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Anisotropy induced director refraction inside inversion walls in nematic liquid crystals

A. M. Figueiredo Neto (*), Ph. Martinot-Lagarde and G. Durand

Laboratoire de Physique des Solides (**), Université de Paris-Sud, Bât. 510, 91405 Orsay Cedex, France

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Abstract. — We compute the texture of the inversion walls which appear in nematics in a magnetic field. In the isotropic case, where the 3 curvature elastic constants are equal, the Brochard planar description is correct. In the anisotropic general case, we find an unpredicted director rotation around the field, which minimizes the elastic free energy of the wall, by transferring some curvature distortion toward the lowest elastic constant curvature mode. This rotation is calculated to first order in the elastic anisotropy. By symmetry, the planar model remains valid when there is no twist in the wall. This rotation explains the recently observed twist of neutral axes along the inversion walls in lyotropic liquid crystals. In the highly anisotropic case (polymeric nematics), the ellipticity of closed loop walls should be twice larger than that predicted.

The textures of nematic liquid crystals can be distorted by magnetic (or electric) fields. In the so-called Freedericksz transition, two symmetrically distorted textures can be created, separated by a « wall ». The structure of this wall has been calculated using the curvature elasticity by Brochard [1]. In the case where the wall makes a closed loop, this model predicts that this loop should be an ellipsis, with the axis ratio equal to the square root of the curvature elastic constants’
ratio. These ellipses have indeed been observed in thermotropic nematics by Léger [2] who
derived the elastic constants by this technique. Recently, Liebert and Figueiredo Neto [3] have
observed these closed loop walls in lyotropic nematics. It appears that the optical neutral axes of
these birefringent walls are twisted. This twist was not predicted by the model of reference [1].
In this Letter, we give an explanation of this twist of birefringence along the walls in terms of a
director « refraction » across the walls. As usual, the « director » n is the local optical axis of
the system. We also explain why this « refraction » was not observed in thermotropic liquid crystals.

The three-dimensional geometry of the wall is sketched in figure 1. In absence of field the nema-
tic sample is uniformly oriented by two rubbed plates, along X, in a planar geometry. The magne-
tic field H is along z. Above the Freedericksz transition threshold $H_c$ the director n is assumed to
tilt toward z, with $(z, n) = \theta(x, y, z)$. The two domains corresponding to symmetrical tilts $\theta_x(z)$
and $\pi - \theta_x(z)$, are separated by a wall oriented along y, with $(x, X) = (y, Y) = \phi_0$. Compared
to reference [1] the new point of our model is the possible existence of a director twist
$\phi = (x, n) = \phi_0 + \delta(x, y, z)$ inside the wall. As in [1], we assume for simplicity that the walls are
straight lines, which drops the y dependence of $\theta$ and $\phi$. Calling as usual $K_{1,2,3}$ the splay, twist and
bend curvature constants and $\chi_a$ the diamagnetic anisotropy, we write the free energy as

$$
F = \frac{1}{2} \int d^3r \left[ K_1 (\text{div } n)^2 + K_2 (n \cdot \text{curl } n)^2 + K_3 (n \times \text{curl } n)^2 - \chi_a (n \cdot H)^2 \right].
$$

The two Euler equations for $\theta$ and $\phi$ are bulky and untractable in general. These equations can be
simply written as $\Delta \delta = 0$ in the isotropic case ($K_1 = K_2 = K_3$), and $\Delta \theta + \left( \frac{1}{\xi^2} \right) \left( \theta - \frac{2}{3} \theta^3 \right) = 0$, for small distortions [4]. $\xi$ is here the usual magnetic coherence length defined by $\chi_a H^2 = K_1/\xi^2$.

We look for a simple perturbation of the approximate planar ($\delta = 0$) solution of reference [1].
This planar solution is correct if the $K_i$ are equal, because an additional $\delta(x, z)$, which converts
some splay and bend into twist or vice versa, cannot then lower $F$. We calculate as a perturbation
the twist $\delta$ produced by the assumed small elastic anisotropies $k_2 = \frac{K_2 - K_1}{K_1}$ and $k_3 = \frac{K_3 - K_1}{K_1}$.
To first order in \( k \), we can keep for \( \theta \) the unperturbed solution of reference [1] for the isotropic case. We are just left with the \( \phi \) equation, which can be written as

\[
\Delta \phi = \Delta \theta = k_2 f_2(\theta, \phi_0) + k_3 f_3(\theta, \phi_0)
\]

where the source terms \( f_{2,3} \) can be estimated for the unperturbed value \( \phi_0 \) of \( \phi \).

We keep only in \( F \) the terms corresponding to a small amplitude distortion \( \epsilon = \frac{\pi}{2} - \theta \). To first order in \( \epsilon \), we find \( f_3 = 0 \) and \( f_2 = -\sin \phi_0 \frac{\partial^2 \epsilon}{\partial x \partial z} \). From [1], in the unperturbed isotropic case, \( \epsilon \) is given by

\[
\epsilon = \epsilon_\alpha \text{ th}\left(\frac{\epsilon_\alpha | x |}{2 \xi}\right) \cos \frac{\pi z}{d},
\]

the natural width of the wall is then : \( \zeta = 2 \xi / | \epsilon_\alpha | \), where \( \xi \) is the magnetic coherence length, of the order of the sample thickness \( d \) above threshold. As \( \epsilon \) is even in \( z \), the twist \( \delta_1 \) induced by the source \( f_2 \) must be odd in \( z \). The order of magnitude of \( \delta_1 \) is \( \delta_1 \sim k_2 \epsilon_\alpha d / 2 \pi \sim k_2 \epsilon_\alpha^2 \). In figure 2 we have plotted the computed solution \( \delta_1(x, z) \) for \( \zeta/d = 0.4/2 \pi \).

we have plotted the computed solution \( \delta_1(x, z) \) for \( \zeta/d = 0.4/2 \pi \). When \( K_2 < K_1 \), the effect of this term is to give to \( n \) a two-dimensional conical twist around \( X \), maximum for \( \phi_0 = \frac{\pi}{2} \), i.e. for the wall of pure twist. It transforms then a splay distortion into a twist. Vice versa, for \( K_2 > K_1 \), it transforms twist into splay (see Fig. 3). To second order in \( \phi \), two additional source terms appear, in the \( \phi \) equation, namely:

\[
\begin{align*}
f_2 &= + \sin \phi_0 \cos \phi_0 \left( \epsilon \frac{\partial^2 \epsilon}{\partial x^2} + 2 \left( \frac{\partial \epsilon}{\partial x} \right)^2 \right) \\
f_3 &= - \sin \phi_0 \cos \phi_0 \left( \frac{\partial \epsilon}{\partial x} \right)^2.
\end{align*}
\]
Molecular arrangement in the xz section of a pure twist wall \( \phi_0 = -\frac{\pi}{2} \). a) unperturbed isotropic wall. b) twist favoured wall. c) splay favoured wall.

The sources now induce a twist \( \delta_2 \) which is even in \( z \). The order of magnitude of \( \delta_2 \) is:

\[
\delta_2 \sim k_i \varepsilon_0^2 d^2/\zeta^2 \sim k_i \varepsilon_0^2.
\]

The \( \sin 2\phi_0 \) symmetry of \( \delta_2 \) is important to notice. \( \delta_2 \) is maximum for \( \phi_0 = \pi/4 + m \pi/2 \) (\( m \) integer). In figure 4 we have plotted the computed solution \( \delta_2(x, z) \) with the same values of the constants as for \( \delta_1 \).

Additional reduced symmetrical twist \( (\phi - \phi_0)/B \) in the wall, versus \( x \) and \( z \). \( B = \sin \phi_0 \times \cos \phi_0 k_2 \varepsilon_0^2 d^2/2 \xi^2 \pi^2 \). \( H \) chosen as in figure 2. \( k_3 = 0 \).

Fig. 4. — Additional reduced symmetrical twist \( \phi - \phi_0 / B \) in the wall, versus \( x \) and \( z \). \( B = \sin \phi_0 \times \cos \phi_0 k_2 \varepsilon_0^2 d^2/2 \xi^2 \pi^2 \). \( H \) chosen as in figure 2. \( k_3 = 0 \).

The physical interpretation of \( \delta_2 \) is simple: the part excited by the source \( f_2 \) transforms a splay distortion into twist, for \( K_2 < K_1 \) and \textit{vice versa}. The part excited by \( f_3 \) transforms bend into splay, for \( K_3 > K_1 \), or splay into bend for \( K_3 < K_1 \) (see Fig. 5). In all cases, the additional \( \phi \) distortion adjusts to minimize \( F \) by transferring curvature distortion from the highest elastic constant curvature distortion, to the smallest one, compatible with the wall symmetry. We must now look at the \( \theta \) equation, to check if the approximate solution used is correct. The \( \theta \) equation writes now as:

\[
\Delta \theta + \xi^{-3}(\theta - (2/3) \theta^3) = g(\theta, \phi).
\]

\( g \) is zero for constant \( \phi = \phi_0 \). It can be expanded in powers of \( \delta \), i.e., of \( k_i \). \( F \) is quadratic in \( k_i \), since the additional twist \( \delta \) decreases \( F \) whatever the sign of \( k_i \) may be. The torque \( g \) acting on \( \theta \) is then also quadratic in \( k_i \), since it is obtained by derivation with respect to \( \theta \). To first order in \( k_i \), the resulting change in \( \theta \) can be neglected, which justifies our previous calculation of \( \phi \).
We will now discuss the case of closed loop walls. In reference [1], the wall energy per unit length (the wall « tension ») was calculated, with the approximation of a straight line shape. Applied to a closed loop of radius of curvature $R$ larger than $d$, an elliptical shape was predicted, with the axes proportional to the square root of the curvature elastic constants. In our perturbation calculation, the wall energy is quadratic in $k_\xi$, so that for small $k_\xi$ the wall tension is unaffected. The prediction of [1] remains valid. However, in the practical case of thermotropic nematics, $k_\xi$ can be of the order of 1, and even larger close to a second-order transition to a smectic phase, so that a new calculation is necessary. We have already seen that the twist $\delta$ across the walls contains parts proportional to $\sin \phi_0$ and $\sin \phi_0 \cos \phi_0$, and not to $\cos \phi_0$. This is a very general property of the system. Because of the symmetry of the texture with respect to the $(z, X)$ plane, the twist inside the wall must remain zero for $\phi_0 = m\pi$ ($m$ integer). The induced twist $\phi$ in a wall must be maximum for $\phi_0 = \pi/2 + m\pi$. Because $\phi$ decreases the energy of the latter walls only, one expects the length of the $Y$ axis of an elliptical loop to decrease in length, whatever the initial ellipticity may be. That part of the twist proportional to $\sin \phi_0 \cos \phi_0$ is not expected, by symmetry, to change the ellipticity of a closed loop wall, but to distort the ellipse toward a lozengic shape. The case of small radius loops ($R < d$) is more delicate to discuss. As these loops are unstable, they contract toward their centre before vanishing. Their exact shape must depend not only on the balance of elastic torque, but also on viscous drag effects. In the extreme case of polymeric nematics [5], one expects $K_1 \gg K_2, K_3$. With our perturbation technique, a quantitative prediction of the wall energies for these very anisotropic cases is difficult. Assume $K_2 = K_3 = \alpha^2 K_1, (\alpha \ll 1)$.

We can use a heuristic argument. One can interpretate simply the wall energy calculated by Brochard [1], in the planar approximation ($\delta \equiv 0$). The wall energy $T$ (per unit length) increases because $\theta$ is no longer tilted toward $H$, with the compensation of the absence of splay, i.e.

$$T \sim K_1 \theta^2 \left( \frac{1}{\xi^2} - \frac{1}{d^2} \right) \xi_T d$$

where $\xi_T$ is the width (along $x$) of the wall. This energy is just equal to the additional energy from the twist $\phi_0 = \pi / 2$ or the bend $\phi_0 = 0$, $T \sim \frac{K_2}{\xi_T^2} \theta^2 \xi_T d$ because $\xi_T \sim \alpha \xi / \theta_\alpha$ and $\theta_\alpha^2 \sim (1 - \xi^2 / d^2)$ [1]. In the presence of a large twist $\delta$ comparable to $\theta$, instead of the two gradient terms $\sim \left( \frac{\partial \theta}{\partial z} \right)^2$ and $\left( \frac{\partial \theta}{\partial x} \right)^2$ in the free energy of the planar solution, one has now four terms $\sim \left( \frac{\partial \delta}{\partial z} \right)^2$ and $\left( \frac{\partial \delta}{\partial x} \right)^2$, which should give equal contributions to $T$. $T$ must now decrease by a factor 2, i.e. closed loop walls in polymeric nematics should be flattened ellipses of axis ratio $\frac{\alpha}{2}$ instead of $\alpha$. 

**Fig. 5.** — Molecular arrangement in the $xz$ section of a mixed splay bend twist wall for $\phi_0 = -\pi/4$. a) unperturbed isotropic wall. b) twist favoured wall. c) splay and bend favoured wall.
We now discuss the optical properties of these twisted walls. When the birefringence $\Delta n$ of the nematic is strong, $(\Delta n . d > \lambda$, wavelength of light) which is the usual case for thermotropics, the twist inside the wall is not visible. We are in the Maughin limit where the light polarization, propagating across the sample, follows adiabatically the director [4]. As the director is anchored on the plates, the output polarization is unaffected. On the other hand, when the birefringence is weak $(\Delta n . d < \lambda)$, one should observe the twist. The antisymmetrical part $\delta_1$, by compensation, gives rise only to a small decrease of the birefringence, probably difficult to observe. The symmetrical part $\delta_2$ gives now, on the average, a local twist of the neutral optical axes, proportional to $\delta_2$, i.e. to $\sin \phi_0 \cos \phi_0$, maximum for $\phi_0 = \frac{\pi}{4} + m \frac{\pi}{2}$. This director rotation around $\mathbf{H}$, inside the wall, explains the recently observed twist of the optical axes in lyotropic nematic walls [3]. Experimentally, this rotation is indeed found maximum for $\phi_0 = \frac{\pi}{4} + m \frac{\pi}{2}$. Its absolute value was not precisely measured, but its order of magnitude is in the $10^\circ$ range. This value is of the order of magnitude of the estimated director rotation. Taking $H \sim 2 H_c$, $\varepsilon_x \sim 1$, $\xi \sim d/2\pi$, $k_i \sim 1$, we find indeed $\delta_1 \sim \delta_2 \sim 0.16 \text{ rad} \sim 10^\circ$. This estimate remains crude, because one can hardly extrapolate a perturbation calculation to $k_i \sim 1$. An exact calculation would necessitate the knowledge of the exact elastic anisotropy of the lyotropic nematic liquid crystal.

In conclusion, we have studied the structure of inversion walls which separate the two symmetrical distorted textures induced by a magnetic field, in a nematic liquid crystal. In a previous work, these walls were described with a planar approximation, where the director was just allowed to bend toward the magnetic field, without rotating around it. We have demonstrated here that the planar approximation is valid only in the isotropic case, where the three curvature elastic constants are equal. In the general anisotropic case, as soon as a twist exists in the planar model, a new director rotation around the field appears inside the walls. The director lines do not remain in a plane. The director rotation around the field favours that curvature distortion which corresponds to the smallest elastic constant. This director « refraction » inside the walls could not be observed in thermotropics, because of their large birefringence. It has been recently observed in weak birefringence nematic lyotropic liquid crystals. It would be interesting to restudy the unexplained tactoidal shell defects observed in PBLG in a magnetic field [6] to check in this case the possible existence of a director refraction.

References