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Surface anchoring energy and the first order Fréedericksz transition of a NLC cell

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Many authors have suggested new forms to describe the surface anchoring energy of the liquid crystal–wall interface, replacing the Rapini-Papoular (RP) formula $g_s = (1/2)A \sin^2 \theta$. If the RP function is considered as the primary approximation, and a lowest order modification is included, then the surface anchoring energy can be represented by $g_s = (1/2)A \sin^2 \theta(1 + \zeta \sin^2 \theta)$. ζ characterizes the modification to the RP formula and varies for the different energy forms. It is well known that the RP formula predicts a second order Fréedericksz transition. This paper points out that the transition can be first order if the modification is taken into account, in which case at the threshold point the tilt angle of the director at the middle layer of the cell, θ_m, is finite. The conditions for the existence of the first order transition are obtained; $\zeta < 0$ is required for a first order transition. The approximate expression of the threshold field is also given.

1. Introduction

Surface effects of liquid crystals are important for both device applications and basic understanding of physical phenomena, and surface-induced alignment has long been used to obtain a single crystalline layer of a nematic liquid crystal (NLC) for practical as well as measurement purposes. To quantify how strongly a NLC is oriented or anchored, the interfacial free energy g_s, also called anchoring energy, has been introduced. Rapini and Papoular have proposed a simple phenomenological expression for the anchoring energy per unit area [1],

$$g_s = \frac{1}{2} A \sin^2 \theta \tag{1}$$

where θ is the angle between the easy direction **e** and the director **n** of the NLC at the nematic–wall interface. This is the so-called RP formula. These, as well as many other authors, have studied the director distribution of a LC medium and the related physical phenomena through continuum theory and have measured A in this way [2]. Formula (1) states the boundary condition on the nematic director. It is important to study the Fréedericksz transition of a NLC cell in theory and practice. It can be strictly proved that when the anchoring energy takes the form of equation (1), only a second order transition will occur [3]. At the transition point, the director changes continuously with the external field. By this property of the second order transition, one can calculate the threshold field as well as the saturation field. This property also underlies the calculation of surface effects and their applications.

The RP formula describes many effects successfully in the presence of a surface. However, it is found that the results calculated from the RP formula do not agree well with the experimental observations in some cases (for instance, the distortions of the director in strong external fields) [4]. Many authors have introduced new anchoring energy forms to replace the RP formula. Yang and Rosenblatt [5], Yang [6], Yokoyama and van Sprang [7], and Barbero and Durand [8] express g_s in Legendre polynomial functions of $\sin \theta$. Barbero [9] expands g_s into a Fourier series. Barnik [10] utilizes the elliptic function of θ as the functional form of g_s.

Because of these new forms of g_s, we should reconsider the physical effects theoretically induced by a surface. The most important effect is the influence of the new forms of g_s on the Fréedericksz transition. In order to study the effects of all these different anchoring energy forms in the same theoretical framework we make the following approximations: we assume that the primary approximation of g_s is the RP formula (1), and that the new form of g_s is obtained by modifying (1). If the lower order modification only is included, then the modified g_s can be expressed as

$$g_s = \frac{1}{2} A \sin^2 \theta(1 + \zeta \sin^2 \theta). \tag{2}$$

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Parameter ζ characterizes the modification. For example, Sonin [4] compared the different forms of g_s by a diagram where the RP form corresponds to the case of $\zeta = 0$; ζ is negative in a Legendre polynomials expression, and positive if expressed by Fourier series or the elliptic function. In fact, g_s is determined by the properties of the interface and the liquid crystal: ζ can be positive even expressed in Legendre polynomials. Yokoyama and van Sprang [7] determined the form of g_s by experiment, which gives $\zeta = -0.22$. Yang and Rosenblatt [5] give $\zeta > 0$. At present the anchoring energy form (2) or its equivalent forms have been accepted by most authors [11].

In this paper we study the relationship between the energy form and the Fréedericksz transition, and prove that when $\zeta < 0$ the transition could be of first order. At the transition point, the director changes discontinuously. The tilt angle θ_m in the middle layer of the LC medium jumps from 0 to a finite value. Conditions for first order behaviour are given.

For a first order transition, the formula of the threshold field given in [1] is not valid. We have developed an approximate expression of the threshold field valid when the critical value of θ_m is small.

First order LC texture transitions have received a great deal of attention. It is known that optical fields can induce first order transitions [12]. External electric and magnetic fields applied together to the cell, one to stabilize, the other to drive the director, can also induce a first order transition [13]. Now we point out that by means of surface anchoring one can induce a first order transition also, with only a d.c. magnetic field or d.c. electric field. This is important not only for understanding the surface effects but also for the practical application (for example, the design and study of storage liquid crystal displays).

2. Fundamental equations

We consider a nematic liquid crystal cell of thickness l. An external magnetic field $\mathbf{H}$ is applied to the LC medium perpendicular to the substrates. Assuming the two substrates are identical, the easy direction $\mathbf{e}$ in both substrates is the same and parallel to the substrate plane. We establish Cartesian coordinate $\hat{z}$ axis perpendicular to the substrates with the two substrates lying in the $z = 0$ and $z = l$ planes, respectively. Suppose $\mathbf{e}$ is parallel to the x axis. The tilt angle of $\mathbf{n}$ at position (x, z) is a function of z and is denoted by $\theta(z)$.

If the anchoring energy takes the form of equation (2), then at $z = 0$ and $z = l$ we have

$$g_s = \frac{1}{2} A \sin^2 \theta_0 (1 + \zeta \sin^2 \theta_0) \tag{3}$$

$$g_s = \frac{1}{2} A \sin^2 \theta_l (1 + \zeta \sin^2 \theta_l) \tag{4}$$

where θ_0 and θ_l are the values of θ at $z = 0$ and $z = l$, respectively. Due to the symmetry of the system, we have $\theta_0 = \theta_l$. The Gibbs free energy of the system can be written as

$$G = S \int_0^l \left[\frac{1}{2} (k_{11} \cos^2 \theta + k_{33} \sin^2 \theta) \left(\frac{d\theta}{dz} \right)^2 - \frac{1}{2} \chi_a \mathbf{H}^2 \sin^2 \theta \right] dz + S[A \sin^2 \theta_0 (1 + \zeta \sin^2 \theta_0)] \tag{5}$$

where S is the area of the substrate, k_{11}, k_{33} are the LC elastic splay and bend constants, and χ_a is the magnetic anisotropy of the NLC medium. Applying the calculus of variations of G yields [14]

$$(k_{11} \cos^2 \theta + k_{33} \sin^2 \theta) \frac{d^2\theta}{dz^2} + \sin \theta \cos \theta (k_{33} - k_{11}) \left(\frac{d\theta}{dz} \right)^2 + \chi_a \mathbf{H}^2 \sin \theta \cos \theta = 0 \tag{6}$$

and the boundary conditions

$$(k_{11} \cos^2 \theta_0 + k_{33} \sin^2 \theta_0) \left(\frac{d\theta}{dz} \right)_{z=0} = A \sin \theta_0 \cos \theta_0 (1 + 2\zeta \sin^2 \theta_0). \tag{7}$$

Equations (6) and (7) can determine $\theta(z)$ completely.

Now we discuss the solution of equation (6) with the boundary condition (7). Obviously there exist two trivial solutions

$$\theta(z) \equiv 0, \quad \text{for all } z \tag{8}$$

$$\theta(z) \equiv \frac{\pi}{2}, \quad \text{for all } z. \tag{9}$$

In addition, there is also a non-trivial solution which satisfies

$$\frac{d}{dz} \left[(k_{11} \cos^2 \theta + k_{33} \sin^2 \theta) \left(\frac{d\theta}{dz} \right)^2 + \chi_a \mathbf{H}^2 \sin^2 \theta \right] = 0. \tag{10}$$

From equation (10) we obtain

$$\frac{d\theta}{dz} = \mathbf{H} \left[\frac{\chi_a (\sin^2 \theta_m - \sin^2 \theta)}{k_{11} (1 + \eta \sin^2 \theta)} \right]^{1/2} \tag{11}$$

where θ_m is the value of θ at the $z = l/2$ plane, and

$$\eta = \frac{k_{33} - k_{11}}{k_{11}}. \tag{12}$$

Equation (11) is a differential equation of θ, which can be transformed to an integral equation

$$\mathbf{H} = \frac{2}{l}\left(\frac{k_{11}}{\chi_a}\right)^{1/2} \int_{\theta_0}^{\theta_m} \left(\frac{1+\eta \sin^2\theta}{\sin^2\theta_m - \sin^2\theta}\right)^{1/2} d\theta. \quad (13)$$

The boundary condition (7) can be expressed as

$$\mathbf{H} = \frac{A}{(\chi_a k_{11})^{1/2}} \frac{\sin\theta_0 \cos\theta_0 (1 + 2\zeta \sin^2\theta_0)}{[(1+\eta\sin^2\theta_0)(\sin^2\theta_m - \sin^2\theta_0)]^{1/2}}. \quad (14)$$

We have seen that equation (6) has three solutions with boundary condition (7). Solution (8) means the director keeps the initial undisturbed spatial distribution. Solution (9) implies that the system reaches saturation. Equations (11) or (13) correspond to the disturbed distribution of the director. Under the same applied external field, the most stable solution is the one with the smallest free energy among the three solutions. Denoting the free energy corresponding to the three solutions (8), (9) (11) by G_0, $G_{\pi/2}$ and G_θ, then

$$G_0 \equiv 0 \quad \text{for all } \mathbf{H} \quad (15)$$

$$G_{\pi/2} = S\left[-\frac{l}{2}\chi_a \mathbf{H}^2 + A(1+\zeta)\right] \quad (16)$$

$$G_\theta = S\left[\frac{l}{2}\chi_a \mathbf{H}^2 \sin^2\theta_m - \int_0^l \chi_a \mathbf{H}^2 \theta\, dz + A\sin^2\theta_0(1+\zeta\sin^2\theta_0)\right]. \quad (17)$$

Generally, when the applied external field begins to increase from zero, G_0 will be the first smallest solution; solution (8) is the most stable. Then when $\mathbf{H}$ increases to some value denoted by H_{th}, G_θ will become the smallest for $\mathbf{H} > \mathbf{H}_{th}$, and solution (11) becomes the most stable equilibrium. $\mathbf{H}_{th}$ is the so-called threshold field. Lastly, when $\mathbf{H}$ increases to another special value denoted by $\mathbf{H}_{sat}$, $G_{\pi/2}$ would become the smallest value for $\mathbf{H} > \mathbf{H}_{sat}$, and solution (9) becomes most stable. $\mathbf{H}_{sat}$ is the so-called saturation field. We can see that $\mathbf{H}_{th}$ is determined by $G_\theta = G_0$.

To determine the order of the Fréedericksz transition we introduce a new parameter

$$u = \sin^2\theta_m. \quad (18)$$

For solution (8), $u = 0$; for solution (9), $u = 1$; and for solution (11), $0 < u < 1$. u is equivalent to the order parameter in Landau–de Gennes theory, see the work by Frisken and Palffy Muhouray [13].

The above formulae can be re-expressed using u. Defining another variable

$$v = \frac{\sin^2\theta}{\sin^2\theta_m}, \quad \left(v_0 = \frac{\sin^2\theta_0}{\sin^2\theta_m}\right) \quad (19)$$

equations (13) and (14) transform to

$$\mathbf{H} = \frac{2}{l}\left(\frac{k_{11}}{\chi_a}\right)^{1/2} \int_{v_0}^{l} \frac{1}{2[v(1-v)]^{1/2}} \left(\frac{1+\eta u v}{1-uv}\right)^{1/2} dv \quad (20)$$

$$\mathbf{H} = \frac{A}{(\chi_a k_{11})^{1/2}} \left(\frac{v_0}{1-v_0}\right)^{1/2} \left(\frac{1-uv_0}{1+\eta u v_0}\right)^{1/2} (1 + 2\zeta u v_0). \quad (21)$$

It is well known that the threshold field in case of rigid anchoring is $\mathbf{H}_c^0 = \pi/l(k_{11}/\chi_a)^{1/2}$, so defining the reduced field

$$h = \frac{\mathbf{H}}{\mathbf{H}_c^0} \quad (22)$$

equation (20) can be expressed as

$$h = \frac{2}{\pi} \int_{v_0}^{l} \frac{1}{2[v(1-v)]^{1/2}} \left(\frac{1+\eta u v}{1-uv}\right) dv. \quad (23)$$

Defining the reduced anchoring strength†

$$\alpha = \frac{Al}{2k_{11}} \quad (24)$$

equation (14) can be represented as

$$h = \frac{2}{\pi}\alpha \left(\frac{v_0}{1-v_0}\right)^{1/2} \left(\frac{1-uv_0}{1+\eta u v_0}\right)^{1/2} (1 + 2\zeta u v_0). \quad (25)$$

The Gibbs free energy can be represented as

$$G_\theta = S\frac{2k_{11}}{l} u[(I_1^2 - 2I_1 I_2) + \alpha v_0 (1 + \zeta u v_0)]$$

where

$$I_1 = \int_{v_0}^{l} \frac{1}{2[v(1-v)]^{1/2}} \left(\frac{1+\eta u v}{1-uv}\right)^{1/2} dv$$

$$I_2 = \int_{v_0}^{l} \frac{v}{2[v(1-v)]^{1/2}} \left(\frac{1+\eta u v}{1-uv}\right)^{1/2} dv.$$

Defining the reduced free energy

$$\mathcal{G} = \frac{lG_\theta}{2k_{11}S} = u[(I_1^2 - 2I_1 I_2) + \alpha v_0 (1 + \zeta u v_0)] \quad (26)$$

$\mathcal{G}$ is a function of u, and can be denoted by $\mathcal{G}(u)$.

† Becker, M. E., *et al.* proposed a similar parameter $\lambda = \pi k_{11}/Al$: obviously $\alpha = (\pi/2)(1/\lambda)$ [15].

By means of equations (23), (25), (26) we can study the Fréedericksz transition. For a given u, from (23) and (25) we can solve v_0 and **H**, if we solve u and v_0 for a given applied external field **H**. From equation (26) we can obtain $\mathcal{G}$ for a given u. Denoting u at the threshold point by u_c, then

$$\mathcal{G}(u_c) = 0. \tag{27}$$

From equation (27) u_c is determined. If $u_c = 0$ the transition is second order, otherwise if $u_c \neq 0$ it is first order. Equations (23), (25), (26) and (27) underpin the discussions of the Fréedericksz transition.

3. Numerical calculations

Equations (23), (25) and (26) can be solved numerically. Combining (23) with (25) results in

$$\alpha\left(\frac{v_0}{1-v_0}\right)^{1/2}\left(\frac{1-uv_0}{1+\eta uv_0}\right)^{1/2}(1+2\zeta uv_0) = \int_{v_0}^{l}\frac{1}{2[v(1-v)]^{1/2}}\left(\frac{1+\eta uv}{1-uv}\right)^{1/2}\mathrm{d}v \tag{28}$$

which defines the implicit function $v_0(u)$. Substituting $v_0(u)$ into (25) and (26) yields $h(u)$ and $\mathcal{G}(u)$, respectively. u_c is determined by $\mathcal{G}(u) = 0$. The threshold field results from $\mathbf{H}_{th} = \mathbf{H}_c^0\ h(u_c)$. The order of the Fréedericksz transition depends on the zero or non-zero value of u_c.

Taking MBBA (4-methoxybenyl idene-4′-*n*-butylaniline) for example, we can develop our numerical results. The elastic constants [16], $k_{11} = 5.8 \times 10^{-12}$ N, $k_{33}/k_{11} \approx 1.25$; the anchoring strength [17], $A \approx 2 \times 10^{-7}$ J m^{-2}. Suppose the cell thickness $l = 5.8\,\mu$m, then $\alpha = 0.1$. In our study we are seeking the influence of ζ on the Fréedericksz transition, so a set of typical value $\zeta = -0.2$, 0, 0.2 is chosen for comparison. The results are illustrated in figures 1–4.

Figure 1 shows that v_0 is a single-valued function of u. The curve of $\zeta = -0.2$ is uppermost in the diagram as expected.

Figure 2 shows the dependence of h on u. h increases monotonically with u in cases $\zeta = 0$, 0.2. But for $\zeta = -0.2$, h first decreases then increases with u. We see one h value may correspond to two different u values; i.e. equations (23) and (25) may possess two sets of solution $[u^{(1)}, v_0^{(1)}]$, $[u^{(2)}, v_0^{(2)}]$ for a given h.

Figure 3 shows the dependence of $\mathcal{G}$ on u. All the three curves are tangential to the horizontal axis $\mathcal{G} = 0$ at $u = 0$. Curves for $\zeta = 0$, 0.2 begin to descend at $u = 0$, which implies $\mathcal{G} \leqslant 0$ for $u \geqslant 0$. So $u_c = 0$, and they are second order transitions. The curve for $\zeta = -0.2$ distinguishes itself by first rising, then falling and intersecting the horizontal axis $\mathcal{G} = 0$ at $u = 0.35$, which implies $\mathcal{G} \leqslant 0$ for $u \geqslant 0.35$. So $u_c = 0.35$, and it is a first order transition.

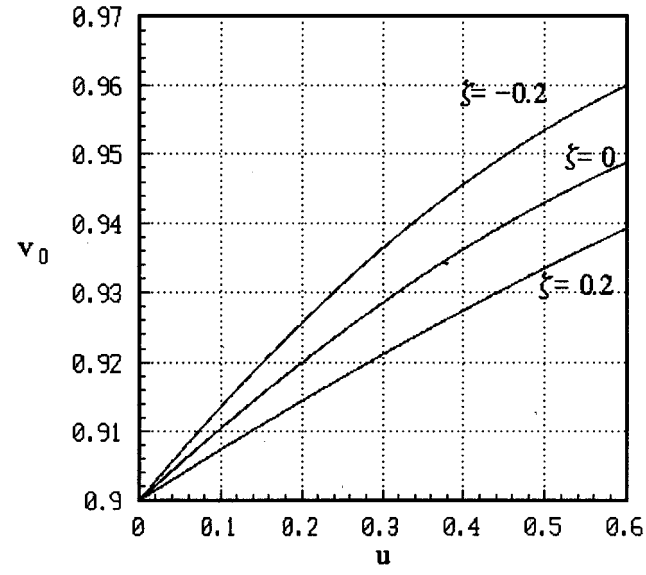

Figure 1. The function $v_0(u)$ for different values of ζ with $\alpha = 0.1$, $k_{33} = 1.25k_{11}$ (refer to MBBA). $v_0 = \sin^2\theta_0/\sin^2\theta_m$, $u = \sin^2\theta_m$.

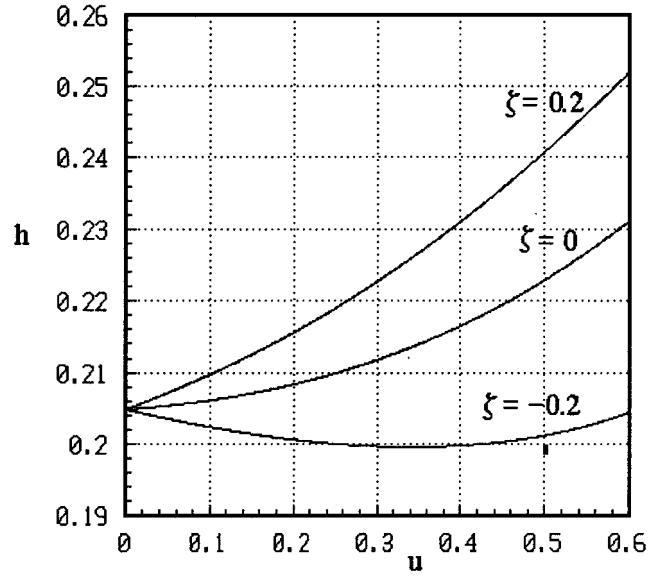

Figure 2. Function $h(u)$ for different values of ζ with $\alpha = 0.1$, $k_{33} = 1.25k_{11}$.

Figure 4 shows the dependence of $\mathcal{G}$ on h. From $\mathcal{G}(u)$ and $h(u)$ we could plot the $\mathcal{G}(h)$ curves. Denoting $(h)_{u=0}$ by h_{th}^0, in curves for $\zeta = 0$, 0.2, $h_{th}^0 = 0.26$, $\mathcal{G} \leqslant 0$ for $h \geqslant 0.26$; so h_{th}^0 is just the reduced threshold field. In § 5 we will show that h_{th}^0 satisfies

$$\cot\left(\frac{\pi}{2}h_{th}^0\right) = \frac{\pi}{2\alpha}h_{th}^0$$

which is the widely used equation to evaluate the threshold field [18]. The curve for $\zeta = -0.2$ intersects

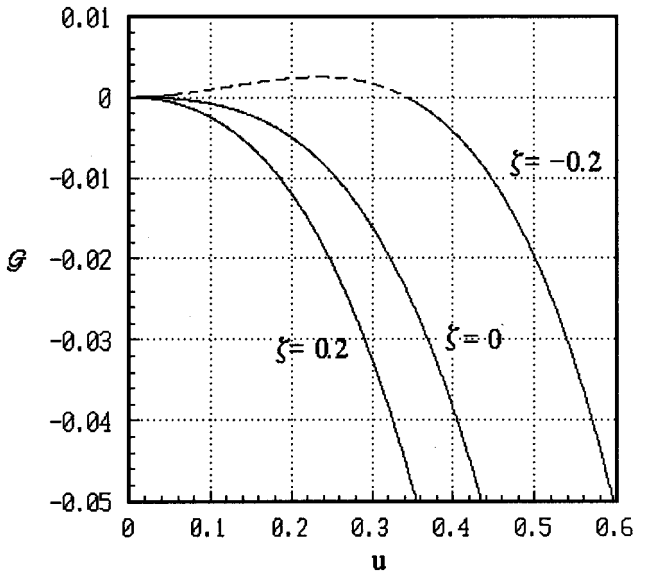

Figure 3. Order parameter u versus reduced Gibbs free energy $\mathcal{G}$ for different ζ with $\alpha = 0.1$, $k_{33} = 1.25k_{11}$.

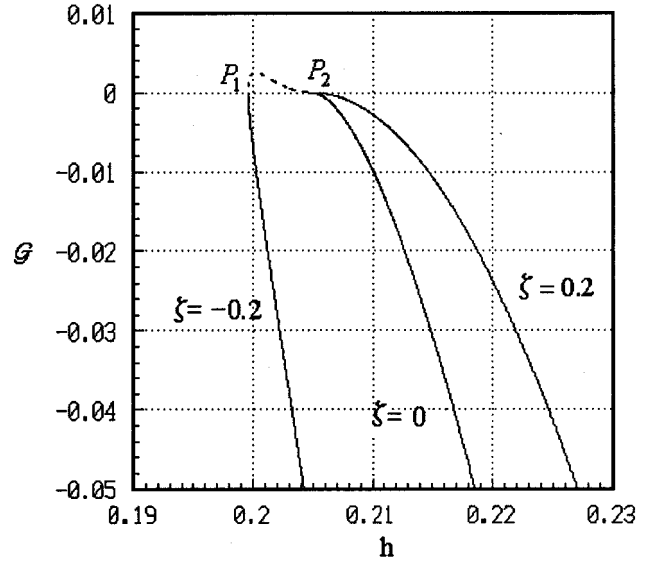

Figure 4. Magnetic field h versus the reduced Gibbs free energy $\mathcal{G}$ for different values of ζ with $\alpha = 0.1$, $k_{33} = 1.25k_{11}$. The unit of h is $(\pi/l)(k_{11}/\chi_a)^{1/2}$. The dashed line means that the corresponding deformed state is less stable than that of the initial uniform state. $P_1 = (0.20, 0.00)$, $P_2 = (0.26, 0.00)$.

the horizontal axis $\mathcal{G} = 0$ at two points P_1 and P_2, which correspond to $[h = 0.20, u = 0.35]$ and $[h = 0.26, u = 0]$, respectively. For the solid line beginning at P_1, $\mathcal{G} \leqslant 0$; for the dashed line between P_1 and P_2, $\mathcal{G} \geqslant 0$. So P_1 corresponds to the threshold point, and $h_{th} = 0.20$, $u_c = 0.35$. h_{th} does not satisfy equation (28) of course.

The above discussions indicate that $\mathcal{G}$ may not be a single-valued function of the external field **H**, but must be single-valued of u. That is why we introduce the parameter u in this approach.

We have discussed only an example; the condition for first order transition needs more general analysis.

4. The condition for the first order transition

From the preceding numerical results, we see that under some conditions the first order Fréedericksz transition may occur. In this section we will determine these conditions.

Frisken and Palffy-Muhoray [13] expanded the Gibbs free energy difference into a series up to the sixth order with respect to the order parameter θ_m when they studied the effects of perpendicular electric and magnetic fields on a liquid crystal sample. We adopt $u = \sin^2 \theta_m$ as the order parameter; similarly $\mathcal{G}(u)$ can be expressed as

$$\mathcal{G}(u) = \mathcal{A}u + \frac{1}{2}\mathcal{B}u^2 + \frac{1}{3}Cu^3 + O(u^4). \tag{29}$$

On the other hand, the Taylor expansion of $\mathcal{G}(u)$ at $u = 0$ is

$$\mathcal{G}(u) = \mathcal{G}(0) + u\mathcal{G}'(0) + \frac{u^2}{2!}\mathcal{G}''(0) + \frac{u^3}{3!}\mathcal{G}'''(0) + O(u^4). \tag{30}$$

Obviously, we have

$$\mathcal{A} = \mathcal{G}'(0), \quad \mathcal{B} = \mathcal{G}''(0), \quad C = \frac{1}{2}\mathcal{G}'''(0). \tag{31}$$

Now we calculate the derivatives of $\mathcal{G}(u)$ at $u = 0$, denoting $V_0 = (v_0)_{u=0}$. From equation (28) we obtain

$$\alpha\left(\frac{V_0}{1 - V_0}\right)^{1/2} = \arccos(V_0)^{1/2} \tag{32}$$

Introducing the parameter β_0 in

$$V_0 = \cos^2 \beta_0 \tag{33}$$

then β_0 satisfies‡

$$\alpha = \beta_0 \tan \beta_0 \tag{34}$$

which shows that V_0 is only a function of α, irrespective of ζ, see figure 5.

Taking the first order u derivative in equation (28) at $u = 0$, we obtain

$$\left(\frac{dv_0}{du}\right) = \left[\frac{\kappa}{2} + \alpha(\kappa - 4\zeta)\frac{V_0}{1 + \alpha - V_0}\right]V_0(1 - V_0) \tag{35}$$

‡In the literature [Sugimura, A., Luckhurst, G. R., and Ou-Yang Zhong-can, 1995, *Phys. Rev. E*, **52,** 681] α^0 is defined by $\sin \theta_0^0 = \sin \theta_m \sin \alpha^0$; here β_0 is equivalent to $\pi/2 - \alpha^0$ [19].

where $\kappa = 1 + \eta = k_{33}/k_{11}$. From (26), through the usual differential calculation and using equations (32) and (35), we can obtain

$$\mathcal{G}(0) = 0, \quad \mathcal{A} = \mathcal{G}'(0) = 0,$$

$$\mathcal{B} = \mathcal{G}''(0) = 2\alpha V_0\left[\frac{\kappa}{8}\left(2V_0 - 1 - \frac{\alpha}{1 - V_0}\right) - \zeta V_0\right] \quad (36)$$

$$C = \frac{1}{2}\mathcal{G}'''(0) = \frac{3}{2}\frac{\alpha}{(1 - V_0 + \alpha)^2}\frac{V_0}{(1 - V_0)}(c_0 + c_1\zeta + c_2\zeta^2) \quad (37)$$

where

$$c_0 = -\frac{\kappa}{8}(2 + \kappa V_0)b^3 + \frac{\kappa V_0}{24}[(25\kappa - 4) + (20 - 17\kappa)V_0 - 16(1 + 2\kappa)V_0^2 + 24\kappa V_0^3]b^2 + \frac{\kappa^2 V_0^2}{8}(-8 + 27V_0 - 26V_0^2 + 8V_0^3)b \quad (38)$$

$$c_1 = \frac{\kappa V_0}{2}b^3 + \frac{\kappa V_0}{2}(-7 - 5V_0 + 28V_0^2 - 16V_0^3)b^2 + \frac{\kappa V_0^2}{2}(16 - 51V_0 + 50V_0^2 - 16V_0^3)b \quad (39)$$

$$c_2 = 16V_0^2(1 - V_0)^2\alpha b \quad (40)$$

$$b = 1 - V_0 + \alpha.$$

Finally we obtain $\mathcal{G}(u)$ up to u^3,

$$\mathcal{G}(u) = \frac{1}{2}\mathcal{B}u^2 + \frac{1}{3}Cu^3. \quad (41)$$

Now we discuss the Fréedericksz transition. Equation (29) is analogous to expression (10) appearing in [13], but they underlie two different approaches. Landau phenomenological theory was used in [13]; the order parameter θ_m in expression (10) of [13] did not minimize the free energy, while in this paper the order parameter u has minimized the free energy already. In our approach θ satisfies equations (6), (7), and the critical order parameter results from $\mathcal{G}(u) = 0$. From (4.13), the equation $\mathcal{G}(u) = 0$ has two solutions

$$u_1 = 0 \quad (42)$$

$$u_2 = -3\mathcal{B}/2C. \quad (43)$$

Generally, (i) if $\mathcal{G}(u) \leqslant 0$ for $u \geqslant 0$, the transition is second order, and occurs at $u = u_1 = 0$; (ii) if $\mathcal{G}(u) \geqslant 0$ for $0 \leqslant u \leqslant u_2$, $\mathcal{G}(u) < 0$ for $u > u_2$, then the transition is first order, occurring at $u = u_2 \neq 0$. In the series expansion of $\mathcal{G}(u)$ only two terms are left; they are relatively accurate for small u, suitable for analysing the second order transition. Obviously the condition for the second order transition is

$$\mathcal{B} < 0 \quad (44)$$

Not being second order, implies first order§, so the condition for the first order transition is

$$\mathcal{B} > 0. \quad (45)$$

From equation (36) we obtain the condition for the first order transition

$$\frac{\zeta}{\kappa} < -\frac{1}{8}\frac{\alpha + (1 - V_0)(1 - 2V_0)}{V_0(1 - V_0)}. \quad (46)$$

Because V_0 is a function of α, equation (46) depends only on the LC and surface parameters α, ζ, κ, as follows:

(i) ζ must be negative. From equations (34) and (35) we obtain $\alpha + (1 - V_0)(1 - 2V_0) = 1/4 \tan\beta_0 \times (4\beta_0 - \sin 4\beta_0) > 0$; the ζ satisfying (46) must be negative.

(ii) The first order transition occurs only when α is small. Figure 5 gives the $V_0 \sim \alpha$ curve. Figure 6 shows the relation between $-\zeta/\kappa$ and α. We see that the diagram is divided into two parts; the left part is the first order transition zone, the right part is the second order zone. Generally $|\zeta| < 1$, and $\kappa = k_{33}/k_{11} > 1$ for most liquid crystals, so $|\zeta|/\kappa$ is about $0.1 \sim 1$; α is required to be $0.1 \sim 1$ for a possible first order transition.

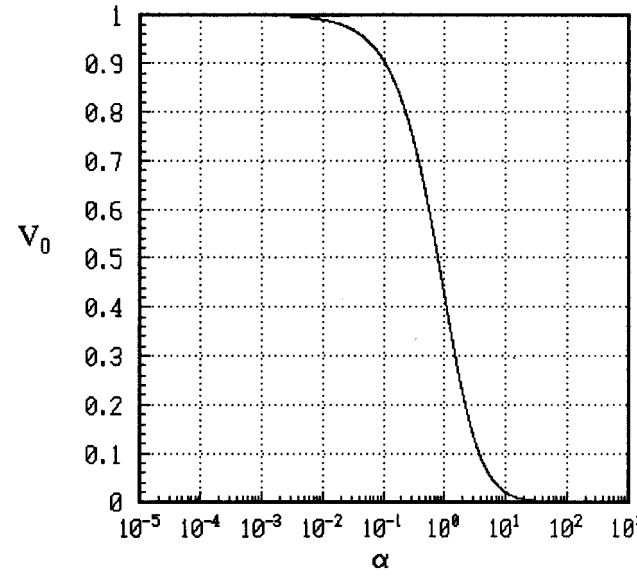

Figure 5. Reduced surface anchoring strength α versus V_0, where $\alpha = Al/2k_{11}$, $V_0 = (v_0)_{u=0}$.

§There are two kinds of first order transitions: (1) from the uniform solution $\theta = 0$ to the deformed solution when $0 < u_2 < 1$, (2) from the uniform solution directly to another uniform solution $\theta = \pi/2$ when $u_2 \geqslant 1$, this is the case for very small α.

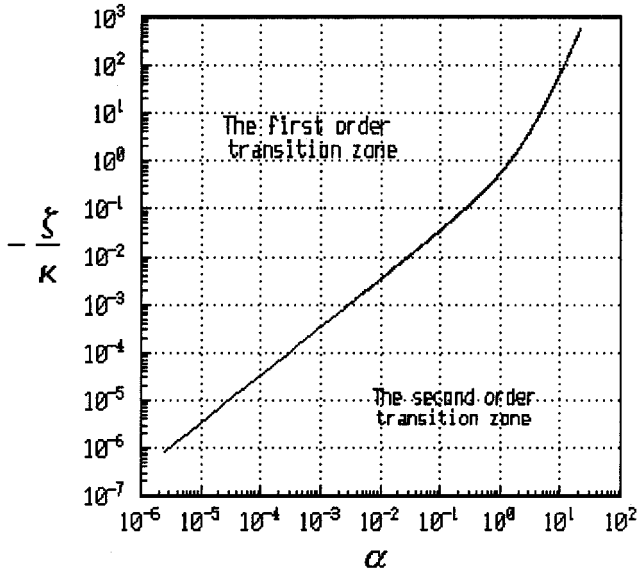

Figure 6. Fréedericksz phase diagram. Surface and material parameters α, ζ, κ determine the Fréedericksz order completely in this diagram.

(iii) If the surfaces of the NLC cell substrates are homeotropically aligned ($\mathbf{e} \| \hat{z}$) initially, the external field is applied parallel to $\hat{x}$, as in the case studied by Yang and Rosenblatt [5]; then the new formulae can be obtained only by swapping k_{11} and k_{33} correspondingly. In this case $\kappa = k_{11}/k_{33} < 1$ for most liquid crystals, and the first order transition can be realized more easily.

5. Approximate expression of the threshold field

This section gives the approximate expression of the threshold field.

Expanding equation (25) up to u yields an approximate expression for h:

$$h = \frac{2}{\pi}\alpha\left(\frac{V_0}{1-V_0}\right)^{1/2}\left\{1 - 2\frac{1-V_0}{1+\alpha-V_0} \times \left[\frac{\kappa}{8}\left(2V_0 - 1 - \frac{\alpha}{1-V_0}\right) - \zeta V_0\right]u\right\} \quad (47)$$

We can now discuss the threshold field.

(1) for the second order transition, $u_c = 0$, then

$$h_{th} = h_{th}^0 = \frac{2}{\pi}\alpha\left(\frac{V_0}{1-V_0}\right)^{1/2}. \quad (48)$$

Applying $V_0 = \cos^2\beta_0$ in the above equation, we have

$$h_{th}^0 = \frac{2}{\pi}\alpha\cos\beta_0. \quad (49)$$

Eliminating α by $\alpha = \beta_0 \tan\beta_0$ results in $\beta_0 = (\pi/2)h_{th}^0$, then substituting into $\alpha = \beta_0 \tan\beta_0$ yields

$$\cot\left(\frac{\pi}{2}h_{th}^0\right) = \frac{1}{\alpha}\frac{\pi}{2}h_{th}^0 \quad (50)$$

which is in agreement with [17].

(2) For the first order transition, if u_c is small, then $u_c \approx 2\mathscr{B}/(2C)$, applying equation (36),

$$h_{th} = h_{th}^0\left[1 + \frac{3(1-V_0)}{\alpha(1+\alpha-V_0)V_0}\mathscr{B}^2/C\right]. \quad (51)$$

Because $C < 0$, then

$$h_{th} < h_{th}^0 \quad (52)$$

Figure 7 shows the curve of h_{th}/h_{th}^0 versus ζ.

6. Discussion and conclusion

We have studied the first order Fréedericksz transition of a NLC cell by adopting surface anchoring energy (2), and concluded that the first order transition is possible only for $\zeta < 0$. If we plot g_s vs. θ diagrams for $\zeta > 0$, $\zeta = 0$, $\zeta < 0$, respectively, the first curve is most steep, the third is least steep. This shows that if the g_s vs. θ curve is more slowly varying than that of the RP formula, the first order transition would be possible.

The conclusion can be generalized to other more general forms of g_s. Taking the RP formula as a referred standard, if the g_s vs. θ curve is less steep than that of the RP formula, then the existence of the first order transition would be possible.

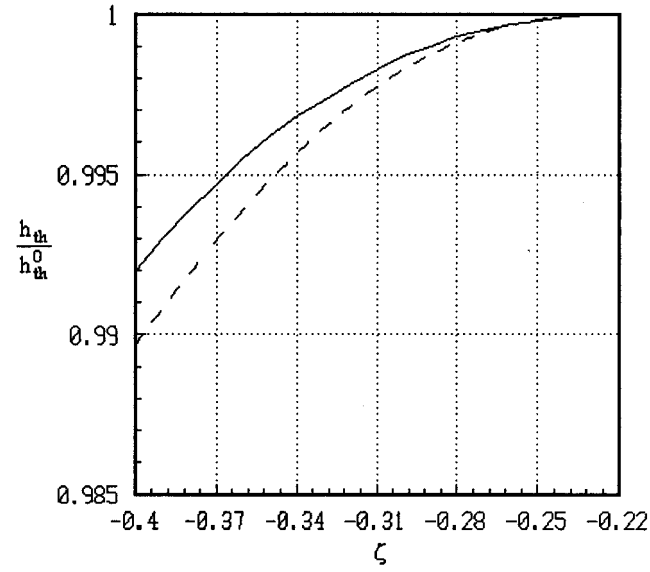

Figure 7. ζ versus ratio of h_{th} to h_{th}^0 with $\alpha = 1.55$, $\kappa = 1.2$. The solid line is the solution from the numerical calculation, the dashed line is the approximation using equation (5.1); the difference is about 1%.

At present, weak anchoring is obtained experimentally in two ways [4]: (1) using a layer of SiO or some kind of organic compound; (2) by rubbing the surface of the substrate. The different surface treatments and different liquid crystals make the form of g_s different, so the adoption of a suitable weak anchoring technique may realize the first order Fréedericksz transition.

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