Surface- and optical-field-induced Fréedericksz transitions and hysteresis in a nematic cell

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For a homeotropic nematic liquid-crystal cell, this paper explores the influence of the surface anchoring and the cell thickness on the first-order optically induced Fréedericksz transitions. The exact criteria for the existence of the first-order transitions at the threshold and at the saturation, respectively, are obtained in terms of material and device parameters for arbitrary anchoring conditions. The critical cell thickness, when thinner than which the first-order transitions will exist, is obtained. A standard for estimating the strength of the first-order transitions is proposed. The group equations for determining the tricritical points are listed. The factors, especially the nonmaterial factors to enhance the first-order transitions are discussed at length.

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I. INTRODUCTION

Particular attention has been devoted to the first-order optical-field-induced Fréedericksz transition (FOFT) in the past two decades. Though theoretical calculations show that, under rigid anchoring boundary conditions, some liquid crystals (LC) that have sufficiently large optical and elastic anisotropy may exhibit first-order transitions induced by only a single optical field [1]. To our knowledge, the reported FOFTs are all induced by two fields, a driving field and a bias field [2]. On the other hand, the single-field-induced Fréedericksz transitions are obviously of great applicative interest. We have investigated the weak anchoring effects on the electromagnetic-field-induced Fréedericksz transition (EMFT) in our other studies [3], found that the first-order Fréedericksz transitions induced by a single dc electric field or a magnetic field may exist under some anchoring conditions. It shows that the first-order transitions may be enhanced by the interfacial interactions, therefore making it possible to observe the FOFT in the absence of any bias fields.

Surface alignment has been widely used to obtain a uniform director configuration. Despite its practical importance, the mechanism of the director alignment of LC films by the substrate surface is not well understood. Rapini and Papoular (RP) proposed a phenomenological formula to describe the weak anchoring potential per unit area [4]

$$g_s(\theta)=\tfrac{1}{2}A_2\sin^2\theta, \tag{1.1}$$

where A_2 is the so-called anchoring strength, and θ is the angle between director $\mathbf{n}$ and easy direction $\mathbf{e}$.

There are a number of theoretical and experimental indications that the surface anchoring potential dependence on the director orientation is much more complicated than described by the RP potential, especially when strong external fields are present [5,6]. Without loss of generality, the expansion of the anchoring potential with respect to $\sin^2\theta$ is usually assumed. Retaining only terms up to second order in $\sin^2\theta$ yields the two-parameter potential

$$g_s(\theta)=\tfrac{1}{2}(A_2\sin^2\theta+A_4\sin^4\theta), \tag{1.2}$$

where A_2 is positive, while A_4 may be negative. It contains the modifications to the RP potential and has been investigated by some authors in experiment [6]. We shall mainly use this form of interfacial potential in this paper.

Ong has made some preliminary investigations on the relationship between the interfacial interactions and the FOFTs [1,7]. This paper dwells on this subject using an approach developed in our other studies when dealing with EMFT [3]. The exact criteria for the existence of the threshold FOFT and the saturation FOFT are obtained in terms of material and device parameters. The group equations for determining the threshold and the saturation tricritical points are given. The bistabilities are discussed exploiting our approach.

II. BASIC EQUATIONS

Consider a homeotropically oriented NLC cell of thickness d confined between planes $z=0$ and $z=d$ of a Cartesian coordinate system. In the cell, the average local orientation of positive nematic molecules is given by $\mathbf{n}(\mathbf{r})$. The NLC director always lies in the xz plane and in the absence of a light beam, the directors are parallel to the z axis everywhere. Denote by $\theta(z)$ the tilt angle between the director and the z axis. Then the director can be described by $\mathbf{n}(z)=(\sin\theta,0,\cos\theta)$. In the presence of a monochromatic laser beam, the NLC molecules can be reoriented. For p polarization, the molecular director moves in the incidence plane xz until a steady-state condition is reached. If the wall-anchoring force is the same for both cell substrates, the solution is symmetric with respect to the $z=d/2$ plane. For incidence intensity I, the total free energy can be written as [1]

$$F=S\int_0^d\left\{\tfrac{1}{2}k_{33}[1+(\kappa-1)\sin^2\theta]\left(\frac{d\theta}{dz}\right)^2-\frac{I}{c}\,\frac{n_o}{\sqrt{1+(\eta-1)\sin^2\theta}}\right\}dz+A_2S\sin^2\theta_0(1+R\sin^2\theta_0), \tag{2.1}$$

where $\kappa=k_{11}/k_{33}$, k_{11}, and k_{33} are elastic splay and bend constants; $\eta=n_o^2/n_e^2$, n_o, n_e are ordinary and extraordinary refractive indices at the optical frequency respectively; $R=A_4/A_2$; c is the light speed; and θ_0 is the value of θ evaluated at $z=0$. Hereafter symbols with subscripts 0 and m denote the corresponding functional values evaluated at $z=0$ and $z=d/2$, respectively, if they are not specified otherwise. Besides κ and R, the following dimensionless parameters will also appear in the rest of this paper for the sake of convenience: $\mu=\eta-1$, $\gamma=\kappa-1$. Remember that we always have $\mu<0$ for the positive nematic liquid crystals.

The variation of the total free energy leads to the bulk equation

$$(1+\gamma\sin^2\theta)\frac{d^2\theta}{dz^2}+\gamma\sin\theta\cos\theta\left(\frac{d\theta}{dz}\right)^2-\frac{In_o}{ck_{33}}\frac{\mu\sin\theta\cos\theta}{(1+\mu\sin^2\theta)^{3/2}}=0, \tag{2.2}$$

and the boundary condition at $z=0$

$$k_{33}[1+\gamma\sin^2\theta_0]\left(\frac{d\theta}{dz}\right)_{z=0}=A_2\sin\theta_0\cos\theta_0(1+2R\sin^2\theta_0). \tag{2.3}$$

The solutions of Eqs. (2.2) and (2.3) describe the equilibrium orientation of the NLC throughout the medium. There exist three solutions. The first one is

$$\theta\equiv 0. \tag{2.4}$$

The second one is

$$\theta\equiv\pi/2. \tag{2.5}$$

The last one is

$$z(\theta)=\sqrt{\frac{ck_{33}}{2\,In_o}}(1+\mu\sin^2\theta_m)^{1/4}\times\int_{\theta_0}^{\theta}\sqrt{\frac{(1+\gamma\sin^2\theta)\sqrt{1+\mu\sin^2\theta}}{\sqrt{1+\mu\sin^2\theta}-\sqrt{1+\mu\sin^2\theta_m}}}\,d\theta. \tag{2.6}$$

The boundary condition for solution (2.6) becomes

$$\frac{(1+\gamma\sin^2\theta_0)J_1^2(\theta_0,\theta_m)}{\alpha^2\sin^2\theta_0\cos^2\theta_0(1+2R\sin^2\theta_0)^2}=\frac{\sqrt{1+\mu\sin^2\theta_0}}{\sqrt{1+\mu\sin^2\theta_0}-\sqrt{1+\mu\sin^2\theta_m}}, \tag{2.7}$$

where

$$\alpha=\frac{A_2d}{2k_{33}},$$

$$J_1(\theta_0,\theta_m)=\int_{\theta_0}^{\theta_m}\sqrt{\frac{[1+\gamma\sin^2\theta]\sqrt{1+\mu\sin^2\theta}}{\sqrt{1+\mu\sin^2\theta}-\sqrt{1+\mu\sin^2\theta_m}}}\,d\theta.$$

The Gibbs free energy corresponding to the three solutions are denoted, respectively, by

$$G_0=-\frac{In_o}{c}Sd, \tag{2.8}$$

$$G_{\pi/2}=-\frac{In_e}{c}Sd+A_2S(1+R), \tag{2.9}$$

$$G_{\rm def}=\frac{A_2S}{\alpha}\{J_1^2(\theta_0,\theta_m)-2J_1(\theta_0,\theta_m)J_2(\theta_0,\theta_m)\times\sqrt{1+\mu\sin^2\theta_m}\}+A_2S\sin^2\theta_0(1+R\sin^2\theta_0), \tag{2.10}$$

where subscripts 0, $\pi/2$ and def stand for the uniform solution $\theta\equiv 0$, $\theta\equiv\pi/2$ and the deformed solution (2.6), where

$$J_2(\theta_0,\theta_m)=\int_{\theta_0}^{\theta_m}\sqrt{\frac{1+\gamma\sin^2\theta}{(1+\mu\sin^2\theta)-\sqrt{(1+\mu\sin^2\theta)(1+\mu\sin^2\theta_m)}}}\,d\theta.$$

The detailed derivation of Eqs. (2.7) and (2.10) are in Appendix A.

The stable or metastable states described by the three solutions correspond to the initial state, the saturation state, and the deformed state, respectively. Near the threshold, solutions (2.4) and (2.6) are the possible stable or metastable states. It is instructive to consider the following dimensionless function for the given intensity I:

$$g_1=\frac{G_{\rm def}-G_0}{A_2S}. \tag{2.11}$$

Due to the same reason, near the saturation, for the given incidence intensity I, we have the function

$$g_2 = \frac{G_{\rm def} - G_{\pi/2}}{A_2 S}. \tag{2.12}$$

We will derive the criteria for the existence of the first-order transitions with the help of g_1 and g_2.

Another important function is the incidence intensity given by solution (2.6). Noting that $\theta = \theta_m$ at $z = d/2$ plane, by (2.6) we obtain

$$I(\theta_0, \theta_m) = \sqrt{1 + \mu \sin^2 \theta_m} J_1^2(\theta_0, \theta_m) \tilde{I}, \tag{2.13}$$

where constant $\tilde{I} = (2ck_{33})/n_o d^2$. The boundary condition (2.7) and the functions (2.11)–(2.13) underlie this paper.

III. THE THRESHOLD FOFT

For convenience, we introduce variables u and ν by $u = \sin^2 \theta_m$, $\sin^2 \theta = u\nu$, ($\sin^2 \theta_0 = u\nu_0$). For the director reorientation near the threshold, u plays the role of an order parameter, $u = 0$ describes the uniform state $\theta \equiv 0$, $u \neq 0$ describes the deformed state. Now the two integrals become

$$J_1(\nu_0, u) = \int_{\nu_0}^1 \sqrt{\frac{[1 + \gamma u \nu]\sqrt{1 + \mu u \nu}}{\sqrt{1 + \mu u \nu} - \sqrt{1 + \mu u}}} \frac{u d\nu}{2\sqrt{u\nu(1 - u\nu)}},$$

$$J_2(\nu_0, u) = \int_{\nu_0}^1 \sqrt{\frac{1 + \gamma u \nu}{(1 + \mu u \nu) - \sqrt{(1 + \mu u \nu)(1 + \mu u)}}}$$

$$\times \frac{u d\nu}{2\sqrt{u\nu(1 - u\nu)}}.$$

The boundary condition transforms to

$$\frac{J_1^2(\nu_0, u)}{\alpha^2} \frac{(1 + \gamma u \nu_0)}{\nu_0(1 - u\nu_0)\sqrt{1 + \mu u \nu_0}} = \frac{u}{\sqrt{1 + \mu u \nu_0} - \sqrt{1 + \mu u}}. \tag{3.1}$$

Condition (3.1) defines an implicit function of $\nu_0(u)$, consequently the two integrals can be written as $J_1(u)$ and $J_2(u)$, then I and g_1 become functions of order parameter u. Equation (2.13) transforms to

$$\sqrt{\frac{I(u)}{\tilde{I}}} = (1 + \mu u)^{1/4} J_1(u). \tag{3.2}$$

Eliminating I in G_0 by Eq. (3.2), then we obtain

$$g_1(u) = \frac{1}{\alpha}\{J_1^2(u) + \sqrt{1 + \mu u}[J_1^2(u) - 2J_1(u)J_2(u)]\}$$

$$+ u\nu_0(u)[1 + Ru\nu_0(u)]. \tag{3.3}$$

The first question of interest is the criterion for the existence of FOFT. We have developed an approach for solving this problem under weak anchoring cases in our other works. The criterion can be obtained from

$$\left(\frac{d^2 g_1}{du^2}\right)_{u=0} > 0, \tag{3.4}$$

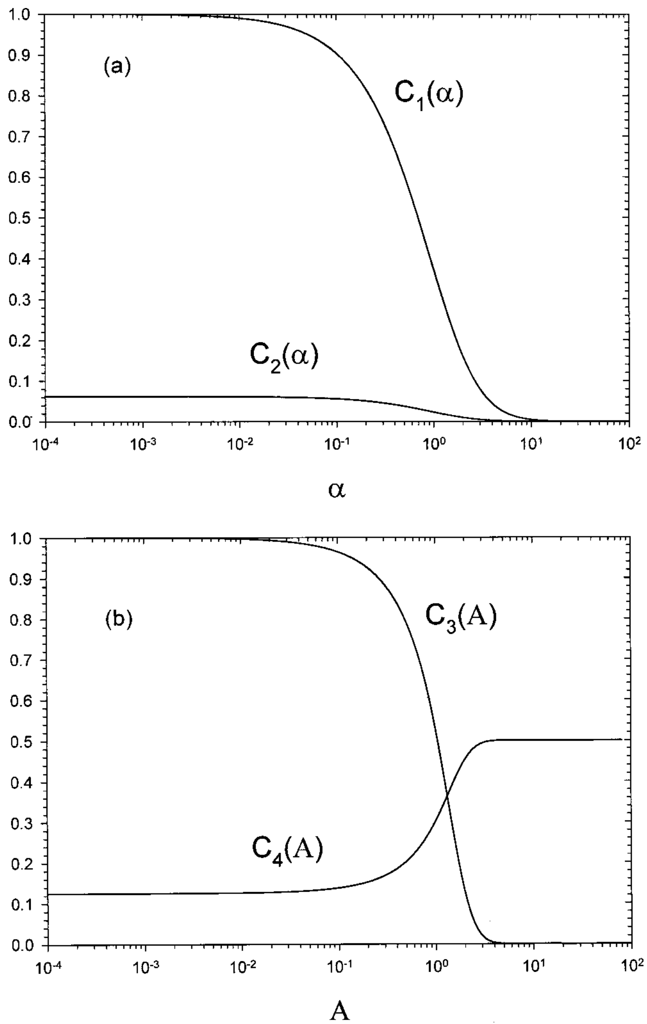

FIG. 1. (a) Implicit functions $C_1(\alpha)$ and $C_2(\alpha)$. They are positive and monotonous functions. $\lim_{a\to 0}[C_1(\alpha) = 1, C_2(\alpha) = \frac{1}{16}]$, $\lim_{a\to +\infty}[C_1(\alpha) = 0, C_2(\alpha) = 0]$. (b) Implicit functions $C_3(A)$ and $C_4(A)$. They are positive and monotonous functions. $\lim_{A\to 0}[C_3(A) = 1, C_4(A) = \frac{1}{8}]$, $\lim_{a\to +\infty}[C_3(A) = 0, C_4(A) = \frac{1}{2}]$.

or from

$$\left(\frac{d}{du}\sqrt{\frac{I}{\tilde{I}}}\right)_{u=0} < 0. \tag{3.5}$$

The reasons are obvious, both Eqs. (3.4) and (3.5) contradict the requirement of the second-order transition at $\theta_m = 0$, so they predict the first-order transition. Direct calculations also show the equivalence of Eqs. (3.4) and (3.5),

$$-f_1(V_0)\sqrt{-\frac{\mu}{2}}\left(\frac{d}{du}\sqrt{\frac{I}{\tilde{I}}}\right)_{u=0} = \frac{\alpha}{2}\left(\frac{d^2 g_1}{du^2}\right)_{u=0}, \tag{3.6}$$

where $f_1(V_0) > 0$ (see Appendix B). After complicated calculations (see Appendix B) we obtain the criterion

$$\frac{n_o^2}{n_e^2} < \left(1 - \frac{4}{9}\frac{k_{11}}{k_{33}}\right) + \frac{4}{9}\frac{k_{11}}{k_{33}}\left[\frac{4\sin 4\beta + 8\sin 2\beta}{\sin 4\beta + 8\sin 2\beta + 12\beta}\right] - \frac{64}{3}\frac{A_4}{A_2}\left[\frac{\sin 2\beta\cos^2\beta}{\sin 4\beta + 8\sin 2\beta + 12\beta}\right], \tag{3.7}$$

where $\beta \in [0, \pi/2]$ is determined by the boundary condition at $u=0$, i.e., by

$$\beta \tan\beta = \frac{A_2 d}{2k_{33}}. \tag{3.8}$$

Besides the criterion for the existence of FOFT, another question of interest is the bistability. The rising and falling transitions are mirrorless, the rising threshold intensity satisfies $I(u_{\rm th}^r) = (I)_{u=0}$, while the falling threshold intensity is the minimal extremum of $I(u)$. For $I_{\rm th}^f < I < I_{\rm th}^r$, there exist two steady states and a hysteresis. Now we give the equations for determining the tricritical points near the threshold.

For the rising threshold, we first determine the critical intensity. Setting $u=0$ at Eq. (3.2) follows that

$$\beta = \sqrt{-\frac{\mu I_{\rm th}^r}{2\tilde{I}}} = \frac{\pi}{2}\sqrt{\frac{I_{\rm th}^r}{I_0}}, \tag{3.9}$$

where

$$I_0 = \frac{ck_{33}}{n_o}\frac{\pi^2}{d^2}\frac{n_e^2}{(n_e^2 - n_o^2)}. \tag{3.10}$$

For the rigid anchoring condition, $A_2 \to +\infty$; from Eq. (3.8) we have $\beta \to \pi/2$; then from Eq. (3.9) we have $I_{\rm th}^r \to I_0$. Therefore I_0 is just the threshold intensity for the rigid anchoring condition, and this is in agreement with what Ong has obtained (see Ref. [1], Table I, $I_{\rm Fr}$). Substituting Eq. (3.9) into Eq. (3.8) yields

$$\left(\frac{\pi}{2}\sqrt{\frac{I_{\rm th}^r}{I_0}}\right)\tan\left(\frac{\pi}{2}\sqrt{\frac{I_{\rm th}^r}{I_0}}\right) = \frac{A_2 d}{2k_{33}}, \tag{3.11}$$

or represented as the well known form

$$\cot\left[\frac{\pi}{2}\sqrt{\frac{I_{\rm th}^r}{I_0}}\right] = \frac{2k_{33}}{A_2 d}\left[\frac{\pi}{2}\sqrt{\frac{I_{\rm th}^r}{I_0}}\right]. \tag{3.12}$$

This is the same as what Ong has obtained [see Eq. (5.14) in Ref. [1]].

The rising threshold order parameter $u_{\rm th}^r$ then can be solved out from

$$I_{\rm th}^r = \frac{2ck_{33}}{n_o d^2}\sqrt{\left(1 + \frac{n_o^2 - n_e^2}{n_e^2}u_{\rm th}^r\right)}J_1^2(u_{\rm th}^r). \tag{3.13}$$

For the falling threshold, we could first determine the order parameter $u_{\rm th}^f$ by solving

$$\frac{d}{du}\sqrt{\frac{I(u)}{\tilde{I}}} = \frac{d}{du}\left[\left(1 + \frac{n_o^2 - n_e^2}{n_e^2}u\right)^{1/4}J_1(u)\right] = 0, \tag{3.14}$$

then obtain the falling threshold intensity by

$$I_{\rm th}^f = \frac{2ck_{33}}{n_o d^2}\sqrt{\left(1 + \frac{n_o^2 - n_e^2}{n_e^2}u_{\rm th}^f\right)}J_1^2(u_{\rm th}^f). \tag{3.15}$$

The above two equations are inspired by what Ong has proposed [see Eq. (4.8) in Ref. [1]].

IV. THE SATURATION FOFT

At the saturation, the results are similar to those of threshold. The order parameter is chosen as $w = \cos^2\theta_m$ instead; the intermediate variable x is introduced by $\cos^2\theta = w/x$, ($\cos^2\theta_0 = w/x_0$). It can be easily proved that $\theta(z) = \pi/2$ throughout the medium when $\theta_m = \pi/2$, so $w=0$ describes the uniform state $\theta(z) = \pi/2$ throughout the medium. The two integrals transform to

$$J_1 = \int_{x_0}^{1}\sqrt{\frac{\kappa\left(1 - \frac{\gamma}{\kappa}\frac{w}{x}\right)\sqrt{1 - \frac{\mu}{\eta}\frac{w}{x}}}{\sqrt{1 - \frac{\mu}{\eta}\frac{w}{x}} - \sqrt{1 - \frac{\mu}{\eta}w}}}\,\frac{w\,dx}{2x^2\sqrt{\frac{w}{x}\left(1 - \frac{w}{x}\right)}},$$

$$J_2 = \int_{x_0}^{1}\sqrt{\frac{\kappa\left(1 - \frac{\gamma}{\kappa}\frac{w}{x}\right)}{\sqrt{\eta\left(1 - \frac{\mu}{\eta}\frac{w}{x}\right)}\left[\sqrt{\eta\left(1 - \frac{\mu}{\eta}\frac{w}{x}\right)} - \sqrt{\eta\left(1 - \frac{\mu}{\eta}w\right)}\right]}}\,\frac{w\,dx}{2x^2\sqrt{\frac{w}{x}\left(1 - \frac{w}{x}\right)}}.$$

The boundary condition becomes

$$\frac{J_1^2}{\alpha^2}\frac{\kappa}{(1+2R)^2}\frac{1}{\sqrt{1-\frac{\mu}{\eta}\frac{w}{x_0}}}\frac{1-\frac{\gamma}{\kappa}\frac{w}{x_0}}{\left(1-\frac{2R}{1+2R}\frac{w}{x_0}\right)^2\left(1-\frac{w}{x_0}\right)}$$
$$=\frac{1}{x_0}\frac{w}{\sqrt{1-\frac{\mu}{\eta}\frac{w}{x_0}}-\sqrt{1-\frac{\mu}{\eta}w}}, \tag{4.1}$$

which defines implicit function $x_0(w)$.

The two important functions I and g_2 are both functions of order parameter w,

$$\sqrt{\frac{I(w)}{\tilde{I}}}=(\eta-\mu w)^{1/4}J_1(w), \tag{4.2}$$

$$g_2(w)=\frac{1}{\alpha}\left\{\left[1+\sqrt{1-\frac{\mu}{\eta}w}\right]J_1^2(w)\right.$$
$$\left.-2J_1(w)J_2(w)\sqrt{\eta}\sqrt{1-\frac{\mu}{\eta}w}\right\}$$
$$-\frac{(1+2R)w}{x_0(w)}+\frac{Rw^2}{[x_0(w)]^2}. \tag{4.3}$$

The criterion for the FOFT at saturation can be derived by either of the following two relations:

$$\left(\frac{d}{dw}\sqrt{\frac{I}{\tilde{I}}}\right)_{w=0}>0 \tag{4.4}$$

and

$$\left(\frac{d^2g_2}{dw^2}\right)_{w=0}>0. \tag{4.5}$$

The equivalence of Eqs. (4.4) and (4.5) also can be seen from

$$\sqrt{\frac{-2\mu\kappa}{\eta}}h_2(X_0)\left(\frac{d}{dw}\sqrt{\frac{I}{\tilde{I}}}\right)_{w=0}=2\alpha\eta^{1/4}\left(\frac{d^2g_2}{dw^2}\right)_{w=0}, \tag{4.6}$$

where $h_2(X_0)>0$ (see Appendix B).

The criterion for the existence of FOFT at saturation is

$$\frac{n_e^2}{n_o^2}>\left(1+\frac{4}{3}\frac{k_{33}}{k_{11}}\right)$$
$$-\frac{4}{3}\frac{k_{33}}{k_{11}}\frac{4B\,\mathrm{sech}^4 B+4\tanh B\,\mathrm{sech}^2 B}{3B\,\mathrm{sech}^4 B+3\tanh B\,\mathrm{sech}^2 B+2\tanh B}$$
$$+\frac{32A_4}{3(A_2+2A_4)}$$
$$\times\frac{\tanh B}{3B\,\mathrm{sech}^4 B+3\tanh B\,\mathrm{sech}^2 B+2\tanh B}, \tag{4.7}$$

where $B\in[0,+\infty]$ is determined by the boundary condition at $w=0$, i.e., by

$$B\tanh B=\frac{(A_2+2A_4)d}{2k_{11}}. \tag{4.8}$$

The rising saturation transition occurs at the maximum extremum of $I(\theta_m)$, the falling saturation critical point satisfies $I(w_{\mathrm{sat}}^f)=(I)_{w=0}$. For $I_{\mathrm{sat}}^f<I<I_{\mathrm{sat}}^r$, bistability and hysteresis exist.

The rising saturation order parameter w_{sat}^r can be determined by solving

$$\frac{d}{dw}\sqrt{\frac{I(w)}{\tilde{I}}}=\frac{d}{dw}\left[\left(\frac{n_o^2}{n_e^2}-\frac{n_o^2-n_e^2}{n_e^2}w\right)^{1/4}J_1^2(w)\right]=0, \tag{4.9}$$

while the rising saturation intensity can be obtained by

$$I_{\mathrm{sat}}^r=\frac{2ck_{33}}{n_od^2}\sqrt{\left(\frac{n_o^2}{n_e^2}-\frac{n_o^2-n_e^2}{n_e^2}w_{\mathrm{sat}}^r\right)}J_1^2(w_{\mathrm{sat}}^r). \tag{4.10}$$

Setting $w=0$ in the right side of Eq. (4.2) yields

$$B=\eta^{-3/4}\sqrt{-\frac{\mu}{2\kappa}\frac{I_{\mathrm{sat}}^f}{\tilde{I}}}=\frac{\pi}{2}\sqrt{\frac{n_e^3k_{33}I_{\mathrm{sat}}^f}{n_o^3k_{11}I_0}}. \tag{4.11}$$

Substituting Eq. (4.11) into Eq. (4.8) follows

$$\left(\frac{\pi}{2}\sqrt{\frac{n_e^3k_{33}I_{\mathrm{sat}}^f}{n_o^3k_{11}I_0}}\right)\tanh\left(\frac{\pi}{2}\sqrt{\frac{n_e^3k_{33}I_{\mathrm{sat}}^f}{n_o^3k_{11}I_0}}\right)=\frac{(A_2+2A_4)d}{2k_{11}}, \tag{4.12}$$

or represented as the well known form

$$\coth\left(\frac{\pi}{2}\sqrt{\frac{n_e^3k_{33}I_{\mathrm{sat}}^f}{n_o^3k_{11}I_0}}\right)=\frac{2k_{11}}{(A_2+2A_4)d}\left(\frac{\pi}{2}\sqrt{\frac{n_e^3k_{33}I_{\mathrm{sat}}^f}{n_o^3k_{11}I_0}}\right), \tag{4.13}$$

which determines the falling saturation intensity. The falling saturation intensity is just the intensity to maintain the saturation state, Ong obtained the above relation in Ref. [1] [see Eq. (5.17) in Ref. [1]]. The falling saturation order parameter then can be obtained from

$$I_{\mathrm{sat}}^f=\frac{2ck_{33}}{n_od^2}\sqrt{\left(\frac{n_o^2}{n_e^2}-\frac{n_o^2-n_e^2}{n_o^2}w_{\mathrm{sat}}^f\right)}J_1^2(w_{\mathrm{sat}}^f). \tag{4.14}$$

V. DISCUSSION AND CONCLUSIONS

A. The boundary conditions, optical anisotropy, and the criteria

The anchoring strength can be characterized by the following two dimensionless parameters:

$$\alpha=\frac{A_2 d}{2k_{33}},\quad A=\frac{(A_2+2A_4)d}{2k_{11}}. \tag{5.1}$$

α and A are related only to material mechanical parameters and cell geometrical parameters. When $\theta_m=0$ and $\theta_m=\pi/2$, the boundary conditions become

$$\beta\tan\beta=\alpha,\quad B\tanh B=A. \tag{5.2}$$

(Here A and B represent upper case Greek alpha and beta.) Due to Eq. (5.2), the criteria (3.7) and (4.7) can be expressed as

$$\frac{n_o^2}{n_e^2}<\left(1-\frac{4}{9}\frac{k_{11}}{k_{33}}\right)+\frac{4}{9}\frac{k_{11}}{k_{33}}C_1(\alpha)-\frac{64}{3}RC_2(\alpha), \tag{5.3}$$

$$\frac{n_e^2}{n_o^2}>\left(1+\frac{4}{3}\frac{k_{33}}{k_{11}}\right)-\frac{4}{3}\frac{k_{33}}{k_{11}}C_3(A)+\frac{32}{3}\frac{R}{1+2R}C_4(A), \tag{5.4}$$

respectively, where $C_1(\alpha)$, $C_2(\alpha)$, $C_3(A)$, and $C_4(A)$ are illustrated in Fig. 1. The material optical parameters appear only in the left-hand sides of Eqs. (5.3) and (5.4). So the above two criteria explicitly prove a law: for the first-order Fréedericksz transition to occur either at threshold or saturation point, n_o/n_e should be small, i.e., optical anisotropy should be large.

The four functions $C_1(\alpha)$, $C_2(\alpha)$, $C_3(A)$, and $C_4(A)$ are all positive and monotonous, so the requirements for the first order transition can be stated as (1) small α and negative R, small n_o/n_e, and small k_{11}/k_{33} favor the threshold FOFT; (2) small A and negative R, small n_o/n_e, and small k_{33}/k_{11} favor the saturation FOFT.

B. The critical cell thickness

When the cell thickness $d\to 0$, the criteria for threshold and saturation FOFT become, respectively,

$$\frac{n_o^2}{n_e^2}<1-\frac{4}{3}\frac{A_4}{A_2}, \tag{5.5}$$

$$\frac{n_e^2}{n_o^2}>1+\frac{4}{3}\frac{A_4}{(A_2+2A_4)}. \tag{5.6}$$

When the cell thickness $d\to+\infty$, the criteria for threshold and saturation FOFT become, respectively,

$$\frac{n_o^2}{n_e^2}<1-\frac{4}{9}\frac{k_{11}}{k_{33}}, \tag{5.7}$$

$$\frac{n_e^2}{n_o^2}>1+\frac{4}{3}\frac{k_{33}}{k_{11}}+\frac{16}{3}\frac{A_4}{(A_2+2A_4)}. \tag{5.8}$$

The definition of B requires $B>0$ (see Appendix B); it follows that $A_2+2A_4>0$. If $A_4\leqslant 0$, we note that Eqs. (5.5) and (5.6) can be met naturally for any positive nematic materials in a homeotropic cell. It follows an interesting conclusion: for any positive nematic materials in a homeotropic cell, if the anchoring conditions at the substrates are kept unchanged, then there exists a critical cell thickness, when thinner than which the first-order transitions will exist. If $A_4>0$, the critical cell thickness may not exist for relatively large A_4.

Exact critical cell thickness can be obtained numerically from Eqs. (5.3) and (5.4), which, for small α and A, can be approximated by

$$\frac{n_o^2}{n_e^2}<1-\frac{4}{9}\frac{k_{11}}{k_{33}}\left[\alpha-\frac{1}{3}\alpha^2\right]-\frac{4}{3}\frac{A_4}{A_2}\left(1-\alpha+\frac{\alpha^2}{3}\right), \tag{5.9}$$

$$\frac{n_e^2}{n_o^2}>1+\frac{4}{9}\frac{k_{33}}{k_{11}}\left(A+\frac{1}{2}A^2\right)+\frac{4}{3}\frac{A_4}{(A_2+2A_4)}\left(1+A+\frac{1}{2}A^2\right), \tag{5.10}$$

respectively, where we employ $\beta^2\approx\alpha-\alpha^2/3$ and $B^2\approx A+A^2/2$. If α^2 and A^2 in Eqs. (5.9) and (5.10) are neglected, then the explicit critical cell thickness, denoted by $d_{\rm th}$ and $d_{\rm sat}$, respectively, can be obtained approximately,

$$d_{\rm th}\approx\frac{\dfrac{2k_{33}}{A_2}\left(1-\dfrac{n_o^2}{n_e^2}-\dfrac{4}{3}\dfrac{A_4}{A_2}\right)}{\left(\dfrac{4}{9}\dfrac{k_{11}}{k_{33}}-\dfrac{4}{3}\dfrac{A_4}{A_2}\right)}, \tag{5.11}$$

$$d_{\rm sat}\approx\frac{\dfrac{2k_{11}}{(A_2+2A_4)}\left(\dfrac{n_e^2}{n_o^2}-1-\dfrac{4}{3}\dfrac{A_4}{A_2+2A_4}\right)}{\left(\dfrac{4}{9}\dfrac{k_{33}}{k_{11}}+\dfrac{4}{3}\dfrac{A_4}{A_2+2A_4}\right)}. \tag{5.12}$$

Yang and Rosenblatt reported an interfacial potential of $g_s=(11.7\sin^2\theta+7.8\sin^4\theta)\times 10^{-3}\ \mathrm{erg/cm^2}$ for a MBBA liquid crystal homeotropic cell [6]. By using the related material parameters listed in Table I, we find that FOFT will not occur for any cell thickness.

The reported measurements of the anchoring strength show that A_2 is about $(10^{-4}-10^{0})\ \mathrm{erg/cm^2}$ [8]. Under the special anchoring conditions $A_2=10^{-4}\ \mathrm{erg/cm^2}$, $A_4=0\ \mathrm{erg/cm^2}$, we calculate the critical cell thickness for some known NLC's in Table I [9].

Obviously the thinner the cell thickness, the stronger the first-order transitions, so

$$d\ll d_{\rm th}\ \text{or}\ d_{\rm sat} \tag{5.13}$$

predicts strong first-order transitions. Table I shows that at 110 °C PAA will be most suitable for observing the first-order transitions in the absence of any bias fields.

C. Criteria for the anchoring limits

The anchoring limits include the rigid anchoring limit and the zero-anchoring limit, which can be attained by taking the limit $A_2\to+\infty$ or 0 in the single parameter RP potential. The

TABLE I. The critical cell thickness for the threshold and saturation FOFTs under special weak anchoring conditions $A_2=10^{-4}$ erg/cm^2, $A_4=0$ erg/cm^2.

NLC	Temp. (°C)	k_{11} (10^{-7} dyn)	k_{33} (10^{-7} dyn)	λ (Å)	n_o	n_e	d_{th} (μm)	d_{sat} (μm)
E_7	30	10.1	16.20	5893	1.524	1.732	264	83
5CB	26	7.20	8.52	5890	1.533	1.703	86	64
5CB	26	7.20	8.52	5890	1.540	1.719	90	67
5CB	26	5.20	7.17	5890	1.533	1.703	84	40
8CB	34	4	7	6328	1.516	1.665	94	21
8CB	34	4	7	6328	1.521	1.670	94	21
MBBA	22	6.95	8.99	6328	1.544	1.758	120	72
PAA	110	9.26	18.10	4800	1.595	1.995	574	120
PAA	120	7.80	13.60	4800	1.600	1.967	361	103
PAA	125	6.94	11.90	4800	1.605	1.949	296	86
PAA	130	5.67	9.05	4800	1.611	1.928	196	69

criteria for the anchoring conditions described by the RP potential can be obtained by setting $A_4=0$ in Eqs. (3.7) and (4.7),

$$\frac{n_o^2}{n_e^2}<\left(1-\frac{4}{9}\frac{k_{11}}{k_{33}}\right)+\frac{4}{9}\frac{k_{11}}{k_{33}}\left[\frac{4\sin 4\beta+8\sin 2\beta}{\sin 4\beta+8\sin 2\beta+12\beta}\right], \tag{5.14}$$

$$\frac{n_e^2}{n_o^2}>\left(1+\frac{4}{3}\frac{k_{33}}{k_{11}}\right)-\frac{4}{3}\frac{k_{33}}{k_{11}}\frac{4B\,\mathrm{sech}^4 B+4\tanh B\,\mathrm{sech}^2 B}{3B\,\mathrm{sech}^4 B+3\tanh B\,\mathrm{sech}^2 B+2\tanh B}. \tag{5.15}$$

Taking the limit of $\beta\rightarrow\pi/2$, $B\rightarrow+\infty$ transforms Eqs. (5.14) and (5.15) into the criteria for the rigid anchoring conditions,

$$\frac{n_o^2}{n_e^2}<\left(1-\frac{4}{9}\frac{k_{11}}{k_{33}}\right), \tag{5.16}$$

$$\frac{n_e^2}{n_o^2}>\left(1+\frac{4}{3}\frac{k_{33}}{k_{11}}\right). \tag{5.17}$$

For the zero-anchoring limit, interestingly both of the two criteria degenerate to

$$n_o<n_e, \tag{5.18}$$

which holds naturally for all positive nematic liquid crystals.

D. Comments on the criteria obtained by Ong

Ong has tried to give the criteria for the transitions to be first order. For the threshold transition, he proposed that $[dI/d(\theta_m^2)]_{\theta_m=0}<0$ predict first-order transition. This is exact and is adopted by us in Eq. (3.5). However, when calculating $[dI/d(\theta_m^2)]_{\theta_m=0}$, the approximation is introduced. It does not cause trouble for rigid anchoring conditions [see Eq. (4.9) in Ref. [1] and Eq. (5.16) in this paper; they are same], while for finite anchoring conditions, he failed to give the correct criterion. Here we copy his criterion for comparison [Eq. (5.16) in Ref. [1]]

$$\left(\frac{k_{11}}{k_{33}}+\frac{9}{4}\frac{n_o^2}{n_e^2}-\frac{9}{4}\right)\pi\sqrt{\frac{I_{th}^r}{I_0}}+\left(\frac{k_{11}}{k_{33}}+\frac{3}{4}\frac{n_o^2}{n_e^2}-\frac{3}{4}\right)\times\sin\left(\pi\sqrt{\frac{I_{th}^r}{I_0}}\right)<0. \tag{5.19}$$

To make a comparison with our criterion (5.14), we apply Eqs. (3.9) to Eq. (5.19) and rewrite it as

$$\frac{n_o^2}{n_e^2}<\left(1-\frac{4}{9}\frac{k_{11}}{k_{33}}\right)-\frac{4}{9}\frac{k_{11}}{k_{33}}\frac{2\sin 2\beta}{6\beta+\sin 2\beta}. \tag{5.20}$$

We see that the difference between Eqs. (5.20) and (5.14) is great. We obtain our criterion through exact calculation, while approximation is introduced in Ong's calculation when employing Landau theory. Therefore the criterion obtained by Ong for the finite anchoring conditions is incorrect and should be revised.

E. Conclusions

We explored in this paper the first-order transitions induced by the surface field and the optical field. For an initially homeotropically aligned LC cell, the exact criteria for the threshold and saturation FOFTs are given under any anchoring conditions. They can be summed up as follows:

(1) Weak interfacial interaction favors FOFT, i.e., small A_2 and negative A_4 may lead to the first-order transitions.

(2) Large material anisotropy favors FOFT, i.e., n_o/n_e should be small for both threshold and saturation FOFT; also, for the threshold FOFT, k_{11}/k_{33} should be small, and for the saturation FOFT, k_{33}/k_{11} should be small.

(3) The thinner cell favors FOFT. There exists a critical cell thickness for any positive nematic liquid-crystal homeotropic cell when A_4 is negative or positively minimal.

The surface interaction remains one of the least understood areas of the liquid-crystal physics; the conclusions obtained in this paper pose a question on the surface technique: how to obtain the surface anchoring condition of minimal A_2 and negative A_4. Under this condition, one may expect to observe the first-order transitions in the absence of any bias fields.

APPENDIX A

We denote $n_p(\theta)=n_o n_e/(\sqrt{n_o^2\sin^2\theta+n_e^2\cos^2\theta})$. Integrating Eq. (2.2) yields

$$\left(\frac{d\theta}{dz}\right)^2=\frac{2I}{ck_{33}}\frac{n_p(\theta_m)-n_p(\theta)}{1+(\kappa-1)\sin^2\theta}, \tag{A1}$$

or it is rewritten as

$$dz=\sqrt{\frac{ck_{33}}{2In_o}}(1+\mu\sin^2\theta_m)^{1/4}\sqrt{\frac{(1+\gamma\sin^2\theta)\sqrt{1+\mu\sin^2\theta}}{\sqrt{1+\mu\sin^2\theta}-\sqrt{1+\mu\sin^2\theta_m}}}d\theta. \tag{A2}$$

Substituting the above relations and Eqs. (2.13) into (2.1) yields

$$\begin{aligned}G_{\rm def}&=2S\int_0^{d/2}\left\{\frac{1}{2}k_{33}[1+(\kappa-1)\sin^2\theta]\left(\frac{d\theta}{dz}\right)^2-\frac{I}{c}n_p\right\}dz+SA_2\sin^2\theta_0(1+R\sin^2\theta_0)\\
&=2S\int_0^{d/2}\left\{\frac{I}{c}[n_p(\theta_m)-n_p(\theta)]-\frac{I}{c}n_p(\theta)\right\}dz+SA_2\sin^2\theta_0(1+R\sin^2\theta_0)\\
&=2S\int_{\theta_0}^{\theta_m}\left\{\frac{I}{c}n_p(\theta_m)-\frac{2I}{c}n_p(\theta)\right\}\sqrt{\frac{ck_{33}}{2I}\frac{[1+(\kappa-1)\sin^2\theta]}{[n_p(\theta_m)-n_p(\theta)]}}d\theta+SA_2\sin^2\theta_0(1+R\sin^2\theta_0)\\
&=S\sqrt{\frac{2Ik_{33}}{cn_o}}(1+\mu\sin^2\theta_m)^{1/4}\int_{\theta_0}^{\theta_m}\{n_p(\theta_m)-2n_p(\theta)\}\sqrt{\frac{(1+\gamma\sin^2\theta)\sqrt{1+\mu\sin^2\theta}}{\sqrt{1+\mu\sin^2\theta}-\sqrt{1+\mu\sin^2\theta_m}}}d\theta+SA_2\sin^2\theta_0(1+R\sin^2\theta_0)\\
&=S\sqrt{\frac{2IK_{33}}{cn_o}}(1+\mu\sin^2\theta_m)^{1/4}\{n_p(\theta_m)J_1-2n_oJ_2\}+SA_2\sin^2\theta_0(1+R\sin^2\theta_0)\\
&=\frac{2S}{d}\frac{k_{33}}{n_o}\sqrt{1+\mu\sin^2\theta_m}\{n_p(\theta_m)J_1^2-2n_oJ_1J_2\}+SA_2\sin^2\theta_0(1+R\sin^2\theta_0)\\
&=\frac{A_2S}{\alpha}\{J_1^2-2J_1J_2\sqrt{1+\mu\sin^2\theta_m}\}+SA_2\sin^2\theta_0(1+R\sin^2\theta_0).\end{aligned} \tag{A3}$$

Applying the same relations on Eq. (2.3) yields Eq. (2.7)

APPENDIX B

We define

$$V_n=\left(\frac{d^n\nu_0}{du^n}\right)_{u=0},\quad f_n(\nu_0)=\int_{\nu_0}^1\frac{\nu^n d\nu}{2\sqrt{\nu(1-\nu)}},$$

and then we have

$$f_0(\nu_0)=\arccos\sqrt{\nu_0},\quad f_1(\nu_0)=\frac{1}{2}[f_0(\nu_0)+\sqrt{\nu_0(1-\nu_0)}],\quad f_2(\nu_0)=\tfrac{3}{8}f_0(\nu_0)+\sqrt{\nu_0(1-\nu_0)}\left[\frac{3}{8}+\frac{\nu_0}{4}\right].$$

The boundary condition at $u=0$ becomes

$$\alpha\sqrt{\frac{V_0}{1-V_0}}=\arccos\sqrt{V_0}. \tag{B1}$$

We define $\beta=\arccos\sqrt{V_0}$, then (B1) becomes $\alpha=\beta tg\beta$. Taking the first-order u derivative at $u=0$ results in

$$\left[\frac{f_1(V_0)}{V_0(1-V_0)}\right]V_1=\frac{\kappa}{2}[f_1(V_0)+V_0f_0(V_0)]+\frac{3\mu}{8}[f_1(V_0)-V_0f_0(V_0)]-2RV_0f_0(V_0). \tag{B2}$$

Because

$$(J_1)_{u=0}=\sqrt{-\frac{2}{\mu}}f_0(V_0), \tag{B3}$$

$$\left(\frac{dJ_1}{du}\right)_{u=0}=\sqrt{-\frac{2}{\mu}}\left\{-\frac{V_1}{2\sqrt{V_0(1-V_0)}}+\frac{1}{8}(3\mu+4\kappa)f_1(V_0)+\frac{1}{8}\mu f_0(V_0)\right\}, \tag{B4}$$

so we have

$$\begin{aligned}\left(\frac{d}{du}\sqrt{\frac{I}{\tilde{I}}}\right)_{u=0}&=\frac{\mu}{4}(J_1)_{u=0}+\left(\frac{dJ_1}{du}\right)_{u=0}\\ &=\frac{\mu}{4}\sqrt{-\frac{2}{\mu}}f_0(V_0)+\sqrt{-\frac{2}{\mu}}\left\{-\frac{V_1}{2\sqrt{V_0(1-V_0)}}+\frac{1}{8}(3\mu+4\kappa)f_1(V_0)+\frac{1}{8}\mu f_0(V_0)\right\}\\ &=\sqrt{-\frac{2}{\mu}}\left\{\frac{\kappa}{4}\left[\frac{2f_1^2(V_0)}{\sqrt{V_0(1-V_0)}}-f_1(V_0)-V_0f_0(V_0)\right]\right.\\ &\quad\left.+\frac{3\mu}{16}\left[[f_1(V_0)+f_0(V_0)]\frac{2f_1(V_0)}{\sqrt{V_0(1-V_0)}}-f_1(V_0)+V_0f_0(V_0)\right]+RV_0f_0(V_0)\right\}.\end{aligned} \tag{B5}$$

We have, by applying Eq. (B1),

$$\left(\frac{dg_1}{du}\right)_{u=0}=\frac{1}{\alpha}[\alpha V_0-\sqrt{V_0(1-V_0)}f_0(V_0)]=0, \tag{B6}$$

and

$$\begin{aligned}\left(\frac{d^2g_1}{du^2}\right)_{u=0}&=\frac{2}{\alpha}\left[\frac{f_1(V_0)}{\sqrt{V_0(1-V_0)}}\right]V_1+\frac{2}{\alpha}\{(\tfrac{3}{4}\mu-\kappa)f_0(V_0)[f_2(V_0)-f_1(V_0)]-(\tfrac{3}{4}\mu+\kappa)f_1^2(V_0)+\alpha RV_0^2\}\\ &=\frac{2}{\alpha}\frac{\kappa}{4}\left[f_1(V_0)+V_0f_0(V_0)-\frac{2f_1^2(V_0)}{\sqrt{V_0(1-V_0)}}\right]+\frac{2}{\alpha}\left(\frac{3\mu}{16}\right)\left\{f_1(V_0)-V_0f_0(V_0)-[f_1(V_0)+f_0(V_0)]\frac{2f_1(V_0)}{\sqrt{V_0(1-V_0)}}\right\}\\ &\quad-\frac{2}{\alpha}RV_0f_0(V_0).\end{aligned} \tag{B7}$$

We define

$$t=\frac{2\alpha(1+2R)}{\kappa},\quad p=\alpha R,\quad s=\frac{\mu\kappa}{\eta},\quad X_n=\left(\frac{d^nx_0}{dw^n}\right)_{w=0},\quad h_n(x_0)=\int_{x_0}^{1}\frac{dx}{x^n\sqrt{1-x}},$$

then we have

$$h_1(x_0)=\ln\left(\frac{1+\sqrt{1-x_0}}{1-\sqrt{1-x_0}}\right),\quad h_2(x_0)=\frac{1}{2}h_1(x_0)+\frac{\sqrt{1-x_0}}{x_0},\quad h_3(x_0)=\frac{3}{8}h_1(x_0)+\frac{1}{2}\frac{\sqrt{1-x_0}}{x_0^2}+\frac{3}{4}\frac{\sqrt{1-x_0}}{x_0}.$$

The boundary condition at $w=0$ becomes

$$\ln\left(\frac{1+\sqrt{1-X_0}}{1-\sqrt{1-X_0}}\right)=\frac{t}{\sqrt{1-X_0}}. \tag{B8}$$

We define $B=\frac{1}{2}\ln[(1+\sqrt{1-X_0})/(1-\sqrt{1-X_0})]$, then we have $2B\tanh B=t$. The first-order derivative is

$$X_1=\frac{1}{\kappa}\left[\left(\frac{4p}{t}+\frac{1}{2}+\frac{3s}{8}\right)\frac{h_1(X_0)}{h_2(X_0)}\frac{(1-X_0)}{X_0}+\left(\frac{1}{2}-\frac{3s}{8}\right)(1-X_0)\right]. \tag{B9}$$

Because

$$(J_1)_{w=0} = \sqrt{-\frac{\kappa\eta}{2\mu}}\, h_1(X_0), \tag{B10}$$

$$\left(\frac{dJ_1}{dw}\right)_{w=0} = \sqrt{-\frac{\kappa\eta}{2\mu}} \left\{ \frac{-X_1}{X_0\sqrt{1-X_0}} + \left[\left(\frac{1}{2}\frac{1}{\kappa} - \frac{3}{8}\frac{\mu}{\eta} \right) h_2(X_0) - \frac{1}{8}\frac{\mu}{\eta} h_1(X_0) \right] \right\}. \tag{B11}$$

So we have

$$\begin{aligned} \left(\frac{d}{dw}\sqrt{\frac{I}{\tilde{I}}}\right)_{w=0} &= \frac{1}{4}\eta^{-3/4}(-\mu)(J_1)_{w=0} + \eta^{1/4}\left(\frac{dJ_1}{dw}\right)_{w=0} \\ &= \frac{1}{4}\eta^{-3/4}\sqrt{-\frac{\kappa\eta}{2\mu}} \left\{ h_1(X_0) + 4\eta \left[\frac{-X_1}{X_0\sqrt{1-X_0}} + \left(\frac{1}{2}\frac{1}{\kappa} - \frac{3}{8}\frac{\mu}{\eta} \right) h_2(X_0) - \frac{1}{8}\frac{\mu}{\eta} h_1(X_0) \right] \right\} \\ &= \frac{\eta^{3/4}}{\sqrt{-2\mu\kappa}\, h_2(X_0)} \left\{ \frac{1}{2}\left(\frac{t^2}{4(1-X_0)} + \frac{t}{2X_0} - \frac{t}{X_0^2} \right) - \frac{3s}{8}\left(\frac{3t^2}{4(1-X_0)} + \frac{3t}{2X_0} + \frac{t}{X_0^2} \right) - \frac{4p}{X_0^2} \right\}. \end{aligned} \tag{B12}$$

We have, by applying Eq. (B8),

$$\alpha\left(\frac{dg_2}{dw}\right)_{w=0} = \frac{\kappa}{2}\left[h_1(X_0)\,\frac{\sqrt{1-X_0}}{X_0} - \frac{t}{X_0} \right] = 0 \tag{B13}$$

and

$$\begin{aligned} \alpha\left(\frac{d^2g_2}{dw^2}\right)_{w=0} &= -\kappa X_1\left[\frac{h_2(X_0)}{X_0\sqrt{1-X_0}} \right] + 2\left\{ \left[\frac{1}{4} + \frac{3s}{16} \right] h_1(X_0)h_3(X_0) + \left[\frac{1}{4} - \frac{3s}{16} \right] h_2^2(X_0) + \left(-\frac{1}{4} - \frac{3s}{16} \right) h_1(X_0)h_2(X_0) + \frac{p}{X_0^2} \right\} \\ &= \frac{1}{2}\left\{ \frac{1}{2}\left(\frac{t^2}{4(1-X_0)} + \frac{t}{2X_0} - \frac{t}{X_0^2} \right) - \frac{3s}{8}\left(\frac{3t^2}{4(1-X_0)} + \frac{3t}{2X_0} + \frac{t}{X_0^2} \right) - \frac{4p}{X_0^2} \right\}. \end{aligned} \tag{B14}$$

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