Reply to ''Comment on 'Periodic distortions in lyotropic nematic calamitic liquid crystals' ''

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We reply to the Comment of Grigutsch and Stannarius [Phys. Rev. E **56**, 7323 (1997)] about our paper [Phys. Rev. E **54**, 3765 (1996)]. It is shown that there are defined conditions in which an elastic approach to study some features of the physics of the walls appearing above the Fréedericksz threshold can be instructive, and even recommended. We analyze the torque balance equation and the exact solution of an equation in our previous paper to show that there are no arbitrary elastic constants to be fixed. Instead of this we show that they arise naturally as integration constants of the Euler-Lagrange equation which must be determined in the transient fluid flow period. Finally, using the exact solution of the elastic problem, we show that there are no mistakes in our computations and interpretations. [S1063-651X(97)09911-X]

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We thank the authors of the Comment [1] for the attention devoted to our paper [2]. They claim that we have described the walls appearing above the Fréedericksz threshold, for some nematic materials, in terms of a purely elastic theory. They observe that we have introduced arbitrary elastic parameters and that with the approach proposed by us we cannot describe the wavelength selection mechanism giving origin to these structures. Afterwards they present a brief historical description of the evolution of the subject in the last twenty years, and suggest that in our paper we have omitted it. Furthermore, they analyze our calculations and conclude (precipitately, as we will show) that, even if our approach could be admitted, our computations were wrong, and that the theory we proposed is not appropriate for the description of the experimental results we reported. In order to respond to all these objections we start by briefly reviewing some fundamental points on this subject.

Let us begin by analyzing the motivations of our static approach. In a remarkable work Lonberg *et al.* [3] showed how these walls arise in the nematic medium. Using the solution of the anisotropic version of the Navier-Stokes equation [4–6], the torque balance equation, and the equation of continuity, they were able to show that the walls formation has an effective viscosity which is lower than the one of the matter movement forming the homogeneous alignment. Their result is based on the fact that at the initial moments there is an exponential growth of the fluid velocity in the direction of the applied magnetic field, as well as a correlated exponential growth in the director bending. In this scenario the fastest growth mode would determine the wavelength of the periodic walls. In another remarkable work Srajer, Fraden, and Meyer [7] studied this selection mechanism a little bit more, and included some nonlinearity. They found (Fig. 7 of [7]) that there is really a fast growth mode of the fluid flow in the initial instants, and that the selection mechanism really works. But this velocity growth rapidly stops: it decreases and becomes nearly zero in a few minutes.

Now, being aware of this well-established theory and phenomenology, let us explicitly write the torque balance equation. In the planar geometry, used in [2], it becomes [8]

$$\gamma_1 d_t \theta = \gamma_1 W_{xy} - \gamma_2 [A_{xy}(n_x^2 - n_y^2) + (A_{xx} - A_{yy}) n_x n_y] + K_{33}[(\partial_x^2 \theta) + (\partial_y^2 \theta)] + K_{22}(\partial_z^2 \theta) + \chi_a H^2 n_x n_y , \tag{1}$$

where, as usual, it is not considered the inertial term, and γ_1 and γ_2 are the shear torque coefficients. Furthermore, in Eq. (1) $A_{\alpha\beta} = \frac{1}{2}(\partial_\alpha \mathcal{V}_\beta + \partial_\beta \mathcal{V}_\alpha)$, $W_{xy} = \frac{1}{2}(\partial_x \mathcal{V}_y - \partial_y \mathcal{V}_x)$, $n_x = \cos\theta(x,y,z)$ and $n_y = \sin\theta(x,y,z)$. This equation indicates that the director bending is fixed by the action of three mechanisms: the flow of the fluid, the elastic resistance of the medium, and the external magnetic field. However, the fluid flow only works for a few minutes in a transient way, and the walls can be observed for a larger time. This means that after some minutes we can consider $A_{\alpha\beta} = W_{xy} = 0$ and $d_t \theta \simeq 0$, and the torque balance equation becomes

$$K_{33}[(\partial_x^2 \theta) + (\partial_y^2 \theta)] + K_{22}(\partial_z^2 \theta) + \chi_a H^2 n_x n_y = 0, \tag{2}$$

which clearly shows that, as soon as the fluid flow stops, the dynamics of the director is determined by the elastic term and the external magnetic field. Moreover, this is the Euler-Lagrange equation obtained from the minimization of the Frank elastic energy, which, of course, cannot describe the arising of the walls. But, once this equation is built up, the metastable walls have to be the solution of it. Consequently, if, for instance, one is interested not in the genesis of these structures, but in their geometrical properties and parameters, the equation to be investigated is this one. It was for this reason that we proposed a static approach in our work: the walls must be the solution of this equation simply because they exist in a quasistatic situation described by this equation.

In the work of Lonberg *et al.* [3] the profile of these walls, along the $\vec{e}_x$ direction, was assumed to be a harmonic func-

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tion (Eq. (1) of [3], in which the $\vec{e}_z$ direction is the $\vec{e}_x$ direction of our paper). Since the purpose of that work was to describe the mechanism of the viscosity reduction this was a very clever insight. But, far from the matter flow initial moments there is no reason to accept a harmonic function describing the profile of these walls along the $\vec{e}_x$ direction. In our paper [2] we assumed that the maximum bend of the director, for large fields, is not achieved just along a line but over a region (see Fig. 2 of [2]). Thus, the purpose of the paper was to correlate the dimensions of this saturated region with the bending of the curve of $1/\lambda^2$ vs h^2. This result is clearly shown in the figures of our paper [2], mainly in Figs. 2 and 4.

To show that there is in fact a saturation of the profile of the director along the $\vec{e}_x$ direction, and that this can indeed be viewed in the bending of the curve of $1/\lambda^2$ vs h^2, we outline the exact solution of these walls that have been found by us after the publication of that paper [9]. This solution has the advantage of giving us exactly the meaning of the integration constants of Eq. (2) and its connection with the transient instants of the walls arising.

Let us consider that $\theta(x,y,z)=\eta(x)\sin(\pi y/b)\sin(\pi z/d)$, and write the magnetic term of the free energy in the form of a functional: $I[\eta(x)]=\int\sin^2\theta dydz\simeq(1/4)\eta(x)-(3/64)\eta^4(x)+O(\eta^6(x))$. By performing some change of scale in the elastic free energy, namely, $\chi_a H_c^2=K_{33}(\pi/b)^2+K_{22}(\pi/d)^2$, $h=H/H_c$, and $x=\sqrt{K_{33}/(\chi_a H_c^2)}t$, $\theta_0^2=8/3$, one can show that Eq. (2) assumes the form

$$\partial_t^2\eta-(1-h^2)\eta-\frac{1}{\theta_0^2}h^2\eta^3=0, \tag{3}$$

which has the conserved quantity $C=\frac{1}{2}(\partial_t\eta)^2-(1/2)(1-h^2)\eta^2-(1/4\theta_0^2)h^2\eta^4$. This equation can be used to find $\eta(t)$. By the usual procedure we find

$$t-t_0=\frac{\sqrt{2\theta_0^2}}{h}\int^{\eta}\frac{d\tilde{\eta}}{\sqrt{(\tilde{\eta}^2-\varphi_0^2)(\tilde{\eta}^2-\varphi_1^2)}}, \tag{4}$$

where φ_0 and φ_1 are the turning points of the oscillating function $\eta(t)$. Since Eq. (4) is an elliptic integral of the first kind, it can be written in terms of elliptic functions [10], giving

$$\eta(t)=\varphi_0\,\mathrm{sn}\left(\varphi_1\sqrt{\frac{h^2}{2\theta_0^2}}t,k\right), \tag{5}$$

where $\mathrm{sn}(u,k)$ is the elliptic sine function of argument k, and we have chosen $t_0$in such a way that $\mathrm{sn}(0,k)=0$. For Eq. (5) we have $k^2=\varphi_0/\varphi_1$. Therefore the argument is limited to the interval $0\leqslant k^2\leqslant 1$.

From Eq. (4) it is also possible to obtain the period τ:

$$\left(\frac{2\pi}{\tau}\right)^2=\left(\frac{\pi}{2}\right)^2(h^2-1)\left[\frac{1}{(1+k^2)}\frac{1}{[K(k)]^2}\right], \tag{6}$$

where $K(k)$ is the complete elliptic integral of the first kind [10].

Using the definition of k^2 given above it is possible to express C, φ_1, and φ_0 in terms of k^2. We obtain $C=\theta_0^2[k^2/(1+k^2)^2](h^2-1)^2/h^2$, $\varphi_0=2\theta_0^2[k^2/(1+k^2)^2](h^2-1)^2/h^2$, $\varphi_1=\varphi_0/k^2$. Therefore, since k^2 is a function of C, we conclude that it is just a constant of integration controlling the shape of the elliptic sine function [10], i.e., when $k\to 0$ we have $\mathrm{sn}(u,k)\to\sin u$, and when $k\to 1$ we have $\mathrm{sn}(u,k)\to\tanh u$. Notice that this was exactly our hypothesis about the shape of the walls. In other words, there is a parameter determined by the initial conditions, in this case k, that controls the shape of the wall. When $k\to 0$ we have a sine function, which indicates that we are close to the critical point. When k increases, a saturated region which reaches the maximum dimension when $k\to 1$ arises. Furthermore, k^2 must be a function of h, otherwise a plot of $1/\lambda^2$ vs h^2 would be a straight line. But, since a bending in the curve has been experimentally obseved, k^2 must change with the magnetic field. The exact determination of this function is now in progress and, of course, it must be fixed at the transient fluid flow period. Moreover, the solution $\eta(t)$ can be separated into two terms: the amplitude of the oscillation, given by φ_0, and the shape of the wall, given by the elliptic sine function. It is exactly what we have supposed in our paper [2]. Hence, to precisely know the shape of the wall and its wavelength, it is enough to determine k^2. But this parameter can not be fixed by an elastic model since it originates from the transient matter flow, and it is an integration constant of Eq. (3).

At this point, the question of why we did not use the exact solution of Eq. (3) in our original work, but an approximated one can be argued. To clearly answer this question let us discuss the nature of the approximation we did and how it is connected to the exact solution. The motivation of our approximation was that, due to the π symmetry of the director, the configurations with $\theta=\varphi_0$ and $\theta=-\varphi_0$ are equivalent. The object making the transition from one configuration to the another one is the wall. In the region between the walls, with length Δ, a constant bend of the director was assumed. Our aim was simply to connect the magnitude of this region with the magnetic field and with the bending of the curve of $1/\lambda^2$ vs h^2. The fact that this can be done has been demonstrated above in the analysis of the exact solution, where it was recognized that, even being distinct parameters, Δ and k^2 have similar meaning: they control the shape of the wall.

Furthermore, it can be argued that our work lost its interest once the exact solution was discovered. This is not true, because, as well known, sometimes an approximated solution is more fruitful than the exact one. For example, the family of walls that we found as the solution of Eq. (2) are known in the statistical mechanics literature [11] as kinks linking two equivalent stable ground states in a model which allows symmetry breaking. Usually it is very important to understand how these structures interact. In fact, it is known that the walls are metastable [12,13] structures that disappear after a long time. Of course these instabilities must follow, in some way, from some kind of interaction among them. Therefore, an easy way to obtain this interaction is to suppose each wall acting as an isolated object and to find the interaction among them which is responsible for the observed structures. This procedure is known as a soap of kinks [11], and it usually requires the isolation of just one kink. Of course, with the exact solution one cannot isolate just one wall in order to get some insight about the interaction. In this situation, the solution must be searched for in another manner.

To conclude, we stress again that the aim of our approach was not to develop a complete expression for the wavelength of the walls in terms of a purely elastic theory. As has been clearly shown above, this would be impossible. But, once the walls have been built in a dynamical transient situation, these structures have to be the solution of Eq. (2), and its parameters; the integration constants of this differential equation, have to be determined by the transient fluid flow. Therefore they are not arbitrary elastics parameters. Furthermore, as pointed out in [1], the amplitude φ_0 is really zero for $l=1$, and there is no mistake about it. To verify that this is indeed true it is enough to recall the exact expression for it, $\varphi_0 = 2\theta_0^2[k^2/(1+k^2)^2](h^2-1)^2/h^2$, and to realize that $l=1$ corresponds to $k^2=0$. Therefore we believe that there was an incorrect interpretation by the authors of [1] about this point, because, as shown by the exact solution, our computations are right.

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