Rigorous analysis of weak boundary-coupling effects in twisted chiral nematic liquid crystals

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General expressions for the threshold and saturation fields are derived analytically for field-controlled twisted chiral nematic layers with weak boundary coupling. The anchoring energy used is the Rapini-Papoular type [J. Phys. (Paris) Colloq. **30**, C4-54 (1969)] in which the azimuthal and the polar anchorings are combined. We can recover the results previously obtained for various limiting cases of the problem, but our results show major differences in detail from other studies in which the azimuthal and polar anchorings are treated as two independent contributions.

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In liquid crystals, surface effects have been studied mainly for nematic liquid crystals (NLC's) [1]. Macroscopically, the surface effects are manifested in the director orientation of the NLC in the bulk. There are two cases: (1) the "strong anchoring" case, in which the director close to the surface takes a fixed mean orientation **e**, which is called the anchoring direction or the "easy" direction as denoted by de Gennes [2]; and (2) the "weak anchoring" case. Practically, in most cases, the surface forces are not strong enough to impose a well-defined director orientation **n**, at the surface. When there are other fields (electric, magnetic, and flow) the director at the interface obviously deviates from the easy direction. To describe a weak anchoring surface for an untwisted NLC sample, Rapini and Papoular [3] (RP) have introduced a simple phenomenological expression for the interfacial energy per unit area for a one-dimensional deformation [3],

$$g_s=\frac{A}{2}\sin^2(\theta^0-\theta_0)\ . \tag{1}$$

Here θ_0 is the tilt angle for the easy direction **e**, and θ^0 is the preferred tilt of the director at the nematic-wall interface. The anchoring strength or anchoring energy proportionality constant A determines the ability of the director to deviate from the easy direction. For a twisted NLC sample the RP energy density must be extended to the more general form [1]

$$g_s=-\frac{A}{2}(\mathbf{n}\cdot\mathbf{e})^2\ , \tag{2}$$

which is a nonlinear combination of the azimuthal and polar angles. On the basis of the RP function, some authors have studied the influence of the bulk orientation of the NLC by an interfacial effect [4–9] and have attempted to measure A [10–13]. However, in [4–9], the unified RP energy form (2) has been written as a linear combination of an azimuthal angle anchoring term $g_\theta=(A_1/2)\sin^2(\theta^0-\theta_0)$ and a polar angle anchoring term $g_\phi=(A_2/2)\sin^2(\phi^0-\phi_0)$. Although such a separation simplifies the mathematical analysis, there is no physical reason to make such a separation. In addition, in Refs. [4–9], the two optimum directions (θ_0,ϕ_0) and $(\theta_0,\phi_0+\pi)$ are inconsistent with the original intention of (2) in that there is only one easy direction at the surface. Since the proposal of (2), the calculation of the field-controlled director orientation in a twisted chiral nematic (TCN) layer with weak anchoring has been an open question for more than 20 years.

In this paper, we give a brief report on our study of the problem. We consider a nematic cell located between the two planes $z=0$ and $z=d$ with mirror symmetry with respect to the middle plane $z=d/2$. The surface tilt angle θ^0 is taken to be the same on both surfaces. The easy direction **e** on the surface of $z=0$ and the director in the z layer may be expressed as

$$\mathbf{e}=(\cos\theta_0,0,\sin\theta_0)\ , \tag{3}$$

$$\mathbf{n}=(\cos\theta\cos\phi,\cos\theta\sin\phi,\sin\theta)\ , \tag{4}$$

respectively, where the polar angle ϕ and tilt angle θ are functions of z. If a magnetic field $\mathbf{H}$ $[=(0,0,H)]$ is applied to the TCN cell, the free energy density in the bulk may be expressed as [2]

$$\begin{aligned}g_b&=\tfrac{1}{2}k_{11}(\nabla\cdot\mathbf{n})^2+\tfrac{1}{2}k_{22}\left[\mathbf{n}\cdot\nabla\times\mathbf{n}+\frac{2\pi}{p_0}\right]^2\\&\quad+\tfrac{1}{2}k_{33}[\mathbf{n}\times(\nabla\times\mathbf{n})]^2-\frac{\Delta\chi}{2}(\mathbf{n}\cdot\mathbf{H})^2\\&=\tfrac{1}{2}[f(\theta)\theta^{(1)2}+h(\theta)\phi^{(1)2}]-\frac{2\pi}{p_0}k_{22}\cos^2\theta\phi^{(1)}\\&\quad+\frac{2\pi^2k_{22}}{p_0^2}-\frac{\Delta\chi}{2}H^2\sin^2\theta\ ,\end{aligned} \tag{5}$$

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where $\theta^{(1)}=d\theta/dz$, $\phi^{(1)}=d\phi/dz$, and

$$f(\theta)=k_{11}\cos^2\theta+k_{33}\sin^2\theta\ , \tag{6}$$

$$h(\theta)=\cos^2(\theta)(k_{22}\cos^2\theta+k_{33}\sin^2\theta)\ . \tag{7}$$

The constants k_{11}, k_{22}, and k_{33} are the splay, twist, and bend elastic constants of the NLC, respectively, p_0 denotes the pitch of the material induced by a chiral dopant, and $\Delta\chi$ is the anisotropy of the diamagnetic susceptibility of the NLC.

The total free energy is the sum of the surface energy [Eq. (2)] and the bulk free energy [the integration of Eq. (5) over the cell volume]. Minimization of the total free energy yields the stable director configuration for any given field. Applying a variational calculation for the two-dimensional problem [14] to the total free energy, we find four equations describing the equilibrium deformation of the director:

$$f(\theta)\theta^{(1)}|_{z=0}=A(\sin\theta_0\sin\theta+\cos\theta_0\cos\theta\cos\phi)\times(\cos\theta_0\sin\theta\cos\phi-\sin\theta_0\cos\theta)\ , \tag{8}$$

$$h(\theta)\phi^{(1)}|_{z=0}=\frac{2\pi k_{22}}{p_0}\cos^2\theta+A(\cos\theta_0\cos\theta\cos\phi+\sin\theta_0\sin\theta)\times\cos\theta_0\sin\phi\cos\theta\ , \tag{9}$$

$$\phi^{(1)}=\frac{1}{h(\theta)}\left[C_1+\frac{2\pi k_{22}}{p_0}\cos^2\theta\right]\ , \tag{10}$$

$$f(\theta)\theta^{(1)2}+\frac{1}{h(\theta)}\left[C_1+\frac{2\pi k_{22}}{p_0}\cos^2\theta\right]^2+\Delta\chi H^2\sin^2\theta=C_2\ , \tag{11}$$

where $\theta^{(2)}=d\theta^{(1)}/dz$, and C_1 and C_2 are two constants of integration. Equations (8) and (9) are the boundary conditions due to the balance of the torque for tilt and twist at $z=0$, respectively. Equations (10) and (11) give the director orientation in the bulk. The surface torque balance equations at $z=d$ are simply equal to the negative of the right-hand side of Eqs. (8) and (9). Essentially, Eqs. (8)–(11) are the basic equations for solving the threshold and the saturation problems analytically. The right-hand side of torque equations (8) and (9) are both functions of θ and ϕ simultaneously. This is entirely different from the corresponding equations obtained in Refs. [4–9], in which one depends only on θ and the other depends only on ϕ. This shows that the challenging problem for the present analysis is to solve the complicated Eqs. (8) and (9).

Under the extreme condition for θ at the midplane of the cell,

$$\theta^{(1)}\left[\frac{d}{2}\right]=0,\quad \theta\left[\frac{d}{2}\right]=\theta_M\ , \tag{12}$$

and the mirror symmetry with respect to $z=d/2$,

$$\phi\left[z=\frac{d}{2}\right]=\tfrac{1}{2}\phi_t\ , \tag{13}$$

integration of Eqs. (8)–(11) gives

$$\frac{d}{2}=\int_{\theta^0}^{\theta_M}N^{1/2}(\theta)d\theta\ , \tag{14}$$

$$\frac{\phi_t}{2}-\phi^0=\int_{\theta^0}^{\theta_M}\frac{N^{1/2}(\theta)}{h(\theta)}\left[C_1+\frac{2\pi k_{22}}{p_0}\cos^2\theta\right]d\theta\ , \tag{15}$$

$$f(\theta^0)N^{-1/2}(\theta^0)=A(\sin\theta_0\sin\theta^0+\cos\theta_0\cos\theta^0\cos\phi^0)\times(\cos\theta_0\sin\theta^0\cos\phi^0-\sin\theta_0\cos\theta^0)\ , \tag{16}$$

$$C_1=A(\cos\theta_0\cos\theta^0\cos\phi^0+\sin\theta_0\sin\theta^0)\cos\theta_0\sin\phi^0\cos\theta^0\ , \tag{17}$$

where $N(\theta)$ is

$$N(\theta)=f(\theta)\left[\Delta\chi H^2(\sin^2\theta_M-\sin^2\theta)+\frac{1}{h(\theta_M)}\left[C_1+\frac{2\pi k_{22}}{p_0}\cos^2\theta_M\right]^2-\frac{1}{h(\theta)}\left[C_1+\frac{2\pi k_{22}}{p_0}\cos^2\theta\right]^2\right]^{-1}\ . \tag{18}$$

It is clear now that for given values of ϕ_t, θ_0, and H, the values of ϕ^0, θ^0, and θ_M can be determined completely from Eqs. (14)–(17).

To derive the threshold magnetic field H_F of the Fréedericksz transition [2], we need to suppose $\theta_0=0$ and $\theta^0=\theta_M=0$ for $H<H_F$ and $\theta_M\to 0$ when $H\to H_F$. With these boundary conditions the limiting integrals in Eqs. (14) and (15) can be solved analytically to give the relationship between the threshold field and the anchoring energy. With a similar process, by taking the limit $\theta_0\to 0$ and $\theta_M\to\pi/2$, we can derive analytically the saturation field H_S, above which the LC layer becomes completely homeotropic from Eqs. (14)–(17). However, in the actual calculations there are some mathematical difficulties to overcome. This is also the case for the previous studies (see the controversy between the authors in Refs. [7–9] and Ref. [10]). The details of the calculation will be given in another paper [14]; here we give only the results.

The threshold magnetic field H_F is

$$H_F=\left[\frac{d^2R+(\phi_t-2\phi^0)[(k_{33}-2k_{22})(\phi_t-2\phi^0)+4\pi dk_{22}/p_0]}{\Delta\chi d^2}\right]^{1/2}\ , \tag{19}$$

where R and ϕ^0 are the solutions of the transcendental equations

$$A\cos^2\phi^0=\sqrt{k_{11}R}\tan\left[\frac{d}{2}\left[\frac{R}{k_{11}}\right]^{1/2}\right], \tag{20}$$

$$\phi_t-2\phi^0-\frac{2\pi d}{p_0}=\frac{Ad}{k_{22}}\sin\phi^0\cos\phi^0 . \tag{21}$$

The saturation field H_S is

$$\frac{Z}{A}=\tanh\left[\frac{Zd}{2k_{33}}\right]\left[1+\frac{\cos^2[\phi_t/2-\pi dk_{22}/(p_0k_{33})]}{\sinh^2[Zd/(2k_{33})]}\right], \tag{22}$$

where

$$Z^2\equiv\Delta\chi H_S^2k_{33}-\left[\frac{2\pi k_{22}}{p_0}\right]^2 . \tag{23}$$

In order to compare our results with previous studies, we consider Eqs. (19)–(23) for the threshold and the saturation properties. It is convenient to introduce the dimensionless coupling parameter

$$\lambda=\frac{\pi k_{22}}{Ad}, \tag{24}$$

and also to use the reduced magnetic field $u'=H/H_c$, where

$$H_c=\frac{\pi}{d}\left[\frac{k_{11}}{\Delta\chi}\right]^{1/2} \tag{25}$$

is the threshold magnetic field for an untwisted nematic slab ($\phi_t=0$) with rigid boundary coupling ($\lambda=0$, i.e., $A\rightarrow\infty$).

For this limit, Eq. (19) reduces to

$$H_Fd=\left[\frac{k_{11}\pi^2+(k_{33}-2k_{22})\phi_t^2+4\pi dk_{22}\phi_t/p_0}{\Delta\chi}\right]^{1/2} . \tag{26}$$

This recovers the result obtained by Becker, Nehring, and Scheffer [10] under the assumption of strong azimuthal anchoring and the consideration of polar anchoring only. This is also the result reported by Hirning *et al.* [11] in treating the tilt anchoring and twist anchoring independently and taking both the anchoring strengths as infinite. In the case of a twisted nematic layer (TN) with strong anchoring and $d/p_0=0$, Eq. (26) reduces to

$$H_Fd=\left[\frac{k_{11}\pi^2+(k_{33}-2k_{22})\phi_t^2}{\Delta\chi}\right]^{1/2} . \tag{27}$$

This is the same result as that derived by Leslie [4] as well as Schadt and Helfrich [5]. Furthermore, for the homogeneous nematic slab with weak anchoring, $d/p_0=0$ and $\phi_t=0$, Eqs. (19)–(21) lead to

$$A=\sqrt{k_{11}\Delta\chi}H_F\tan\left[\frac{d}{2}\left[\frac{\Delta\chi}{k_{11}}\right]^{1/2}H_c\right], \tag{28}$$

which is the same result as that obtained by Rapini and Papoular [3]. These agreements for various limiting conditions offer a good check on the present general theory. However, in order to demonstrate the difference between the present theory and previous studies, it is necessary to consider other special cases.

For an isotropic surface ($\lambda\rightarrow\infty$, $A=0$), in other words, where there is no anchoring energy, we have

$$\Delta\chi H_F^2=k_{33}\left[\frac{2\pi}{p_0}\right]^2 . \tag{29}$$

This provides the reasonable result that the Fréedericksz transition does not exist for a nematic slab ($p_0\rightarrow\infty$) coupling with an isotropic surface. We have also calculated numerically the λ dependencies of the threshold and the saturation fields for a 90° twisted layer with the same material parameters as those used in [10], i.e., $k_{33}/k_{11}=1.5$, $k_{22}/k_{11}=0.6$, and $d/p_0=0$. The result is shown in Fig. 1, where the solid lines give the results for the present calculations and the dashed lines are those reported in [10]. From Fig. 1 it is clear that the results of the previous studies may give the correct threshold fields only in the limiting case of $A\rightarrow\infty$.

To discuss the saturation properties, as defined in Ref. [10], we introduce the parameter

$$Y\equiv\left[u''^2\left[\frac{k_{11}}{k_{33}}\right]-\left[\frac{2k_{22}d}{k_{33}p_0}\right]^2\right]^{1/2}, \tag{30}$$

where the reduced saturation field u'' is defined as $u''=H_S/H_c$. Using Eqs. (24), (30), and $R'\equiv\phi_t/2+\pi dk_{22}/k_{33}p_0$, with a lengthy calculation, we find that Eq. (22) reduces to

$$\lambda\left[\frac{k_{33}}{k_{11}}\right]=\frac{\tanh(\pi Y/2)}{Y}\left[1+\frac{\cos^2R'}{\sinh^2(\pi Y/2)}\right], \tag{31}$$

and that

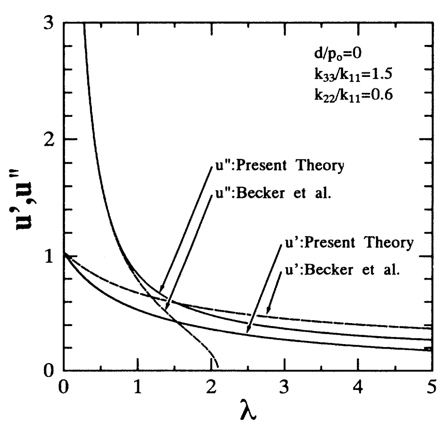

FIG. 1. λ dependence of the reduced threshold (u') and saturation (u'') fields of a 90° twisted slab. Solid lines show the present theoretical results and dashed lines show those reported in Ref. [10]. Material parameters used in the computation are $k_{33}/k_{11}=1.5$, $k_{22}/k_{11}=0.6$, and $d/p_0=0$.

$$\tan\phi^0 = \frac{\frac{1}{2}|\sin 2R'|}{\cos^2 R' + \sinh^2(\pi Y/2)} . \tag{32}$$

For the TCNLC of very short pitch, where $[2k_{22}d/(k_{33}p_0)]^2 - u''^2 k_{11}/k_{33} > 0$, Eqs. (31) and (32) can be rewritten as

$$\lambda\left[\frac{k_{33}}{k_{11}}\right] = \frac{\tan(\pi Y'/2)}{Y'}\left[1 - \frac{\cos^2 R'}{\sin^2(\pi Y'/2)}\right] , \tag{33}$$

$$\tan\phi^0 = \frac{\frac{1}{2}|\sin 2R'|}{\cos^2 R' - \sin^2(\pi Y'/2)} , \tag{34}$$

respectively, where

$$Y' \equiv Y/i' = \sqrt{[2k_{22}d/(k_{33}p_0)]^2 - u''^2 k_{11}/k_{33}} .$$

The relationship between λ and u'' given by Eqs. (30)–(32) has been calculated numerically with the same values of the physical parameters given previously. The result is shown in Fig. 1. One notices that, in the limit of $Y \to \infty$, Eq. (31) leads to nearly the same result as reported in Refs. [8] and [10]. However, in the limit of $Y \to 0$, we have

$$u'' \to 2\left[\frac{k_{22}^2}{k_{11}k_{33}}\right]^{1/2} \frac{d}{|p_0|} . \tag{35}$$

Equation (35) shows that, for a NLC slab, $u'' \to 0$ because $|p_0| \to \infty$ (see the solid line shown in Fig. 1). This differs from the result in which the saturation voltage vanished at some value of λ_0 (see the dashed line shown in Fig. 1) as reported in Refs. [8] and [10]. Therefore, the present theory is the only one which leads to the natural conclusion that decreasing the anchoring strength reduces the saturation field and that, in the limit, free anchoring (i.e., $A = 0$) gives a zero saturation field.

In summary, in keeping with the model of Rapini and Papoular, we have made a rigorous analysis of weak boundary coupling effects for nematic liquid crystals. Instead of using two different anchoring strengths, polar and azimuthal, we need only one unified anchoring strength A in the derivation of the threshold field and the saturation field. Calculations of the director configuration for NLC cells with different surface anchoring and external fields becomes much easier. This may be significant in the development of LC display devices.

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