Fréedericksz transition in the director-density coupling theory

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We show that the director-density coupling theory gives rise to a singular behavior for the mass density. To overcome this drawback, we propose to supplement the theory with a term that can be derived by regarding liquid crystals as anisotropic Korteweg fluids. We thus show that the static bevahior of the resulting theory predicts a Fréedericksz transition accompanied by a modulation in the mass density.

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I. INTRODUCTION

The acousto-optic effect in nematic liquid crystals [1–4] has provided the impetus for generalizing the Oseen-Frank energy by including effects due to the coupling between the liquid-crystal director $\hat{\mathbf{n}}$ and inhomogeneities in the mass density ρ [5,6]. In the framework in which liquid crystals are regarded as anisotropic Korteweg fluids [6–12], the usual Oseen-Frank energy density

$$f_{\text{of}} = \tfrac{1}{2}K_1(\nabla\cdot\hat{\mathbf{n}})^2 + \tfrac{1}{2}K_2[\hat{\mathbf{n}}\cdot(\nabla\times\hat{\mathbf{n}})]^2 + \tfrac{1}{2}K_3|\hat{\mathbf{n}}\times(\nabla\times\hat{\mathbf{n}})|^2, \tag{1}$$

where K_1, K_2, and K_3 are, respectively, the Frank constants for splay, twist, and bend, is supplemented with the elastic energy density

$$f_{\text{kf}} = \rho\left\{\sigma_0(\rho) + \tfrac{1}{2}B_0|\nabla\rho|^2 + \tfrac{1}{2}u_2[(\nabla\rho)\cdot\hat{\mathbf{n}}]^2\right\}, \tag{2}$$

where $\rho^2(d\sigma_0/d\rho)$ is an increasing function of ρ and B_0 and u_2 are acoustic susceptibilities.

Quite recently, the authors of Ref. [12] considered a nematic liquid-crystal cell with strong planar anchoring conditions at the boundaries. Assuming $K_1 = K_2 = K_3 \propto \rho$, they have shown that the static behavior of the theory [6] predicts a Fréedericksz-type transition followed by a mass density undulation. The critical threshold voltage of the transition coincides with that predicted by the Oseen-Frank static theory. In addition, expressions for the director and mass density profiles were also derived and discussed.

A few years before Virga's proposal [6], Selinger and collaborators [5] (see also Refs. [13–15]) introduced the elastic energy density,

$$f_{\text{ddc}} = \sum_{i,j}\left[u_1\left(\frac{\partial^2\rho}{\partial x^i\partial x^j}\right) + u_2\left(\frac{\partial\rho}{\partial x^i}\right)\left(\frac{\partial\rho}{\partial x^j}\right)\right]n_i n_j, \tag{3}$$

as a supplement to the Oseen-Frank energy density and, subsequently, applied the model to explain several experimental results [5,16–18]. Here u_1 and u_2 are the acoustic susceptibilities of the director-density coupling theory. We should like to observe in this connection that the u_1 term is essential for explaining the experimental data [19] for the action of ultrasonic waves on homeotropically aligned nematic liquid-crystal cells [20–23]. In discussing the Fréedericksz transition in nematic liquid crystals on the basis of the director-density coupling theory, we have found that f_{ddc} alone gives rise to a singular behavior for ρ [see Eq. (75) below]. Due to this difficulty, the proposal is to add the second term appearing in Eq. (2) to f_{ddc} in order to prevent the mass density from becoming singular. Thus, by retaining terms up to second order in $\partial\rho/\partial x^i$ [to be consistent with Eq. (3)], a more general elastic energy density thus obtained is given by

$$f = f_{\text{of}} + f_{\text{ddc}} + \tfrac{1}{2}B|\nabla\rho|^2, \tag{4}$$

where $B = \rho_0 B_0$ and ρ_0 is the average mass density. Here it is very important to emphasize that the inclusion of the B-dependent term does not alter our previous results reported in Refs. [21–23], since it would be reduced to a constant value with no influence on the dynamic of the director.

The rest of the paper is organized in the following way. In Sec. II we consider a liquid-crystal cell connected to a constant voltage source and derive the set of equations that determines the equilibrium configuration for ρ and $\hat{\mathbf{n}}$. We thus particularize the equations to the cases of homeotropic and planar alignments in Secs. III and IV, respectively. Finally, a summary and concluding remarks are provided in Sec. V.

II. THEORY

Consider a liquid-crystal cell consisting of a nematic liquid-crystal layer of thickness a sandwiched between two large parallel plates: The alignment can be either homeotropic [Fig. 1(a)] or planar [Fig. 1(b)]. A fixed voltage V is applied across the cell and hence an electric field

$$\mathbf{E} = E(z)\hat{\mathbf{z}} \tag{5}$$

along the z direction appears inside the cell. The electric displacement reads [24]

$$\mathbf{D} = \varepsilon_0[\varepsilon_\perp\mathbf{E} + (\Delta\varepsilon)(\mathbf{E}\cdot\hat{\mathbf{n}})\hat{\mathbf{n}}], \tag{6}$$

where ε_0 is the permittivity of vacuum; $\varepsilon_\perp$ and $\varepsilon_\parallel$ are, respectively, dielectric susceptibilities perpendicular and parallel to the director; $\Delta\varepsilon = \varepsilon_\parallel - \varepsilon_\perp$ denotes the dielectric anisotropy; and $\hat{\mathbf{n}} = \hat{\mathbf{n}}(z)$. In the absence of free charge one has $\nabla\cdot\mathbf{D} = 0$ and thus the z component of $\mathbf{D}$ is constant across the cell; in addition, it is related to the surface free charge density $\sigma = \hat{\mathbf{z}}\cdot\mathbf{D}$ on the bottom surface of the nematic cell. If we now return to Eq. (6), we find that

$$E(z) = \frac{\sigma}{\varepsilon_0[\varepsilon_\perp + (\Delta\varepsilon)(\hat{\mathbf{n}}\cdot\hat{\mathbf{z}})^2]}. \tag{7}$$

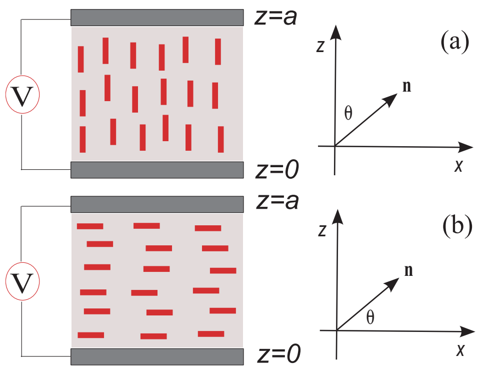

FIG. 1. (Color online) Cell of thickness a containing nematic liquid crystal connected to a fixed voltage source: (a) homeotropic alignment and (b) planar alignment. On the right, the coordinate system defines the angles θ for the director.

The equilibrium configuration of the director is found by minimizing [24]

$$g = \int_0^a \left(f - \frac{1}{2}\mathbf{D}\cdot\mathbf{E} \right) dz \tag{8}$$

with respect to $\theta(z)$ and $\rho(z)$ and subject to the constraint of global mass conservation

$$\int_0^a \rho(z)\, dz = M \tag{9}$$

and fixed voltage

$$\int_0^a E(z)\, dz = V. \tag{10}$$

In contrast to the assumption made in Ref. [12] (see the Introduction), we emphasize that no relevant dependence of the Frank constants on ρ is assumed from now on [5]. Applying techniques from the calculus of variations to isoperimetric problems [25], the equilibrium configuration is obtained by solving the following set of coupled equations:

$$\frac{\partial \tilde{f}}{\partial \sigma} = 0, \tag{11}$$

$$\frac{d^2}{dz^2}\left(\frac{\partial \tilde{f}}{\partial \rho_{zz}}\right) - \frac{d}{dz}\left(\frac{\partial \tilde{f}}{\partial \rho_z}\right) + \frac{\partial \tilde{f}}{\partial \rho} = 0, \tag{12}$$

$$\frac{\partial \tilde{f}}{\partial \theta} - \frac{d}{dz}\left(\frac{\partial \tilde{f}}{\partial \theta_z}\right) = 0, \tag{13}$$

in which $\theta_z \equiv d\theta/dz$, $\rho_z \equiv d\rho/dz$, $\rho_{zz} \equiv d^2\rho/dz^2$,

$$\begin{aligned} \tilde{f} &= f - \frac{1}{2}\mathbf{D}\cdot\mathbf{E} + \mu\rho + \lambda E \\ &= f + \mu\rho + \frac{2\lambda\sigma - \sigma^2}{2\varepsilon_0[\varepsilon_\perp + (\Delta\varepsilon)(\hat{\mathbf{n}}\cdot\hat{\mathbf{z}})^2]}, \end{aligned} \tag{14}$$

μ and λ are (constant) Lagrange multipliers, and use of $\mathbf{D}\cdot\mathbf{E} = \sigma E(z)$ has been made. The substitution of $\tilde{f}$ in Eq. (11) gives us directly

$$\lambda = \sigma \tag{15}$$

and then the case of constant voltage is mapped onto the case of constant charge [24]. In addition, since $\partial \tilde{f}/\partial\rho = \mu$, we see that Eq. (12) can be immediately integrated to yield

$$\frac{d}{dz}\left(\frac{\partial \tilde{f}}{\partial \rho_{zz}}\right) - \left(\frac{\partial \tilde{f}}{\partial \rho_z}\right) + \mu z = C, \tag{16}$$

where C is a constant of integration. In order to compare our results with those reported in Ref. [12], we shall assume throughout the paper the strong-anchoring boundary condition, i.e.,

$$\theta(0) = \theta(a) = 0 \tag{17}$$

and

$$\left(\frac{d\rho}{dz}\right)_{z=0} = \left(\frac{d\rho}{dz}\right)_{z=a} = 0. \tag{18}$$

III. HOMEOTROPIC ALIGNMENT

For homeotropic geometry, the case of interest is that of negative dielectric materials. In considering this, we set

$$\Delta\varepsilon = -|\Delta\varepsilon| \tag{19}$$

for convenience. Now we see from Fig. 1(a) that

$$\hat{\mathbf{n}}\cdot\hat{\mathbf{z}} = \cos\theta(z) \tag{20}$$

and thus Eq. (14) becomes

$$\begin{aligned} \tilde{f} &= \frac{1}{2}(K_1\sin^2\theta + K_3\cos^2\theta)\left(\frac{d\theta}{dz}\right)^2 + \frac{1}{2}B(\rho_z)^2 + \mu\rho \\ &\quad + [u_1\rho_{zz} + u_2(\rho_z)^2]\cos^2\theta + \frac{\sigma^2}{2\varepsilon_0(\varepsilon_\perp - |\Delta\varepsilon|\cos^2\theta)}. \end{aligned} \tag{21}$$

When we insert Eq. (21) into Eq. (16) we obtain

$$-u_1\left(\frac{d\theta}{dz}\right)\sin(2\theta) - (B + 2u_2\cos^2\theta)\left(\frac{d\rho}{dz}\right) + \mu z = C. \tag{22}$$

By virtue of (17) and (18), it is straightforward to find that $C = 0$ and also $\mu = 0$. Therefore, the space derivatives of ρ and θ are interrelated as follows:

$$\frac{d\rho}{dz} = -\frac{u_1\sin(2\theta)}{B + 2u_2\cos^2\theta}\left(\frac{d\theta}{dz}\right). \tag{23}$$

Now we substitute Eq. (21) into Eq. (13). A little calculation yields

$$\begin{aligned} &(K_1\sin^2\theta + K_3\cos^2\theta)\frac{d^2\theta}{dz^2} + \frac{1}{2}(K_1 - K_3)\left(\frac{d\theta}{dz}\right)^2\sin(2\theta) \\ &+ \frac{|\Delta\varepsilon|\sigma^2\sin(2\theta)}{2\varepsilon_0[\varepsilon_\perp - |\Delta\varepsilon|\cos^2\theta]^2} + \left[u_1\frac{d^2\rho}{dz^2} + u_2\left(\frac{d\rho}{dz}\right)^2\right] \\ &\times\sin(2\theta) = 0. \end{aligned} \tag{24}$$

In the following, we explore the consequences of Eqs. (23) and (24).

A. Uniform density

First, we examine the equilibrium configuration with uniform mass density as follows:

$$\rho(z) = \frac{M}{a}. \tag{25}$$

When this is put into Eq. (23), we find that the relationship

$$u_1\left(\frac{d\theta}{dz}\right)\sin(2\theta) = 0 \tag{26}$$

must be satisfied for all values of z between 0 and a. This, together with the boundary condition (17), implies

$$\theta(z) = 0, \tag{27}$$

which also satisfies Eq. (24). Upon returning to Eq. (10), we thus eliminate σ in favor of V,

$$\sigma = \frac{\varepsilon_0\varepsilon_\parallel}{a}V. \tag{28}$$

Finally, Eq. (8) furnishes the corresponding free energy for the nondistorted director profile,

$$g = -\frac{\varepsilon_0\varepsilon_\parallel}{2a}V^2. \tag{29}$$

B. Nonuniform density

Next we shall discuss the case in which inhomogeneities in density appear. To proceed with the analytical calculation, it is necessary to employ a simplifying approximation. Specifically, we limit ourselves to describe the vicinity of the Fréedericksz transition in which $\theta \ll 1$. Thus, by neglecting terms of $\mathcal{O}(\theta^5)$, we find that

$$\left[u_1\frac{d^2\rho}{dz^2} + u_2\left(\frac{d\rho}{dz}\right)^2\right]\sin(2\theta) = -\frac{4u_1^2}{B+2u_2}\left(\frac{d^2\theta}{dz^2}\right)\sin^2\theta - \frac{2u_1^2}{B+2u_2}\left(\frac{d\theta}{dz}\right)^2\sin(2\theta) + \mathcal{O}(\theta^5). \tag{30}$$

The reason for keeping $\sin^2\theta$ and $\sin(2\theta)$ in the right-hand side of Eq. (30), instead of replacing them with θ^2 and 2θ, respectively, as would expected, lies in the fact that after the substitution of Eq. (30) in Eq. (24) we arrive at

$$(K_1'\sin^2\theta + K_3\cos^2\theta)\frac{d^2\theta}{dz^2} + \frac{1}{2}(K_1' - K_3)\left(\frac{d\theta}{dz}\right)^2\sin(2\theta) + \frac{|\Delta\varepsilon|\sigma^2\sin(2\theta)}{2\varepsilon_0[\varepsilon_\parallel + |\Delta\varepsilon|\sin^2\theta]^2} = 0, \tag{31}$$

where

$$K_1' = K_1 - \frac{4u_1^2}{B+2u_2} \tag{32}$$

is the renormalized constant for splay and assumed to be positive. Here we have eliminated $\cos^2\theta$ that is present in the third term of Eq. (24) in favor of $\sin^2\theta$ in going to Eq. (31). Therefore, the net result of considering inhomogeneities in density is to renormalize the constant for splay only [see Eq. (24) with $u_1 = u_2 = 0$] and we can proceed, within an error of $\mathcal{O}(\theta^5)$, without more approximations. It turns out that the differential equation (31) is exactly soluble [24]. In fact, after multiplying it by $d\theta/dz$, it can be cast in the form

$$\frac{d}{dz}\left[\frac{1}{2}(K_1'\sin^2\theta + K_3\cos^2\theta)\left(\frac{d\theta}{dz}\right)^2\right] - \frac{d}{dz}\left[\frac{\sigma^2}{2\varepsilon_0[\varepsilon_\parallel + |\Delta\varepsilon|\sin^2\theta]}\right] = 0, \tag{33}$$

which is immediately integrated to yield

$$(K_1'\sin^2\theta + K_3\cos^2\theta)\left(\frac{d\theta}{dz}\right)^2 - \frac{\sigma^2}{\varepsilon_0[\varepsilon_\parallel + |\Delta\varepsilon|\sin^2\theta]} = C'. \tag{34}$$

The constant

$$C' = -\frac{\sigma^2}{\varepsilon_0[\varepsilon_\parallel + |\Delta\varepsilon|\sin^2\theta_m]} \tag{35}$$

is determined by imposing symmetric distortion around $z = \frac{a}{2}$, that is,

$$\left(\frac{d\theta}{dz}\right)_{z=\frac{a}{2}} = 0, \tag{36}$$

$$\theta\left(z = \frac{a}{2}\right) = \theta_m, \tag{37}$$

where θ_m is the maximum angle. The solution with $d\theta/dz \geqslant 0$ and valid in the range $0 \leqslant z \leqslant a/2$ is given by the following pair of coupled equations:

$$\int_0^{\theta} I(\alpha)\,d\alpha = \frac{z\sigma}{\sqrt{\varepsilon_0}}, \tag{38}$$

$$\int_0^{\theta_m} I(\alpha)\,d\alpha = \frac{a\sigma}{2\sqrt{\varepsilon_0}}, \tag{39}$$

where

$$I(\alpha) = \sqrt{K_1'\sin^2\alpha + K_3\cos^2\alpha}\times\left(\frac{1}{\varepsilon_\parallel + |\Delta\varepsilon|\sin^2\alpha} - \frac{1}{\varepsilon_\parallel + |\Delta\varepsilon|\sin^2\theta_m}\right)^{-1/2} = \frac{\varepsilon_\parallel\sqrt{K_3}}{\sqrt{|\Delta\varepsilon|}\sqrt{\theta_m^2 - \alpha^2}}(1 + A_1\alpha^2 + A_2\theta_m^2 + A_3\alpha^4 + A_4\alpha^2\theta_m^2 + A_5\theta_m^4 + \cdots), \tag{40}$$

and

$$A_1 = \frac{K_1'}{2K_3} + \frac{|\Delta\varepsilon|}{2\varepsilon_\parallel} - \frac{1}{3}, \tag{41}$$

$$A_2 = \frac{|\Delta\varepsilon|}{2\varepsilon_\parallel} + \frac{1}{6}, \tag{42}$$

$$A_3 = \frac{K_1'|\Delta\varepsilon|}{4K_3\varepsilon_\parallel} + \frac{K_1'}{6K_3} - \frac{1}{8}\left(\frac{K_1'}{K_3}\right)^2 - \frac{|\Delta\varepsilon|}{3\varepsilon_\parallel} - \frac{1}{8}\left(\frac{|\Delta\varepsilon|}{\varepsilon_\parallel}\right)^2 - \frac{1}{45}, \tag{43}$$

$$A_4 = \frac{K_1'|\Delta\varepsilon|}{4K_3\varepsilon_\parallel} + \frac{K_1'}{12K_3} + \frac{1}{4}\left(\frac{|\Delta\varepsilon|}{\varepsilon_\parallel}\right)^2 - \frac{|\Delta\varepsilon|}{12\varepsilon_\parallel} - \frac{1}{45}, \quad (44)$$

$$A_5 = \frac{7}{360} - \frac{|\Delta\varepsilon|}{12\varepsilon_\parallel} - \frac{1}{8}\left(\frac{|\Delta\varepsilon|}{\varepsilon_\parallel}\right)^2. \quad (45)$$

For $z > a/2$, one has

$$\theta(z) = \theta(a - z). \quad (46)$$

The above expansion is useful to proceed with the analytical discussion and, in addition, is in agreement with our observation below Eq. (32). Indeed, substituting this result back into Eq. (39) yields, putting $\alpha = \theta_m \sin\phi$,

$$1 + A\theta_m^2 + D\theta_m^4 + \cdots = \frac{\sigma}{\sigma_c}, \quad (47)$$

in which

$$A \equiv \frac{A_1}{2} + A_2, \quad (48)$$

$$D \equiv \frac{3A_3}{8} + \frac{A_4}{2} + A_5, \quad (49)$$

$$\sigma_c \equiv \frac{\pi\varepsilon_\parallel}{a}\sqrt{\frac{\varepsilon_0 K_3}{|\Delta\varepsilon|}}. \quad (50)$$

It is clear that Eq. (47) admits solution only if $\sigma \geqslant \sigma_c$. In this case, one finds

$$\theta_m = \frac{1}{\sqrt{A}}\left(\frac{\sigma - \sigma_c}{\sigma_c}\right)^{1/2}\left[1 - \frac{D}{2A^2}\left(\frac{\sigma - \sigma_c}{\sigma_c}\right) + \cdots\right]. \quad (51)$$

To illustrate that the calculation is working properly, in Fig. 2 we show a graphical comparison between Eqs. (39) and (51). We now substitute expansion (40) into Eq. (38) and, after integrating, we obtain

$$\phi_0 + \left[A\phi_0 - \frac{A_1}{4}\sin(2\phi_0)\right]\theta_m^2 + \mathcal{O}\left(\frac{\sigma - \sigma_c}{\sigma_c}\right)^2 = \frac{\pi\sigma z}{a\sigma_c}, \quad (52)$$

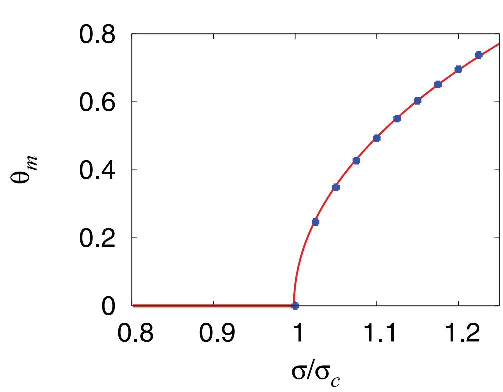

FIG. 2. (Color online) Maximum angle versus σ/σ_c for $K_1 = 6.4 \times 10^{-12}$ N, $K_3 = 10 \times 10^{-12}$ N, $|\Delta\varepsilon| = 1.0$, and $\varepsilon_\parallel = 3.0$. The solid line is obtained from Eq. (39) and the dots are calculated using Eq. (51).

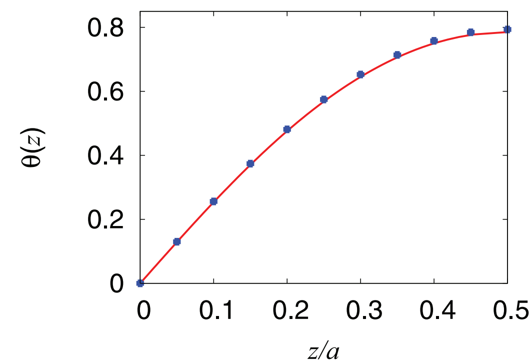

FIG. 3. (Color online) $\theta(z)$ versus z/a for $K_1 = 6.4 \times 10^{-12}$ N, $K_3 = 10 \times 10^{-12}$ N, $|\Delta\varepsilon| = 1.0$, and $\varepsilon_\parallel = 3.0$. The solid line is obtained from Eq. (38) using $\theta_m = 0.7854$ and $\sigma/\sigma_c = 1.2602$, and the dots are calculated using Eq. (56).

where

$$\theta(z) = \theta_m \sin(\phi_0). \quad (53)$$

Next we put

$$\phi_0 = \frac{\pi\sigma z}{a\sigma_c} + \delta\phi_0 \quad (54)$$

into Eq. (52) and, after retaining terms up to first order in $\delta\phi_0$, we obtain

$$\delta\phi_0 = \left[\frac{A_1}{4}\sin\left(\frac{2\pi\sigma z}{a\sigma_c}\right) - \frac{A\pi\sigma z}{a\sigma_c}\right]\theta_m^2 + \mathcal{O}\left(\frac{\sigma - \sigma_c}{\sigma_c}\right)^2. \quad (55)$$

The use of Eqs. (51), (54), and (55) in Eq. (53) enables us to write

$$\theta(z) = \frac{1}{\sqrt{A}}\left(\frac{\sigma - \sigma_c}{\sigma_c}\right)^{1/2}\sin\left(\frac{\pi z}{a}\right) \times\left\{1 + \frac{1}{2A}\left[A_1\cos^2\left(\frac{\pi z}{a}\right) - \frac{D}{A}\right]\left(\frac{\sigma - \sigma_c}{\sigma_c}\right) + \cdots\right\}, \quad (56)$$

which is valid in the entire range of the variable z, since Eq. (56) satisfies the relationship given by Eq. (46). We should like to observe here that $\theta(z = \frac{a}{2}) = \theta_m$ [see Eq. (51)] and $(d\theta/dz)_{z=\frac{a}{2}} = 0$, as required by Eqs. (36) and (37); moreover, up to $\mathcal{O}(\frac{\sigma-\sigma_c}{\sigma_c})^{3/2}$, $\theta(z)$ given by Eq. (56), satisfies Eq. (24). Finally, a graphical comparison between Eqs. (38) and (56) is also shown in Fig. 3, in which the numerical values $\theta_m = 0.7854$ and $\sigma/\sigma_c = 1.2602$ were previously calculated using Eq. (39). It remains to eliminate σ in favor of V. First, we manipulate Eq. (10) to bring it into the form

$$\frac{\sigma}{\varepsilon_0\varepsilon_\parallel}\int_0^a\left[1 - \frac{|\Delta\varepsilon|}{\varepsilon_\parallel}\theta^2 + \frac{|\Delta\varepsilon|}{\varepsilon_\parallel}\left(\frac{|\Delta\varepsilon|}{\varepsilon_\parallel} + \frac{1}{3}\right)\theta^4 + \cdots\right] \times dz = V. \quad (57)$$

The integration is straightforward and, after a little algebra, we find that

$$G\left(\frac{\sigma - \sigma_c}{\sigma_c}\right) + H\left(\frac{\sigma - \sigma_c}{\sigma_c}\right)^2 + \cdots = \frac{V - V_c}{V_c}, \quad (58)$$

where

$$G = \frac{K_1'\varepsilon_\parallel + K_3|\Delta\varepsilon|}{K_1'\varepsilon_\parallel + 3K_3|\Delta\varepsilon|}, \tag{59}$$

$$H = \frac{|\Delta\varepsilon|(3|\Delta\varepsilon|A + \varepsilon_\parallel A - 4\varepsilon_\parallel A^2 - \varepsilon_\parallel A_1 A + 4\varepsilon_\parallel D)}{8\varepsilon_\parallel^2 A^3}, \tag{60}$$

$$V_c = \pi\sqrt{\frac{K_3}{\varepsilon_0|\Delta\varepsilon|}}. \tag{61}$$

Resolving Eq. (58) for $(\frac{\sigma-\sigma_c}{\sigma_c})$ yields

$$\left(\frac{\sigma-\sigma_c}{\sigma_c}\right) = \frac{1}{G}\left(\frac{V-V_c}{V_c}\right) - \frac{H}{G^3}\left(\frac{V-V_c}{V_c}\right)^2 + \cdots. \tag{62}$$

This must be substituted back into Eq. (56), and the final expression for $\theta(z)$ as a function of the measurable quantity V is given by

$$\theta(z) = \frac{1}{\sqrt{AG}}\left(\frac{V-V_c}{V_c}\right)^{1/2}\left\{\sin\left(\frac{\pi z}{a}\right) + \left[A_6\sin\left(\frac{\pi z}{a}\right) + A_7\sin\left(\frac{3\pi z}{a}\right)\right]\left(\frac{V-V_c}{V_c}\right) + \cdots\right\}, \tag{63}$$

where

$$A_6 = \frac{A_1}{8AG} - \frac{H}{2G^2} - \frac{D}{2A^2G}, \tag{64}$$

$$A_7 = \frac{A_1}{8AG}. \tag{65}$$

Having obtained $\theta(z)$, the next step is to return to Eq. (23) in order to calculate the corresponding mass density profile. After a little inspection, we see that

$$\frac{d\rho}{dz} = -\frac{u_1}{B+2u_2}\frac{d}{dz}\left[\theta^2 + \frac{u_2-B}{3(B+2u_2)}\theta^4\right] + \mathcal{O}(\theta^6) \tag{66}$$

and thus we obtain

$$\rho(z) = \frac{M}{a} + \frac{u_1}{2AG(B+2u_2)}\left(\frac{V-V_c}{V_c}\right)\left(\cos\left(\frac{2\pi z}{a}\right) + \left\{\frac{1}{G}\left[\frac{u_2-B}{3A(B+2u_2)} - \frac{H}{G} - \frac{D}{A^2}\right]\cos\left(\frac{2\pi z}{a}\right) - \frac{1}{4AG}\left[\frac{u_2-B}{3(B+2u_2)} - A_1\right]\cos\left(\frac{4\pi z}{a}\right)\right\} \times\left(\frac{V-V_c}{V_c}\right) + \cdots\right), \tag{67}$$

where we have used Eq. (9) to calculate the constant of integration. We are now in a position to obtain the energetic cost, via Eq. (8), associated with the distortion given by Eq. (63). The calculation is lengthy albeit straightforward. We give, therefore, only the final result,

$$g = -\frac{\varepsilon_0\varepsilon_\parallel V_c^2}{2a}\left[1 + 2\left(\frac{V-V_c}{V_c}\right) + Z\left(\frac{V-V_c}{V_c}\right)^2 + \cdots\right], \tag{68}$$

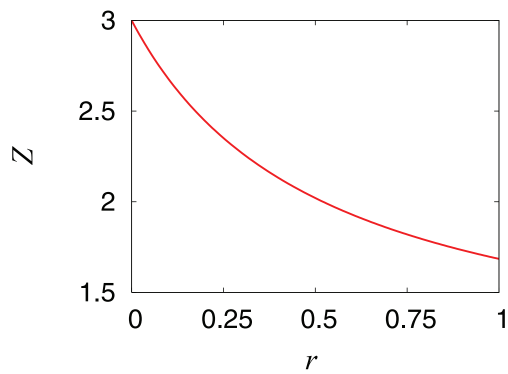

FIG. 4. (Color online) Plot of Z as a function of $r \equiv K_1'/K_1$ for $K_1 = 6.4\times10^{-12}$ N, $K_3 = 10\times10^{-12}$ N, $|\Delta\varepsilon| = 1.0$, and $\varepsilon_\parallel = 3.0$.

where

$$Z = \frac{G-2H}{G^3} + \frac{|\Delta\varepsilon|}{\varepsilon_\parallel(AG)^2}\left(\frac{AH}{G} + \frac{D}{A} - A_1\right). \tag{69}$$

It is interesting to call attention to the contribution of $f_{\rm ddc}$ for the free energy,

$$\int_0^a f_{\rm ddc}\,dz = -\frac{\pi^2u_1^2(B+u_2)}{2a(AG)^2(B+2u_2)^2}\left(\frac{V-V_c}{V_c}\right)^2 + \cdots. \tag{70}$$

A representative plot of Z as a function of $r \equiv K_1'/K_1$ is shown in Fig. 4. Since $Z > 1$, the free energy (68) is smaller than that given by Eq. (29): $g = -\frac{\varepsilon_0\varepsilon_\parallel V_c^2}{2a}[1 + 2(\frac{V-V_c}{V_c}) + (\frac{V-V_c}{V_c})^2]$. Therefore, the elastic energy (4) predicts a Fréedericksz transition accompanied by inhomogeneities in density.

Moreover, the critical threshold voltage, see Eq. (61), coincides with that predicted by the Oseen-Frank static theory.

IV. PLANAR ALIGNMENT

For planar geometry, the case of interest is that of positive dielectric anisotropy,

$$\Delta\varepsilon > 0. \tag{71}$$

Almost all we need to proceed with the discussion has been already presented in Secs. II and III. This helps us, therefore, to simplify the analysis. Noting from Fig. 1(b) that

$$\hat{\mathbf{n}}(z) = \hat{\mathbf{x}}\cos\theta(z) + \hat{\mathbf{z}}\sin\theta(z), \tag{72}$$

we thus find that Eq. (14) becomes

$$\tilde{f} = \frac{1}{2}(K_1\cos^2\theta + K_3\sin^2\theta)\left(\frac{d\theta}{dz}\right)^2 + \frac{1}{2}B(\rho_z)^2 + \mu\rho + [u_1\rho_{zz} + u_2(\rho_z)^2]\sin^2\theta + \frac{\sigma^2}{2\varepsilon_0(\varepsilon_\perp + \Delta\varepsilon\sin^2\theta)}. \tag{73}$$

The substitution of Eq. (73) into Eq. (16) now implies

$$\frac{d\rho}{dz} = \frac{u_1\sin(2\theta)}{B+2u_2\sin^2\theta}\left(\frac{d\theta}{dz}\right), \tag{74}$$

which should be contrasted with Eq. (23). Note that for $B = 0$, the above equation makes the disconcerting prediction that

$$\lim_{z\to 0^+} \frac{d\rho}{dz} = \infty, \quad (75)$$

which we have removed in advance by considering a term coming from Virga's theory, without fully adhering to it. In addition, one sees clearly from Eqs. (23) and (74) [and confirmed by Eq. (67) and Eq. (84) below] that the u_1 term in Eq. (3) is crucial to trigger density instability and it helps to reduce the free energy [see Eq. (70) and Eq. (86) below]. After these comments to justify the introduction of $\frac{1}{2}B|\nabla\rho|^2$ into $f_{\rm ddc}$, we note that the substitution of Eq. (73) into Eq. (13) results in

$$(K_3\sin^2\theta + K_1\cos^2\theta)\frac{d^2\theta}{dz^2} + \frac{1}{2}(K_3 - K_1)\left(\frac{d\theta}{dz}\right)^2\sin(2\theta) + \frac{(\Delta\varepsilon)\sigma^2\sin(2\theta)}{2\varepsilon_0[\varepsilon_\perp + (\Delta\varepsilon)\sin^2\theta]^2} - \left[u_1\frac{d^2\rho}{dz^2} + u_2\left(\frac{d\rho}{dz}\right)^2\right] \times \sin(2\theta) = 0. \quad (76)$$

A. Uniform density

A nondistorted director profile coexisting with an uniform mass density profile is compatible with Eqs. (74) and (76). Therefore, the corresponding free energy reads

$$g = -\frac{\varepsilon_0\varepsilon_\perp}{2a}V^2, \quad (77)$$

where we have used $\sigma = (\varepsilon_0\varepsilon_\perp/a)V$ to eliminate σ in favor of V. This expression should be compared with Eq. (29).

B. Nonuniform density

Following the previously developed scheme of approximation [see Eq. (30)], we substitute

$$\left[u_1\frac{d^2\rho}{dz^2} + u_2\left(\frac{d\rho}{dz}\right)^2\right]\sin(2\theta) = \frac{4u_1^2}{B}\left(\frac{d^2\theta}{dz^2}\right)\sin^2\theta + \frac{2u_1^2}{B}\left(\frac{d\theta}{dz}\right)^2\sin(2\theta) + \mathcal{O}(\theta^5) \quad (78)$$

in Eq. (76) to obtain

$$(K_3'\sin^2\theta + K_1\cos^2\theta)\frac{d^2\theta}{dz^2} + \frac{1}{2}(K_3' - K_1)\left(\frac{d\theta}{dz}\right)^2\sin(2\theta) + \frac{(\Delta\varepsilon)\sigma^2\sin(2\theta)}{2\varepsilon_0[\varepsilon_\perp + (\Delta\varepsilon)\sin^2\theta]^2} = 0, \quad (79)$$

where the renormalized constant for bend

$$K_3' = K_3 - \frac{4u_1^2}{B} \quad (80)$$

is assumed to be positive. Note that the above Euler-Lagrange equation for θ is mapped onto the one given by Eq. (31) by the correspondence $K_1' \leftrightarrow K_3'$, $K_3 \leftrightarrow K_1$, $\varepsilon_\parallel \leftrightarrow \varepsilon_\perp$, and $|\Delta\varepsilon| \leftrightarrow (\Delta\varepsilon)$. This correspondence also applies to establish a map between Eq. (57) and the corresponding one for the planar alignment case:

$$\frac{\sigma}{\varepsilon_0\varepsilon_\perp}\int_0^a\left[1 - \frac{\Delta\varepsilon}{\varepsilon_\perp}\theta^2 + \frac{\Delta\varepsilon}{\varepsilon_\perp}\left(\frac{\Delta\varepsilon}{\varepsilon_\perp} + \frac{1}{3}\right)\theta^4 + \cdots\right]dz = V. \quad (81)$$

Since $\theta(z)$ also satisfies the conditions given by Eqs. (36), (37), and (46), the solution of (79) thus may be immediately deduced from Eq. (63). In particular, the threshold voltage is given by

$$V_c' = \pi\sqrt{\frac{K_1}{\varepsilon_0(\Delta\varepsilon)}}. \quad (82)$$

Our prediction for $\theta(z)$ differs significantly from that reported in Ref. [12] [see Eq. (4.24) in which $\epsilon \to \sqrt{(V - V_c')/V_c'}$],

$$\theta(z) = \overline{A}\left(\frac{V - V_c'}{V_c'}\right)^{1/2}\sin\left(\frac{\pi z}{a}\right) + \overline{B}\left(\frac{V - V_c'}{V_c'}\right)\sin\left(\frac{\pi z}{a}\right) + \cdots. \quad (83)$$

The mass density profile follows from Eq. (74). Up to $\mathcal{O}(\frac{V-V_c'}{V_c'})$, we find

$$\rho(z) = \frac{M}{a} - \frac{2u_1K_1\varepsilon_\perp}{B[K_3'\varepsilon_\perp + K_1(\Delta\varepsilon)]}\left(\frac{V - V_c'}{V_c'}\right)\cos\left(\frac{2\pi z}{a}\right) + \cdots, \quad (84)$$

whose dependence on V and z coincides with that obtained in Ref. [12]. Finally, we give the free energy for $V \geqslant V_c'$ as follows:

$$g = -\frac{\varepsilon_0\varepsilon_\perp V_c'^2}{2a}\left[1 + 2\left(\frac{V - V_c'}{V_c'}\right) + Z'\left(\frac{V - V_c'}{V_c'}\right)^2 + \cdots\right], \quad (85)$$

where Z' is obtained from Eq. (69) by using the correspondence described in the text below Eq. (80). A representative plot of Z' versus $r' \equiv K_3'/K_3$ is shown in Fig. 5. In passing, we note that the contribution of $f_{\rm ddc}$ for g is given by

$$\int_0^a f_{\rm ddc}\,dz = -\frac{\pi^2u_1^2}{2a(A'G')^2B}\left(\frac{V - V_c'}{V_c'}\right)^2 + \cdots. \quad (86)$$

We thus arrive at the same conclusion as in the case of homeotropic alignment, namely that the system undergoes

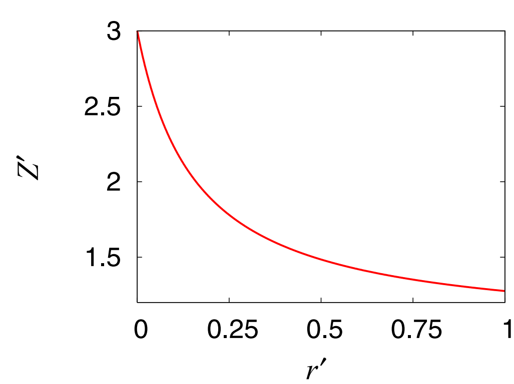

FIG. 5. (Color online) Plot of Z' as a function of $r' \equiv K_3'/K_3$ for $K_1 = 6.4 \times 10^{-12}$ N, $K_3 = 10 \times 10^{-12}$ N, $\Delta\varepsilon = 1.0$, and $\varepsilon_\perp = 4.0$.

a Fréedericksz transition driven by V followed by inhomogeneities in density. As before, V_c' coincides with the critical voltage predicted by the Oseen-Frank static theory.

V. CONCLUDING REMARKS

In conclusion, we have discussed the Fréedericksz transition in nematic liquid crystals in the framework of the director-density coupling theory and have found that $f_{\rm ddc}$ alone predicts a singular behavior for ρ. To avoid this nonphysical divergence, we have then supplemented the theory with the term $\frac{1}{2}B|\nabla\rho|^2$ that penalizes rapid changes in ρ independently of the orientation of $\hat{\mathbf{n}}$. In doing so, we have shown that the theory predicts that the Fréedericksz transition is necessarily accompanied by inhomogeneities in the mass density. It is a remarkable fact that, within an error of $\mathcal{O}(\theta^5)$, the effect of $f_{\rm ddc} + \frac{1}{2}B|\nabla\rho|^2$ on $\hat{\mathbf{n}}$ is to renormalize the Frank constants K_1 (homeotropic alignment) and K_3 (planar alignment) only. Finally, we point out that our results differ from the ones reported in Ref. [12] and only experimental data can validate (or invalidate) the competing theories.

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