Director deformation of a twisted chiral nematic liquid crystal cell with weak anchoring boundaries

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On the basis of a generalization of the Rapini-Papoular expression [J. Phys. (Paris) Colloq. **30**, C4-54 (1969)] for the anchoring energy, the rigorous expressions for the threshold and saturation fields are derived analytically, in detail, for a field-controlled twisted chiral nematic slab with weak boundary coupling. The surface anchoring energy of the Rapini-Papoular type for a twisted nematic slab should be generally expressed as the interfacial energy per unit area for a two-dimensional deformation which is a nonlinear combination of the azimuthal and polar angles. Applying a variational calculation method for the two-dimensional problem to the total free energy, that is the sum of the bulk energy and the surface energy, we derive general torque balance equations which describe the equilibrium deformation of the director.

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I. INTRODUCTION

In liquid crystals (LCs), surface effects have been studied mainly for nematic phases [1]. The structure of liquid crystalline phases in close proximity to an interface is different than that in the bulk, and this "surface structure" changes the boundary conditions and influences the behavior of the liquid crystal in the bulk. The nematic phase is especially sensitive to external agents, in particular, to surface forces [2]. Macroscopically, the surface effects are manifested in the director orientation in the bulk. There are two cases of particular interest: first, the strong anchoring case, in which the director near the surface adopts a fixed orientation $\vec{e}$, which is called the anchoring direction or the "easy" direction as denoted by de Gennes [3]; second, the weak anchoring case where the surface forces are not strong enough to impose a well-defined director orientation $\vec{n}$ at the surface; this is the situation for the majority of systems. 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 nematic liquid crystal (NLC) sample, Rapini and Papoular (RP) have introduced a simple phenomenological expression for the interfacial energy per unit area for a one-dimensional deformation [4],

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

Here θ_0 is the angle between the easy direction $\vec{e}$ and the layer parallel while θ^0 is the orientation of the director at the nematic-wall interface. The anchoring strength parameter A determines the ability of the director to deviate from the easy direction. For a twisted nematic (TN) LC sample the RP anisotropic energy density for the director orientation must be extended to the more general form [1]

$$g_s = -\frac{A}{2}(\vec{n}\cdot\vec{e})^2 \ , \tag{1}$$

which is a nonlinear combination of the azimuthal and polar angles. Using the RP function, some authors have studied the influence of the interfacial effect [5–12] on the bulk orientation of NLCs and in this way attempted to measure A [13–16]. However, in Refs. [5–12], the unified RP energy form Eq. (1) has been written as a linear combination of a polar angle anchoring term $g_\theta=(A_1/2)\sin^2(\theta^0-\theta_0)$ and an azimuthal 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 a separation. In addition, from a mathematical point of view, this linear combination is not invariant with respect to rotation of the axis system; therefore, the two optimum directions (θ_0,ϕ_0) and $(\theta_0,\phi_0+\pi)$ in Refs. [5–12] are inconsistent with the original intention of Eq. (1) that there is only one easy axis at the surface. Although the expression for the surface energy can be predicted for other shapes of the surface potential, such as the elliptic type, Legendre expansion, and so on [2], it cannot be expressed as a sum of independent terms $g_s(\theta)$ and $g_s(\phi)$ for the polar and azimuthal angles, but is expressed by the two-dimensional function $g_s(\theta,\phi)$. Since the proposal of Eq. (1), the calculation of the field-controlled director orientation in a twisted chiral nematic (TCN) slab with weak anchoring has been an open question for more than 20 years. Recently, on the basis of a general RP expression for the anchoring energy, Eq. (1),

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two of us have reported briefly our results for the general expressions for the threshold and saturation fields [17]. This follows from a rigorous treatment on the variational problem with special variable boundaries. The method is significant both for fundamental and the applied research in the LC field.

In this paper, we describe the variational method for the two-dimensional variation problem on the energy including the bulk and surface energy, and give the detailed derivation of our results reported in [17]. In Sec. II the general torque equations are derived using a technique based on the special functions. By using the general torque equations the basic equations needed to calculate the threshold field are derived in Sec. III. With a limiting calculation for the equations obtained the result of the threshold field is shown in Sec. IV. Following a similar procedure to that in Sec. IV, we show the derivation of the saturation field in Sec. V. Finally, Sec. VI contains our conclusions.

II. GENERAL TORQUE BALANCE EQUATIONS

We first give the derivation of the general torque balance equation. We consider a nematic cell located between the two planes located at $X_3=0$ and $X_3=l$, as illustrated schematically in Fig. 1. The easy directions at the top and bottom substrate surfaces are denoted by the unit vectors $\vec{e}^{\,+}$ and $\vec{e}^{\,-}$, respectively. Using Eq. (1), the corresponding surface energy densities are given by

$$g_s^+=-\frac{A^+}{2}(\vec{n}\cdot\vec{e}^{\,+})^2 \quad (X_3=l)\ , \tag{2}$$

$$g_s^-=-\frac{A^-}{2}(\vec{n}\cdot\vec{e}^{\,-})^2 \quad (X_3=0)\ , \tag{3}$$

where A^+ and A^- are the anchoring strength at the top and bottom substrate surfaces, respectively. The total free energy density in the bulk may be expressed as [3]

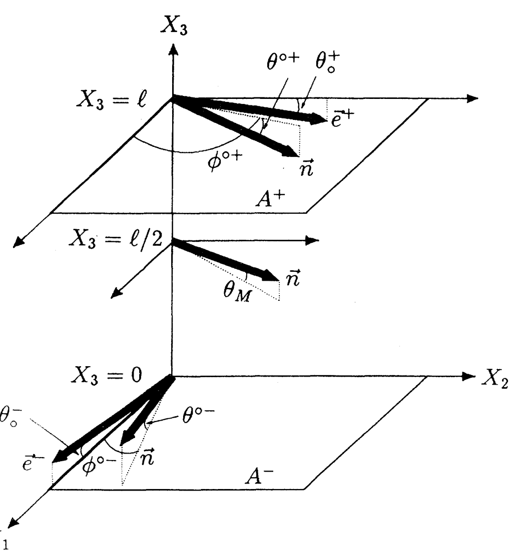

FIG. 1. The geometry of the twisted chiral nematic cell located between the two planes $X_3=0$ and $X_3=l$.

$$g_b=\frac{1}{2}\left[k_{11}(\vec{\nabla}\cdot\vec{n})^2+k_{22}\left[\vec{n}\cdot\vec{\nabla}\times\vec{n}+\frac{2\pi}{p_0}\right]^2 +k_{33}[\vec{n}\times(\vec{\nabla}\times\vec{n})]^2\right]+g_f(\vec{n})\ , \tag{4}$$

where 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 $g_f(\vec{n})$ represents the interaction energy between the director and an external field which depends on $\vec{n}$ but not on $\nabla\vec{n}$. The total free energy F is the sum of the bulk energy and the surface free energy

$$F=\int g_b dv+\int g_s^- ds^- +\int g_s^+ ds^+\ , \tag{5}$$

where dv is the volume element of the bulk and ds is the surface area element. Minimization of the total free energy yields the stable director configuration. The equilibrium condition is then determined by the variation equation $\delta F=0$. For many years the determination of the equilibrium condition for a weak anchoring coupling has been an unsolved problem because of the complicated form of Eq. (5). No solution for a variational problem under boundary conditions including integral forms can be found in literature and books on the variational problem. In order to change Eq. (5) into a form which can be solved by the normal variational approach, we introduce two special functions, the unit step function

$$\mu(X_3)=\begin{cases}1 & (X_3\geq 0)\\ 0 & (X_3<0)\ ,\end{cases}$$

and the Dirac function

$$\delta(X_3)=\begin{cases}\infty & (X_3=0)\\ 0 & (X_3\neq 0)\ ,\end{cases}$$

$$\int_{-\infty}^{\infty}\delta(X_3)dX_3=1 \quad \left[\delta(X_3)=\frac{d\mu(X_3)}{dX_3}\right]\ .$$

Then Eq. (5) reduces to the unified integral

$$F=\int_{-\infty}^{\infty} g^* dv=\int_{-\infty}^{\infty}(g_b^*+g_s^*)dv\ , \tag{6}$$

where g_b^* and g_s^* are defined by

$$g_b^*=\left[g_b+\frac{\nu}{2}(1-\vec{n}\cdot\vec{n})\right][\mu(X_3)-\mu(X_3-l)]\ , \tag{7}$$

$$g_s^*=-\frac{1}{2}\left[A^-(\vec{n}\cdot\vec{e}^{\,-})^2+\frac{\zeta^-}{2}(1-\vec{n}\cdot\vec{n})\right]\delta(X_3) -\frac{1}{2}\left[A^+(\vec{n}\cdot\vec{e}^{\,+})^2+\frac{\zeta^+}{2}(1-\vec{n}\cdot\vec{n})\right]\delta(X_3-l)\ . \tag{8}$$

Here ν, ζ^+, and ζ^- are Lagrange multipliers to be determined by the constraint $\vec{n}\cdot\vec{n}=1$ in the bulk and at the substrate surfaces. In previous work [10–12] on the same problem, the Dirac function was used to unify the integral form of F; however, the unit step function has not been included because it was not necessary for the problems being addressed. On the other hand, the normal Euler-Lagrange approach used to minimize F is

$$\frac{\partial g^*}{\partial n_i}-\frac{\partial}{\partial X_j}\frac{\partial g^*}{\partial n_{i,}}=0 \quad (i,j=1,2,3)\ , \tag{9}$$

where $n_{i,j}=\partial n_i/\partial X_j$. Substitution of Eqs. (7) and (8) into Eq. (9) leads to

$$\left[\frac{\partial g_b}{\partial n_i}-\frac{\partial}{\partial X_j}\left[\frac{\partial g_b}{\partial n_{i,j}}\right]-\nu n_i\right][\mu(X_3)-\mu(X_3-l)] + \left[\frac{\partial g_b}{\partial n_{i,3}}-A^+(\vec{n}\cdot\vec{e}^{\,+})e_i^+-\zeta^+n_i\right]\delta(X_3-l) + \left[-\frac{\partial g_b}{\partial n_{i,3}}-A^-(\vec{n}\cdot\vec{e}^{\,-})e_i^--\zeta^-n_i\right]\delta(X_3)=0\ . \tag{10}$$

This leads to the following equilibrium conditions:

$$\frac{\partial g_b}{\partial n_i}-\frac{\partial}{\partial X_j}\left[\frac{\partial g_b}{\partial n_{i,j}}\right]=\nu n_i \quad (0\le X_3\le l)\ , \tag{11}$$

$$\frac{\partial g_b}{\partial n_{i,3}}=A^+(\vec{n}\cdot\vec{e}^{\,+})e_i^++\zeta^+n_i \quad (X_3=l)\ , \tag{12}$$

$$\frac{\partial g_b}{\partial n_{i,3}}=-A^-(\vec{n}\cdot\vec{e}^{\,-})e_i^--\zeta^-n_i \quad (X_3=0)\ . \tag{13}$$

Equation (11) comes from the coefficient of the function $[\mu(X_3)-\mu(X_3-l)]$ of Eq. (10), and Eqs. (12) and (13) come from the coefficients of $\delta(X_3)$ and $\delta(X_3-l)$, respectively. Equation (11) is the torque balance equation in the bulk. General surface torque balance equations at the top and the bottom surfaces are given by Eqs. (12) and (13), respectively. Equations (11)–(13) and the constraint $\vec{n}\cdot\vec{n}=1$ determine the solutions for $\vec{n}$, ν, and $\zeta^{\pm}$ completely. The problem for a weak anchoring surface using the RP function can now be solved generally.

III. BASIC EQUATIONS FOR THRESHOLD PROBLEMS

In the case of strong anchoring, the Fréedericksz transition gives us a simple method to determine the physical parameters for NLCs by measuring the deformation induced by an external magnetic or electric field. To understand the generalized torque balance equations derived in Eqs. (11)–(13) we may consider the threshold problems of the Fréedericksz transition and the saturation transition in the case of weak anchoring.

First, based on the general torque balance equations, we derive the basic equations necessary to deal with threshold problems. We consider simply a TCN cell located between the two planes $X_3=0$ and $X_3=l$ with a symmetry with respect to the middle plane $X_3=l/2$. Then for any ϕ_t the symmetry, $\phi(X_3)=\phi_t-\phi(l-X_3)$ and $\theta(X_3)=\theta(l-X_3)$ in a range of $0<X_3<l/2$, obtains. The surface tilt angles are taken to be the same at both surfaces, $\theta^0=\theta(0)=\theta(l)$ and $A=A^+=A^-$. The easy direction $\vec{e}$ at $X_3=0$ and the direction at the X_3 layer may be expressed as

$$\vec{e}=(\cos\theta_0,0,\sin\theta_0)\ , \tag{14}$$

$$\vec{n}=(\cos\theta\cos\phi,\cos\theta\sin\phi,\sin\theta)\ , \tag{15}$$

where the azimuthal angle ϕ and the tilt angle θ are functions of X_3. With Eqs. (4) and (15), $\partial g_b/\partial n_{i,3}$ is given by

$$\frac{\partial g_b}{\partial n_{i,3}}=\begin{cases} k_{33}\sin^3\theta\cos\phi\theta^{(1)}-(k_{22}\cos^2\theta+k_{33}\sin^2\theta)\cos\theta\sin\phi\phi^{(1)}-k_2\cos\theta\sin\phi & (i=1)\\ k_{33}\sin^3\theta\sin\phi\theta^{(1)}+(k_{22}\cos^2\theta+k_{33}\sin^2\theta)\cos\theta\cos\phi\phi^{(1)}+k_2\cos\theta\cos\phi & (i=2)\\ -(k_{11}+k_{33}\sin^2\theta)\cos\theta\theta^{(1)} & (i=3)\ , \end{cases} \tag{16}$$

where $\theta^{(1)}=d\theta/dX_3$, $\phi^{(1)}=d\phi/dX_3$, and $k_2=-2\pi k_{22}/p_0$, where positive and negative signs of k_2 correspond to left- and right-handed helixes, respectively. Substitution of Eqs. (14) and (15) into Eq. (13) leads to

$$\frac{\partial g_b}{\partial n_{i,3}}=-A(\vec{n}\cdot\vec{e})e_i-\zeta n_i = \begin{cases} -A(\cos\theta_0\cos\theta\cos\phi+\sin\theta_0\sin\theta)\cos\theta_0-\zeta\cos\theta\cos\phi & (i=1)\\ -\zeta\cos\theta\sin\phi & (i=2)\\ -A(\cos\theta_0\cos\theta\cos\phi+\sin\theta_0\sin\theta)\sin\theta_0-\zeta\sin\theta & (i=3)\ . \end{cases} \tag{17}$$

Elimination of ζ with Eqs. (16) and (17) gives the surface torque balance equations at $X_3=0$ as

$$f(\theta)\theta^{(1)}|_{X_3=0}=A(\sin\theta_0\sin\theta+\cos\theta_0\cos\theta\cos\phi)(\cos\theta_0\sin\theta\cos\phi-\sin\theta_0\cos\theta)\ , \tag{18}$$

$$h(\theta)\phi^{(1)}|_{X_3=0}=-k_2\cos^2\theta+A(\cos\theta_0\cos\theta\cos\phi+\sin\theta_0\sin\theta)\cos\theta_0\sin\phi\cos\theta\ , \tag{19}$$

where

$$f(\theta)=k_{11}\cos^2\theta+k_{33}\sin^2\theta\ ,\qquad h(\theta)=\cos^2\theta(k_{22}\cos^2\theta+k_{33}\sin^2\theta)\ . \tag{20}$$

The surface torque balance equations at $X_3=l$ can be obtained simply by reversing the signs of the right-hand sides of Eqs. (18) and (19).

When a magnetic field $\vec{B}=(0,0,B)$ is applied to the TCN cell, i.e., $g_f=-(\Delta\chi/2)(\vec{n}\cdot\vec{B})^2$ in Eq. (4), with Eqs. (4) and (15) the free energy density in the bulk may be expressed as

$$g_b=\frac{1}{2}[f(\theta)\theta^{(1)2}+h(\theta)\phi^{(1)2}]+k_2\cos^2\theta\phi^{(1)}+\frac{k_2^2}{2k_{22}}-\frac{\Delta\chi}{2}B^2\sin^2\theta\ , \quad (21)$$

where $\Delta\chi$ is the anisotropy of the diamagnetic susceptibility of the NLC. Minimization of the free energy in the bulk yields the stable director configuration for any given field. Applying variational calculus to Eq. (21), we find that the bulk equations (11) lead to

$$f(\theta)\theta^{(2)}+\tfrac{1}{2}f_\theta\theta^{(1)2}-\tfrac{1}{2}h_\theta\phi^{(1)2}+2k_2\sin\theta\cos\theta\phi^{(1)}+\Delta\chi B^2\sin\theta\cos\theta=0\ , \quad (22)$$

$$\phi^{(1)}=\frac{1}{h(\theta)}(C_1-k_2\cos^2\theta)\ , \quad (23)$$

whre C_1 is a constant of integration, $f_\theta=df/d\theta$, $h_\theta=dh/d\theta$, and $\theta^{(2)}=d\theta^{(1)}/dX_3$. Subsitution of Eq. (23) into Eq. (22) leads to the torque balance equation in the bulk,

$$f(\theta)\theta^{(1)2}+\frac{1}{h(\theta)}(C_1-k_2\cos^2\theta)^2+\Delta\chi B^2\sin^2\theta=C_2\ , \quad (24)$$

where C_2 is a constant of integration.

Applying a variational calculation to the total free energy for the two-dimensional problem described in the preceding section, we find four equations describing the equilibrium director deformtion. Equations (18) and (19) are the boundary conditions due to the balance of the torque for tilt and twist at $X_3=0$, respectively. Equations (23) and (24) give the director orientation in the bulk. Essentially, Eqs. (18), (19), (23), and (24) are the basic equations for solving the threshold and the saturation problems analytically. The right-hand side of the torque equations (18) and (19) are both functions of θ and ϕ, simultaneously. This is entirely different from the corresponding equations obtained in Refs. [5–10] in which one depends only on θ and the other only on ϕ. This shows that the challenging problem for the present analysis is to solve the complicated equations (18) and (19).

Further calculation of Eqs. (18), (19), (23), and (24) may give us more useful forms to consider the threshold problems. Substitution of Eq. (23) into Eq. (19) leads to

$$C_1=A(\cos\theta_0\cos\theta^0\cos\phi^0+\sin\theta_0\sin\theta^0)\cos\theta_0\cos\theta^0\sin\phi^0\ , \quad (25)$$

where $\theta^0=\theta(X_3=0)$ and $\phi^0=\phi(X_3=0)$. Let us consider the extreme condition for θ at the midplane of the cell,

$$\left.\frac{d\theta}{dX_3}\right|_{x_3=l/2}=0\ ,\quad \theta\left[\frac{l}{2}\right]=\theta_M\ . \quad (26)$$

Substitution of Eq. (26) into Eq. (24) leads to

$$C_2=\frac{1}{h(\theta_M)}(C_1-k_2\cos^2\theta_M)^2+\Delta\chi B^2\sin^2\theta_M\ . \quad (27)$$

Substituting Eq. (27) into Eq. (24), we obtain

$$\theta^{(1)}=N^{-1/2}(\theta)\ , \quad (28)$$

where $N(\theta)$ is defined by

$$N(\theta)=f(\theta)\left[\Delta\chi B^2(\sin^2\theta_M-\sin^2\theta)+\frac{1}{h(\theta_M)}(C_1-k_2\cos^2\theta_M)^2-\frac{1}{h(\theta)}(C_1-k_2\cos^2\theta)^2\right]^{-1}\ .$$

With Eq. (26) the integration of Eq. (28) changes to

$$\frac{l}{2}=\int_{\theta^0}^{\theta_M}N^{1/2}(\theta)d\theta\ . \quad (29)$$

On the other hand, Eqs. (23) and (28) lead to

$$d\phi=\frac{N^{1/2}(\theta)}{h(\theta)}(C_1-k_2\cos^2\theta)d\theta\ . \quad (30)$$

If ϕ_t is the angle of twist from $\phi(X_3=0)$ to $\phi(X_3=l)$, the symmetry with respect to $X_3=l/2$ gives us the condition

$$\phi\left[X_3=\frac{l}{2}\right]=\frac{1}{2}\phi_t\ .$$

Integration of Eq. (30) then leads to

$$\frac{\phi_t}{2}-\phi^0=\int_{\theta^0}^{\theta_M}\frac{N^{1/2}(\theta)}{h(\theta)}(C_1-k_2\cos^2\theta)d\theta\ . \quad (31)$$

Substitution of Eq. (28) into Eq. (18) gives

$$f(\theta^0)N^{-1/2}(\theta^0)=A(\sin\theta_0\sin\theta^0+\cos\theta_0\cos\theta^0\cos\phi^0)\times(\cos\theta_0\sin\theta^0\cos\phi^0-\sin\theta_0\cos\theta^0)\ . \quad (32)$$

Now for given values of ϕ_t, θ_0, and B, it is clear that the values of ϕ^0, θ^0, and θ_M can be determined completely from the basic equations (25), (29), (31), and (32). Once they are known, by using Eqs. (28) and (30), we can obtain the director deformation in the bulk, $\theta(X_3)$ and $\phi(X_3)$.

IV. FRÉEDERICKSZ TRANSITION

To derive the threshold magnetic field B_F of the Fréedericksz transition, we suppose that $\theta_0=0$ and $\theta^0=\theta_M=0$ for $B<B_F$ and $\theta_M \to 0$ when $B \to B_F$. With these boundary conditions the limiting integrals in Eqs. (29) and (31) can be solved analytically to give the relationship between the threshold field and the anchoring energy. We introduce a new variable α under the condition of $\theta \le \theta_M$ such that

$$\sin\theta=\sin\theta_M \sin\alpha \quad (\sin\theta^0=\sin\theta_M \sin\alpha^0) ;$$

Eq. (29) then becomes

$$\frac{l}{2}=\int_{\alpha^0}^{\pi/2}\left[\frac{k_{11}(1+\eta\sin^2\theta_M\sin^2\alpha)}{\Delta\chi B^2+S}\right]^{1/2} \times\frac{d\alpha}{\sqrt{1-\sin^2\theta_M\sin^2\alpha}} , \tag{33}$$

where

$$S=\frac{1}{h(\theta_M)h(\theta)}\{\psi(C_1-k_2)^2+2k_2(C_1-k_2) \times[h(\theta_M)+\psi\sin^2\theta_M] +k_2^2[h(\theta_M)(\sin^2\theta_M+\sin^2\theta) +\psi\sin^4\theta_M]\} ,$$

$$\psi=[2k_{22}-k_{33}+(k_{33}-k_{22})(\sin^2\theta_M+\sin^2\theta)] ,$$

$$\eta=\frac{k_{33}-k_{11}}{k_{11}} .$$

Taking the limit $\theta_M \to 0$ at $B=B_F$, we have $\theta \to 0$, $h(\theta) \to k_{22}$, $\psi \to \psi_0=2k_{22}-k_{33}$, and Eq. (25) reduces to

$$C_1=A\sin\phi^0\cos\phi^0 . \tag{34}$$

Then the integration of Eq. (33) can be performed analytically to give

$$\frac{l}{2}=\int_{\alpha^0}^{\pi/2}\left[\frac{k_{11}}{\Delta\chi B_F^2+k_{22}^{-2}[\psi_0(C_1-k_2)^2+2k_2k_{22}(C_1-k_2)]}\right]^{1/2} d\alpha = \left[\frac{\pi}{2}-\alpha_0\right]\left[\frac{k_{11}}{\Delta\chi B_F^2+k_{22}^{-2}[\psi_0(C_1-k_2)^2+2k_2k_{22}(C_1-k_2)]}\right]^{1/2} . \tag{35}$$

With a similar process, Eq. (31) can be solved analytically and gives

$$\frac{\phi_t}{2}-\phi^0=\left[\frac{\pi}{2}-\alpha_0\right]\left[\frac{C_1-k_2}{k_{22}}\right]\left[\frac{k_{11}}{\Delta\chi B_F^2+k_{22}^{-2}[\psi_0(C_1-k_2)^2+2k_2k_{22}(C_1-k_2)]}\right]^{1/2} . \tag{36}$$

The ratio of Eq. (36)/Eq. (35) leads to the relation

$$C_1-k_2=\frac{k_{22}}{l}(\phi_t-2\phi^0) . \tag{37}$$

Equations (34) and (37) then lead to the important relationship between A and ϕ^0, namely,

$$\phi_t-2\phi^0-\frac{2\pi l}{p_0}=\frac{Al}{k_{22}}\sin\phi^0\cos\phi^0 . \tag{38}$$

Equation (38) may give us the simplest way to evaluate the anchoring strength. In other words, the anchoring energy can be calculated from the measurment of ϕ^0 as a zero-field technique.

Substitution of Eq. (37) into Eq. (35) leads to

$$\cot\alpha^0=\tan\left[\frac{l}{2}\left[\frac{\Delta\chi B_F^2+\psi_0(\phi_t-2\phi^0)^2/l^2+2k_2(\phi_t-2\phi^0)/l}{k_{11}}\right]^{1/2}\right] . \tag{39}$$

Equation (32) at $B=B_F$ changes to

$$A\cos^2\phi^0=\sqrt{k_{11}}\left[\Delta\chi B_F^2+\frac{\psi_0(\phi_t-2\phi^0)^2}{l^2}-\frac{4\pi k_{22}(\phi_t-2\phi^0)}{lp_0}\right]^{1/2}\cot\alpha^0 . \tag{40}$$

Elimination of $\cot\alpha^0$ from Eqs. (39) and (40) gives

$$A\cos^2\phi^0=\sqrt{k_{11}R}\,\tan\left[\frac{l}{2}\left[\frac{R}{k_{11}}\right]^{1/2}\right] , \tag{41}$$

where

$$R=\Delta\chi B_F^2+\frac{(2k_{22}-k_{33})(\phi_t-2\phi^0)^2}{l^2}-\frac{4\pi k_{22}(\phi_t-2\phi^0)}{lp_0} . \tag{42}$$

With Eq. (42), the threshold magnetic field B_F is given by

$$B_F=\left[\frac{l^2R+(\phi_t-2\phi^0)[(k_{33}-2k_{22})(\phi_t-2\phi^0)+4\pi l k_{22}/p_0]}{\Delta\chi l^2}\right]^{1/2}. \tag{43}$$

In Eq. (43), R and ϕ^0 are the solutions of the transcendental equations (38) and (41).

In order to compare our results with previous studies, we consider Eqs. (38), (41), and (43) for the threshold properties. It is convenient to introduce the dimensionless parameter

$$\lambda=\frac{\pi k_{22}}{Al}, \tag{44}$$

and also to use the reduced magnetic field $u'=B/B_c$, where

$$B_c=\frac{\pi}{l}\sqrt{k_{11}/\Delta\chi} \tag{45}$$

is the threshold magnetic field for an untwisted nematic slab ($\phi_t=0$) with rigid boundary coupling ($\lambda=0$, i.e., $A\rightarrow\infty$). In this limiting case of $A\rightarrow\infty$ ($\phi^0\rightarrow 0$ [see Eq. (38)] and $\frac{1}{2}\sqrt{l^2R/k_{11}}\rightarrow\pi/2$ [see Eq. (41)]), Eq. (43) reduces to

$$B_F l=\left[\frac{k_{11}\pi^2+(k_{33}-2k_{22})\phi_t^2+4\pi l k_{22}\phi_t/p_0}{\Delta\chi}\right]^{1/2}. \tag{46}$$

This recovers the result obtained by Becker *et al.* [11] under the assumption of strong azimuthal anchoring and the consideration of polar anchoring only. This is also the result reported by Hirning *et al.* [12] in treating the tilt anchoring and twist anchoring independently and taking both anchoring strengths as infinite. In the case of a twisted nematic cell with strong anchoring and $p_0\rightarrow\infty$, Eq. (46) reduces to

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

This is the same result as that derived by Leslie [5] as well as by Schadt and Helfrich [6]. Furthermore, for the homogeneous nematic (HN) slab with weak anchoring, $l/p_0=0$ and $\phi_t=0$, Eqs. (38), (41), and (43) lead to

$$A=\sqrt{k_{11}\Delta\chi}B_F\tan\left[\frac{l}{2}\sqrt{\Delta\chi/k_{11}}B_F\right],$$

which is the same result as that obtained by Rapini and Papoular [4]. The agreements for these various limiting conditions provide a good check on the present general theory. However, in order to demonstrate the differences 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 there is no anchoring energy for the director orientation, we obtain from Eqs. (38), (41), and (43),

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

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 now discuss our present results in comparison with previous results by using numerical calculations. Figure 2, in which we show the present results and those reported in Ref. [11], shows the λ dependence of the threshold fields for a HN cell ($\phi_t=0$, $l/p_0=0$), a twisted cell ($\phi_t=90°$, $l/p_0=0$), and the supertwist slab ($\phi_t=270°$, $l/p_0=0.7$) with the same material parameters as those used in [11], i.e., $k_{33}/k_{11}=1.5$ and $k_{22}/k_{11}=0.6$. In a supertwist birefringent effect (SBE) cell the previous report [2] shows that the ratio $l/p_0=0.75$ fits within the layer thickness. In the present result, however, the ratio may be less than 0.75 because of the effect of the pretwist angle ϕ^0 [see Eq. (38)]. So $l/p_0=0.7$ is used in our calculation for a SBE cell. The significance of the sign of $(k_{33}-2k_{22})$ in the threshold properties is apparent from Eq. (46) as discussed in [9]. It is clear from Fig. 2 that the results of the previous studies only give the correct threshold fields in the limiting case of $A\rightarrow\infty$. The result for a HN cell is same as that reported in Ref. [4].

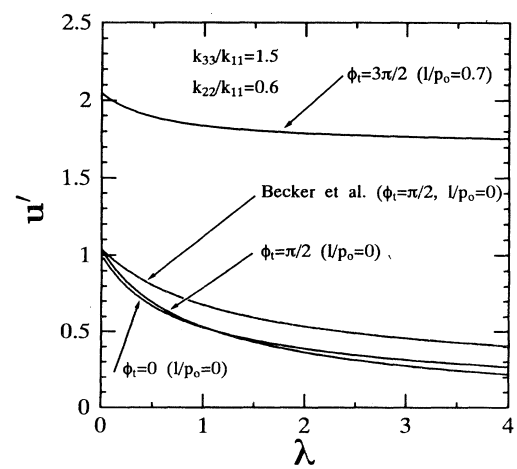

FIG. 2. The λ dependence of the reduced threshold fields u' for homogeneous nematic, twisted nematic, and supertwist birefringent effect cells. We show the present theoretical results and those reported in Ref. [11]. The material parameters used in the calculation are $k_{33}/k_{11}=1.5$ and $k_{22}/k_{11}=0.6$.

V. SATURATION FIELD

We can also derive analytically the saturation field B_S, above which the director becomes complely homeotropic. However, in actual calculations we have to overcome some mathematical difficulties (see the controversy mentioned in Refs. [8–10] and Ref. [11]).

To derive the saturation field B_S, we need to suppose $\theta_0=0$ and $\theta_M \to \pi/2$ when $B \to B_S$. With these boundary conditions the limiting integrals in Eqs. (29) and (31) can be solved analytically to give the relationship between the saturation field and the anchoring energy. Introducing a new variable, β for θ_M in the range $\pi/2 \geq \theta_M > \theta$, given by

$$\cos\theta = \frac{\cos\theta_M}{\cos\beta} \quad \left[\cos\theta^0 = \frac{\cos\theta_M}{\cos\beta^0} \right],$$

and with $C_1 = q\cos^2\theta_M$ from Eq. (25) at $\theta_0=0$, Eq. (29) becomes

$$\frac{l}{2} = \int_0^{\beta^0} \frac{1}{\cos\beta} \left[\frac{f(\theta)}{[\Delta\chi B^2 + W(\theta)](1-\cos^2\theta_M/\cos^2\beta)} \right]^{1/2} d\beta , \tag{47}$$

where

$$W(\theta) = \frac{-(q-k_2)^2 - (1+\gamma\cos^2\theta_M)[-2q(q-k_2)+q^2\sin^2\beta]}{k_{33}(1+\gamma\cos^2\theta_M)(1+\gamma\cos^2\theta_M/\cos^2\beta)} ,$$

$$q = \frac{A\cos\phi^0 \sin\phi^0}{\cos^2\beta^0} ,$$

$$\gamma = \frac{k_{22}-k_{33}}{k_{33}} .$$

In the limit $\theta_M \to \pi/2$, Eq. (47) becomes

$$\frac{l}{2} = \int_0^{\beta^0} \frac{k_{33}\,d\beta}{\cos\beta\sqrt{Z^2+q^2\cos^2\beta}} , \tag{48}$$

where

$$Z^2 \equiv \Delta\chi B_S^2 k_{33} - k_2^2 .$$

The limiting integral of Eq. (48) can be obtained analytically as

$$\frac{\sin\beta^0}{\sqrt{Z^2+q^2\cos^2\beta^0}} = \frac{1}{Z}\tanh\left[\frac{lZ}{2k_{33}}\right] . \tag{49}$$

With a similar process, in the limit of $\theta_M \to \pi/2$, the limiting integral of Eq. (31) can be obtained analytically as

$$\frac{\phi_t}{2} - \phi^0 - \frac{\pi l k_{22}}{p_0 k_{33}} = -\sin^{-1}\left[\frac{q\sin\beta^0}{\sqrt{Z^2+q^2}}\right] . \tag{50}$$

On the other hand, the boundary condition of Eq. (32) at

$\theta_0=0$,

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

in the limit of $\theta_M \to \pi/2$ and $\theta^0 \to \pi/2$, leads to

$$\sin\beta^0\sqrt{Z^2+q^2\cos^2\beta^0} = A\cos^2\phi^0 . \tag{51}$$

Now for given values of ϕ_t, the values of B_S, ϕ^0, and β^0 (i.e., θ^0) can be determined completely from Eqs. (49)–(51). Elimination of β^0 in Eqs. (49) and (51) leads to

$$\cos^2\phi^0 = \frac{\xi^2}{\xi^4(A/Z)^2(1-\xi^2)} , \tag{52}$$

where $\xi^2 = (A/Z)\tanh(lZ/2k_{33})$. Equation (52) is an important equation which gives the relationship between B_S and ϕ^0.

We now show the derivation of the relationship between B_S and A. Eliminating β^0 and ϕ^0 in Eqs. (49)–(51), we obtain

$$\left\{ \sin(T)\left[1-\frac{A}{Z}\tanh\left[\frac{lZ}{2k_{33}}\right]\right]^{1/2} - \cos(T)\left[\frac{A}{Z}\coth\left[\frac{lZ}{2k_{33}}\right]-1\right]^{1/2} \right\} \times \left[1+\tanh^2\left[\frac{lZ}{2k_{33}}\right] - \frac{A}{Z}\tanh\left[\frac{lZ}{2k_{33}}\right]\right] = 0 , \tag{53}$$

where $T \equiv \phi_t/2 - \pi l k_{22}/(p_0 k_{33})$. Because the second factor of Eq. (53) leads to an unreasonable result of $\tan^2\phi^0 = -1$, only one reasonable solution is derived analytically with the first term of Eq. (53) to give the important relationship between B_S and A as

$$\frac{Z}{A} = \tan\left[\frac{lZ}{2k_{33}}\right]\left[1+\frac{\cos^2(T)}{\sinh^2[lZ/(2k_{33})]}\right] . \tag{54}$$

To discuss the saturation properties, as defined in Ref. [11], we introduce a parameter

$$Y \equiv \left[u''^2 \left[\frac{k_{11}}{k_{33}} \right] - \left[\frac{2lk_{22}}{p_0 k_{33}} \right]^2 \right]^{1/2}, \tag{55}$$

where the reduced saturation field u'' is defined as $u''=B_S/B_c$. With Eqs. (44) and (55), we find that Eq. (54) reduces to

$$\lambda \left[\frac{k_{33}}{k_{11}} \right] = \frac{\tanh(\pi Y/2)}{Y} \left[1 + \frac{\cos^2(T)}{\sinh^2(\pi Y/2)} \right]. \tag{56}$$

Next we show the relationship between ϕ_0 and Y. The substitution of Eq. (54) into Eq. (52) gives

$$\tan\phi^0 = \frac{|\sin 2T|}{2[\sinh^2(\pi Y/2)+\cos^2 T]}. \tag{57}$$

For TCN LC of very short pitch, where $[2lk_{22}/(k_{33}p_0)]^2 - u''^2 k_{11}/k_{33} > 0$, Eqs. (56) and (57) can be rewritten as

$$\lambda \left[\frac{k_{33}}{k_{11}} \right] = \frac{\tan(\pi Y'/2)}{Y}, \left[1 - \frac{\cos^2 T}{\sin^2(\pi Y'/2)} \right], \tag{58}$$

$$\tan\phi^0 = \frac{|\sin 2T|}{2[\cos^2 T - \sin^2(\pi Y'/2)]}, \tag{59}$$

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

The relationship between λ and u'' given by Eqs. (55)–(57) has been calculated numerically using the same values of the physical parameters used in Fig. 2. The result is shown in Fig. 3. We notice that, in the limit $Y \to \infty$, Eq. (56) leads to nearly the same result as that reported in Refs. [9] and [11]. However, in the limit $Y \to 0$, we have

$$u'' \to 2\sqrt{k_{22}^2/k_{11}k_{33}} \frac{l}{|p_0|}. \tag{60}$$

Equation (60) shows that, for a HN cell and TN cells, $u'' \to 0$ because $|p_0| \to \infty$, and for a SBE cell, u'' follows Eq. (60) for the value of $l/|p_0|$ given. This differs from the result that the saturation voltage vanished as some value of λ_0 as reported in Refs. [9] and [11]. The present theory is therefore the only one which leads to the natural conclusion that decreasing the anchoring strength reduces the saturation field and that the free anchoring limit (i.e., $A=0$) gives a zero saturation field for HN and TN cells and a constant value for a SBE cell. The significance of the ratio of k_{22}/k_{33} in a TCN cell is apparent from Eqs. (56) and (60). It is clear from Eq. (56) that the saturation field for a HN cell is always larger than that for a TN cell. It can be deduced from Eqs. (43) and (56) that for typical values of l/p_0 and the elastic constant ratios the $u'(\lambda)$ and $u''(\lambda)$ curves always intersect, as shown in Figs. 2 and 3. For a weak anchoring condition with λ larger than the value of λ at the point of

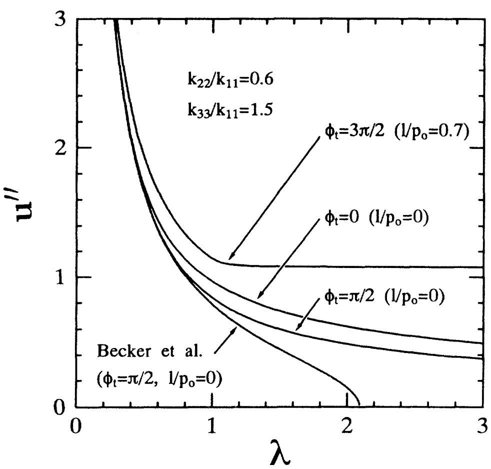

FIG. 3. The λ dependence of the reduced saturation fields (u'') for homogeneous nematic, twisted nematic, and supertwist birefringent effects cells. This shows the present theoretical results and those reported in Ref. [11]. The material parameters used in the calculation are $k_{33}/k_{11}=1.5$ and $k_{22}/k_{11}=0.6$.

intersection, a LC cell has a bistable property discussed in Refs. [9] and [11]. More detailed consideration of this property may help us in the design of a SBE cell with a weak anchoring.

Finally, we discuss the saturation property for strong anchoring. The saturation threshold field for strong anchoring has been predicted theoretically [8] and is observed experimentally [15]. In the limit of $A \to \infty$, Eqs. (54) and (55) lead to $Z \to \infty$ and then $Y \to \infty$. As a result, Eq. (57) gives the condition of $\phi^0 \to 0$ for strong anchoring. On the other hand, strong anchoring leads to $\beta^0 \to \pi/2$ with Eq. (51). Then the result of $\theta^0 \to 0$ is found. Both results of $\phi^0 \to 0$ and $\theta^0 \to 0$ are reasonable conditions for strong anchoring.

VI. CONCLUSION

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 only need a single 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 conditions and external fields become much easier. A variational calculation method for the two-dimensional problem introduced in this paper may allow us to minimize the total free energy, which is the sum of the bulk energy and the surface energy for a two-dimensional deformation. This may be significant in the development of LC display devices.

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