos \tilde{\theta}^j + \Pi \xi \frac{\sin^2 \tilde{\theta}^j}{r} = \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial \theta^{j+1}}{\partial r} \right) \qquad (15)$$

$$where: \quad (e_S - e_B) E = \Pi \xi$$
$$b = WR / K$$

After the numerical solution, in Ref.[9], we gave several figures illustrating the role of anchoring parameter *b* and the dimensionless electric field parameter ξ.

Discussion

As it is intuitively expected, when the electric field is higher that a threshold value, the angle θ goes to zero and the director field is parallel to the cylinder axis, in all the cell. If the flexoelectric parameter Π is large, a distorted configuration (see the Figure 2) is favoured, and the threshold field required for suppressing this configuration is increased. Moreover, if the flexoelectric parameter is large, the angle θ starts to oscillate as the field increases. We must have a huge electric field to suppress the oscillating distortion and have cosθ=0, that is, with all the nematic aligned parallel to the field, in a uniform configuration.

In the Figure 2, the phase diagram is shown, when anchoring parameter *b* is fixed and equal to 6. We see three regions, denoted by U for uniform alignment of director parallel to *z*-axis, D for the director with a deformed configuration, and O when the director is oscillating and cosine becomes negative too. Angle θ turns more than π/2 on the distance *R*.

A last note on the flexoelectric term. The flexoelectric vector is a sum of two contributions:

$$\vec{P} = \left(e_S \, \vec{n} \, div \, \vec{n} + e_B \, \vec{n} \times rot \, \vec{n} \right) = \qquad (16)$$

$$= e_S D(\sin \theta \vec{u}_r + \cos \theta \vec{u}_z) + e_B R(-\cos \theta \vec{u}_r + \sin \theta \vec{u}_z) = e_S D \vec{n} + e_B R \vec{t}$$

$$where: \quad D = div \, \vec{n}, \; R = (rot \, \vec{n})_\varphi$$

These two components which are perpendicular each other: when they are coupled with the electric field, parallel to the cylinder axis, we have then the two contributions in the bulk energy with an opposite sign. To conclude, let us discuss the saddle-splay contribution to the free energy. In the previously made assumptions, (θ=θ(r), φ=0), this is a term which is simply renormalizing the value of the surface energy and then it does not need a further discussion.

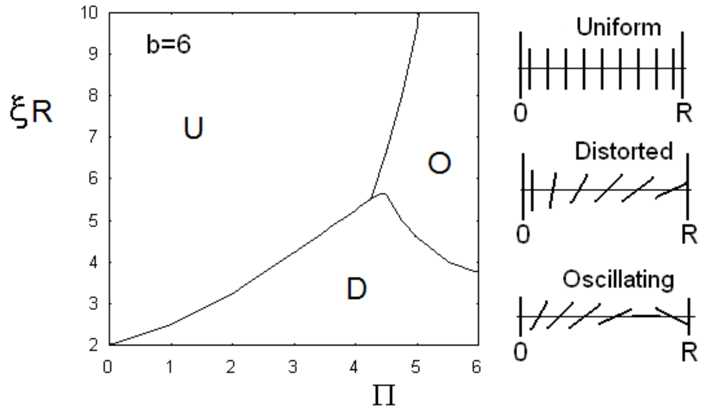

Figure 2. Phase diagram of the cylindrical confinement, when the anchoring parameter b is fixed. The three regions are denoted by U for the uniform alignment of director parallel to the cylinder axis, D when the director has a deformed configuration, and O if director is oscillating and cosine becomes negative too.

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