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Periodicity in nematic liquid crystal walls

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The elastic continuum theory of nematic liquid crystals is used to show that the periodicity of the walls that are observed above the critical Frederick's field in nematic liquid crystals is closely related to the dimensionality of these structures, and that the π symmetry of the director and the fluid flow mechanism, usually regarded as responsible for these walls, are not enough to fully explain the observed periodicity. [S1063-651X(96)07912-3]

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The observation of periodic structures in liquid crystal systems is commonplace [1]. Sometimes such structures arise where we do not expect to find them [2]. Some nonlinear and unstable systems show metastable, but periodic, configurations. The periodic unidimensional walls of the nematic liquid crystals (NLC) are examples of such structures [3]. Even being nonlinear and unstable, they have attracted the attention of a broad audience that studied them for many years [3–8]. In this work we will give a mathematically simple and general demonstration of a profound connection between the periodicity of these nematic structures and its dimensionality. In spite of the fact that such systems have been widely studied, we believe that this important connection has not been put into evidence.

When a previously uniformly oriented sample of NLC is submitted to a magnetic field perpendicular to the direction of the director, it tends to bend to the direction of the magnetic field if the field is greater than a critical field H_c, which defines Frederick's threshold [9]. For many compounds it is observed that this bending is not uniform along the sample. Due to the π symmetry ($\vec{n}$ and $-\vec{n}$ are equivalent) in some regions of the sample the director presents a clockwise bending, and in other regions it presents a counterclockwise bending. In the regions of the space where the director links these two configurations, turning from one to the another, we say that there is a wall. As soon as we turn on the external magnetic field, these walls appear as a one-dimensional array perpendicular to the external magnetic field [10–15].

Recently it has been shown that the behavior of the wavelength of the periodic distortion (λ) can be properly understood if an interaction is assumed between these walls [16]. In that work, motivated by the fact that the one-dimensional array of walls appears to us a sequence of equidistant lines crossing the sample along the y axis (the axis of the external magnetic field), it was assumed that these walls form a periodic structure along the x axis. But why is this so? Why is a nonperiodic sequence of walls not shown by the system? The answer is clearly related to another question: why does the system not show a homogeneous alignment in all of the sample? These questions are usually answered grasping two fundamental points. The first one, and the more important, is the π symmetry. The other one is a fluid flow that generates a nonuniform rotation pattern of the director which reinforces opposite rotations of neighboring regions of the sample leading to an effective lower viscosity of the matter movement which forms the walls in relation to the viscosity of the matter movement which forms the homogeneous alignment [3]. Even when we claim this beautiful mechanism, the question about the origin of the periodicity is not completely answered because it must be assumed at the beginning. So, we should ask: why does a nonperiodic, but oscillating, pattern of the director not show an even lower viscosity? As we will show, the answer to this question transcends the π symmetry and the fluid flow mechanism. It lies in a simple feature of the system that is beyond these principles: its dimensionality.

It is usual to divide the walls' kind in splay, twist, and bend, according to the geometry and the term of the Frank free energy which dominates its configuration [1]. But irrespective of the walls' kind that we consider, we always find the same mathematical structure [5]. Without losing the generality, we will choose here a particular geometry for our analysis. To do this, we consider a slab with dimensions a along the x axis, b along the y axis, and d along the z axis, in such a way that $a \gg b \gg d$. The director was previously prepared in such a way that it is initially uniformly aligned along the x axis and strong boundary conditions, with the usual boundary conditions of $\theta(x,y,z)$ at the sample's edge, assumed [1]. The external controlled magnetic field H is applied along the y axis.

With this geometry we suppose that the components of the director can be expressed by

$$n_x = \cos\theta(x,y,z), \quad n_y = \sin\theta(x,y,z), \quad n_z = 0, \tag{1}$$

where $\theta(x,y,z)$ is the angle between the director $\vec{n}$ and the x axis direction.

The expression of the free energy density in the two elastic constant approximations ($K_1 = K_3$), taking into account the magnetic field coupling, is [1,5]

$$F = \int_V \{ \tfrac{1}{2} K_3 [(\partial_x \theta)^2 + (\partial_y \theta)^2] + \tfrac{1}{2} K_2 (\partial_z \theta)^2 - \tfrac{1}{2} \chi_a H^2 \sin^2\theta \} dV, \tag{2}$$

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where K_1, K_2, and K_3 $(=K_1)$ are, respectively, the elastic constants of splay, twist, and bend, and V is the volume of the system. Since we are dealing with a one-dimensional structure that spreads along the x axis, the function $\theta(x,y,z)$, which represents the spacial configuration of director $\vec{n}$, can assume the form

$$\theta(x,y,z)=\eta(x)\sin\left(\frac{\pi y}{b}\right)\sin\left(\frac{\pi z}{d}\right), \tag{3}$$

for $0\leqslant x\leqslant a$, $0\leqslant y\leqslant b$, $0\leqslant z\leqslant d$, where $\eta(x)$ is the configuration of the nematic structure along the x axis. With these replacements and with the approximation $\sin^2\theta\approx\theta^2-2/3!\,\theta^4$ in the last term of Eq. (2), and assuming that $\chi_a H_c^2=K_3(\pi/b)^2+K_2(\pi/d)^2$, $h=H/H_c$, $x=\sqrt{K_3/(\chi_a H_c^2)},t$, and $\theta_0^2=8/3$, we arrive at

$$F=\frac{1}{4}bd\sqrt{K_3(\chi_a H_c^2)}\int_0^{\tilde{a}}\mathcal{F}\;dt,$$

where

$$\mathcal{F}=\frac{1}{2}(\partial_t\eta)^2+\frac{1}{2}(1-h^2)\eta^2+\frac{1}{4\theta_0^2}h^2\eta^4, \tag{4}$$

and $\tilde{a}=\sqrt{(\chi_a H_c^2)/K_3}\;a$. Observe that the free energy density $\mathcal{F}$ does not have any particular constant that characterizes the actual system. The elastic constants, the critical field, and sample dimensions have been put aside. Therefore the resulting equation for $\eta(t)$ will be, save for the geometry, completely independent of the NLC sample and, as h is the ratio between the actual magnetic field H and the critical Frederick's field H_c, the equation for the field $\eta(t)$ describes a kind of equation of corresponding states for walls [17], which assumes the form

$$\partial_t^2\eta-(1-h^2)\eta-\frac{3}{8}h^2\eta^3=0, \tag{5}$$

with the boundary conditions $\eta(0)=\eta(\tilde{a})=0$. In his work about the mathematical structure of the nematic walls, Brochard [5] found, save for the constants, exactly this equation and solved it for one wall. It is important to observe that this equation does not only describe the geometry of the twist walls. As can be seen in the work quoted above, all the walls can be reduced to this mathematical form. The multiwall integration of Eq. (5) is a difficult task [18], but it is easy to find the integration's constant associated with it, which is

$$\mathcal{C}=\frac{1}{2}(\partial_t\eta)^2-\frac{1}{2}(1-h^2)\eta^2-\frac{3}{32}h^2\eta^4. \tag{6}$$

We will use this equation to show that if there is any oscillatory solution of Eq. (5) it will necessarily be a periodic solution. So, supposing that it admits an oscillatory solution, it follows that there will be a set of points $S=\{t_1,t_2,t_3,\dots\}$ for which $\eta(t_1)=\eta(t_2)=\eta(t_3)=\cdots=0$. So, at each point of this set, we have

$$\mathcal{C}=\tfrac{1}{2}(\partial_t\eta)^2/_{t=t_i},\quad t_i\in S. \tag{7}$$

Therefore, for any two distinct points t_i and t_j of the set S we have

$$\partial_t\eta/_{t=t_i}=\pm\partial_t\eta/_{t=t_j}. \tag{8}$$

Let $t_b\in S$ be the closest point to $t_a\in S$ for which we have simultaneously

$$\eta(t_a)=\eta(t_b)=0$$

and

$$\partial_t\eta/_{t=t_a}=\partial_t\eta/_{t=t_b}. \tag{9}$$

Using Eq. (5) and the equations above, we can compute the second derivative of $\eta(t)$ and find that it assumes the same value at these two points. That is, $\partial_t^2\eta/_{t=t_a}=\partial_t^2\eta/_{t=t_b}$. We can continue this process and compute, using Eq. (5), the n order derivative of $\eta(t)$ at these points. For example, for the third-order derivative of $\eta(t)$ we get $\partial_t^3\eta=(1-h^2)(\partial_t\eta)+\frac{9}{8}h^2\eta^2(\partial_t\eta)$, and using Eq. (9) we conclude that $\partial_t^3\eta/_{t=t_a}=\partial_t^3\eta/_{t=t_b}$. In this way, for any n, we will always arrive at

$$\partial_t^n\eta/_{t=t_a}=\partial_t^n\eta/_{t=t_b}. \tag{10}$$

Now, as at points t_a and t_b, the function $\eta(t)$ and all its derivatives assume the same values we see, using a Taylor series argument, that for any ε, $\eta(t_a+\varepsilon)=\eta(t_b+\varepsilon)$. Setting $t_b-t_a=P$, we obtain $\eta(t_a+\varepsilon)=\eta(t_a+\varepsilon+P)$. And, due to the fact that the equality in Eq. (10) is independent of the order n, we do not have any limit for ε and can set $t=t_a+\varepsilon$ to obtain

$$\eta(t)=\eta(t+P), \tag{11}$$

which is exactly the definition of a periodic function with period $P=t_b-t_a$.

The cornerstone of this demonstration is Eq. (6), and to arrive at it we have made some simplifications, upon which we now comment. We assumed strong anchoring boundary conditions, but we did not use them in our demonstration. They only had the role of being an easy way of obtaining the one-dimensional Eq. (4). So, the exact way by which the molecules touch the edges of the sample seen to be not important for our conclusion, because the condition that the function $\eta(t)$ vanishes at the set S, follows directly from the fact that $\eta(t)$ was supposed to be an oscillatory function. We have also used the two elastic constant approximations $(K_1=K_3)$. Again this was done in the name of simplicity of the resulting equation. If we do not assume the two elastic constant approximations, Eq. (4) would result in a tantamount and awkward equation that, with the use of Eq. (3), could also be put in the form of a one-dimensional expression for the free energy. Finally we have assumed that the last term in Eq. (2), the $\sin^2\theta$ term, can be expanded in a polynomial approximation. If this simplification procedure were not used, Eq. (5) would have a cumbersome form, but a constant of integration would follow in the same way. Therefore, we conclude that the key to understanding the periodicity of the walls is its one-dimensional character, which we used when we stated Eq. (3), and which has allowed us to construct the constant of integration given in Eq. (6). It is important to observe that this kind of constant of integration, which imitates the energy in mechanical problems, can only be found for one-dimensional functionals [19] and these periodic walls are unstable structures which decay in closed bidimensional walls that, of course, do not present any periodicity in their distribution along the sample. This fact is therefore strong, and pleasing, evidence of the relation between their periodicity and their dimensionality.

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