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Surface anchoring and the saturation behaviour of a NLC cell under external electric and magnetic fields

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Based on the modified Rapini–Papoular formula for surface anchoring energy, the saturation behaviour of a weak anchoring nematic liquid crystal cell under electric and magnetic fields has been studied by the methods of analytical derivation and numerical calculation. The results show that the transition at saturation point may be second order, as many authors have predicted. However, it may also be first order. The condition for the first order transition is deduced; it is related to the anchoring parameters. The influence of anchoring on the saturation field strength is also discussed, both for second and for first orders; the results are shown by graphically.

1. Introduction

Liquid crystal surface anchoring is an important subject from both academic and applications points of view. Most liquid crystal devices require very strong anchoring energy, and during their operation the orientation of the director **n** close to the substrate remains unchanged. Many earlier investigations treated the problems only for this type of cell [1, 2]. Frisken and Palffy-Muhoray [3] found that a first order transition occurs at a threshold point for a strong anchoring nematic liquid crystal (NLC) cell under external electric and magnetic fields which are perpendicular to each other. Meanwhile, a theoretical analysis for the condition of the first order transition was made, and the existence of a bistable state predicted [4]. Cells with strong anchoring and under external electric and magnetic fields have aroused considerable attention from researchers. However, for NLC cells, surface forces are generally too weak to impose a well defined orientation of **n** along the surface of the cell. For an untwisted NLC sample with a weak anchoring surface, Rapini and Papoular [5] proposed a phenomenological expression for a one-dimensional deformation of the interfacial energy per unit area to quantify the strength of anchoring:

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

where θ is the angle between the easy direction **e** and the director **n** of the NLC at the nematic–wall interface and A is the anchoring parameter measuring the ability of **n** to deviate from **e**. This is the so-called RP formula; it states the boundary condition of the nematic director. It can be strictly proved that when the weak anchoring energy takes the form of equation (1), only a second order transition will occur and the critical fields can be calculated from this property [6]. The RP formula successfully describes many effects for a weak anchoring surface. However, it has been found gradually that the results calculated from RP formulae, in some cases do not agree well with the experimental observations [7]. Many authors have introduced new anchoring energy forms to replace the RP formula [8–13]. At present the single-order modified RP formula has been accepted by most people [14]

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

In recent years, physical effects have been theoretically studied on the basis of the modified RP formula (2). It has been pointed out that, if adopting equation (2), a first order transition at the threshold point may also be possible for a weak anchoring NLC cell under a single magnetic field [15].

In fact, there are two transitions in a NLC cell with increasing external field, one is at the threshold point and the other is at the saturation point. The existence of a saturation transition had been predicted by several authors [16–18] and was first experimentally demonstrated by Yokoyama and van Sprang [10]. All these previous investigations show that the saturation transition is of second order, which means that the director **n**

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and its distribution change continuously at the transition point, and the saturation field formula is obtained from this view. In fact, the value of θ at the saturation point is greater than for the threshold point. So the adoption of the modified RP formula is important in studying saturation behaviour.

In this paper, we study the saturation behaviour of a weak anchoring NLC cell under external electric and magnetic fields. We will show that, if the surface anchoring energy is described by equation (2) and $\zeta<0$, a first order transition may occur at the saturation point, as at the threshold point, under certain conditions. In §2, the liquid crystal cell model for the investigated system is given, and the equilibrium equation and boundary condition of the director are obtained by the analytical method. The solutions of the equations are discussed. In §3, the property of the saturation transition is discussed in detail by means of numerical calculation. The results show that for the cell studied, we may expect the usual second order transition; as many authors predicted, the first order transition can also be induced by a suitable surface anchoring. The condition for existence of the first order transition is deduced by means of the analytical method in §4; it is related to the anchoring parameters. In §5, the influence of the anchoring parameters on the saturation field strength is discussed by giving the calculation formula for the second order transition, and the method for the first order transition.

2. Fundamental equations

As shown in figure 1, we consider a weak anchoring NCL cell of thickness l. A voltage V is applied to the LC medium by placing electrically conducting glass plates at both ends of the cell; an external magentic field $\mathbf{B}$ is also applied to the LC medium. Both the glass plates and the external magnetic field $\mathbf{B}$ are perpendicular to the substrates of the cell. If the distance between the electrodes is d, and the easy direction $\mathbf{e}$ in both substrates is the same and parallel to the substrates, we

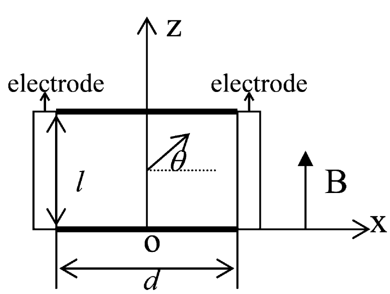

Figure 1. The weak anchoring NLC cell in external electric and magnetic fields.

establish a Cartesian coordinate system with the z-axis perpendicular to the two substrates, which lie at the $z=0$ and $z=l$ positions. The easy direction $\mathbf{e}$ is along the x-axis. Clearly, the external electric field is parallel to the initial alignment of the molecules and stabilizes the alignment. The external magentic field is perpendicular to the initial alignment of the molecules and drives the director to rotate to the z-axis, which has the same direcation as the field. The tilt angle of the director $\mathbf{n}$ is a function of z and is denoted by $\theta(z)$.

The surface energy per unit area at $z=0$ and $z=l$ can be expressed as

$$F_s\Big|_{z=l} = \frac{1}{2}A\sin^2\theta_l\left(1+\zeta\sin^2\theta_l\right) \quad \text{for } z=l \tag{3}$$

$$\text{and } F_s\Big|_{z=0} = \frac{1}{2}A\sin^2\theta_0\left(1+\zeta\sin^2\theta_0\right) \quad \text{for } z=0 \tag{4}$$

where θ_0 and θ_l are the values of θ at the two substrates where $z=0$ and $z=l$, respectively. Based on the symmetry of the system, we have $\theta_0=\theta_l$.

The Gibbs free energy per unit volume in the cell can be written

$$\begin{aligned} g_b &= f_{\text{elas}}+f_{\text{elec}}+f_{\text{mag}} \\ &= \left[\frac{1}{2}k_{11}(\nabla\cdot\mathbf{n})^2+\frac{1}{2}k_{22}(\mathbf{n}\cdot\nabla\times\mathbf{n})^2+\frac{1}{2}k_{33}(\mathbf{n}\times\nabla\times\mathbf{n})^2\right] \\ &\quad -\frac{1}{2}\mathbf{D}\cdot\mathbf{E}-\frac{1}{2}\chi_a(\mathbf{H}\cdot\mathbf{n})^2 \\ &= \frac{1}{2}\left(k_{11}\cos^2\theta+k_{33}\sin^2\theta\right)\cdot\left(\frac{d\theta}{dz}\right)^2 \\ &\quad -\frac{1}{2}\frac{\varepsilon_0\varepsilon_\parallel V^2}{d^2}\frac{1}{1+\omega\sin^2\theta}-\frac{1}{2}\chi_a\frac{\mathbf{B}^2}{\mu_0}\sin^2\theta \end{aligned}$$

where k_{11}, k_{33} are the Frank splay and bend elastic constants, respectively; χ_a is the magnetic anisotropy of the NLC medium, and $\omega=(\varepsilon_\parallel-\varepsilon_\perp)/\varepsilon_\perp=\Delta\varepsilon/\varepsilon_\perp$, $\varepsilon_\parallel$ and $\varepsilon_\perp$ are the principal values of the dielectric tensor, parallel and perpendicular to the director, respectively. ε_0 is the dielectric constant of vacuum. The total energy of the system is therefore

$$\begin{aligned} G &= S\int_0^l\left[\frac{1}{2}\left(k_{11}\cos^2\theta+k_{33}\sin^2\theta\right)\left(\frac{d\theta}{dz}\right)^2\right. \\ &\quad \left.-\frac{1}{2}\frac{\chi_a\mathbf{B}^2}{\mu_0}\sin^2\theta-\frac{1}{2}\frac{\varepsilon_0\varepsilon_\parallel V^2}{d^2}\frac{1}{1+\omega\sin^2\theta}\right]dz \\ &\quad +SA\sin^2\theta_0\left(1+\zeta\sin^2\theta_0\right) \end{aligned} \tag{5}$$

where S is the area of the substrate. Because the free energy G is a minimum in the stable director distribution state, we can obtain the equilibrium equation and boundary condition for director distribution θ from the first order variation $\delta G=0$ [19]. The equation is

$$\cos\theta\sin\theta(k_{33}-k_{11})\left(\frac{\mathrm{d}\theta}{\mathrm{d}z}\right)^2-\frac{\varepsilon_0\varepsilon_\parallel V^2}{d^2}\frac{\omega\sin\theta\cos\theta}{\left(1+\omega\sin^2\theta\right)^2}+\frac{\chi_a\mathbf{B}^2}{\mu_0}\sin\theta\cos\theta+\left(k_{11}\cos^2\theta+k_{33}\sin^2\theta\right)\frac{\mathrm{d}^2\theta}{\mathrm{d}z^2}=0 \tag{6}$$

and the boundary condition is

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

equation (6) with the boundary condition (7) has three solutions when the external voltage V is fixed. Obviously, there are two trivial solutions

$$\theta(z)\equiv 0 \tag{8}$$

$$\theta(z)\equiv\frac{\pi}{2}. \tag{9}$$

We call them the uniform solution and saturation solution, respectively. In addition, there is also the third non-trivial solution, which is called the disturbed solution. From equation (6), we obtain

$$\frac{\mathrm{d}}{\mathrm{d}z}\left[\left(k_{11}\cos^2\theta+k_{33}\sin^2\theta\right)\left(\frac{\mathrm{d}\theta}{\mathrm{d}z}\right)^2+\frac{\varepsilon_0\varepsilon_\parallel V^2}{d^2}\frac{1}{1+\omega\sin^2\theta}+\frac{\chi_a\mathbf{B}^2}{\mu_0\sin^2\theta}\right]=0 \tag{10}$$

that is,

$$\frac{\mathrm{d}\theta}{\mathrm{d}z}=\left[\frac{c(\theta_m)-c(\theta)}{k_{11}\left(1+\gamma\sin^2\theta\right)}\right]^{\frac{1}{2}},\quad\left(0\le z\le\frac{l}{2}\right) \tag{11}$$

where $(k_{33}-k_{11})/k_{11}$, and θ_m is the tilt angle of the director **n** at the middle layer $z=l/2$. From the symmetry of the surface anchoring at the top and bottom substrates, we know that θ reaches a maximum at $z=l/2$ and satisfies $\frac{\mathrm{d}\theta}{\mathrm{d}z}\big|_{z=\frac{l}{2}}=0$. $c(\theta)$ is a term related to θ, and is expressed as

$$c(\theta)=\frac{\varepsilon_0\varepsilon_\parallel V^2}{d^2}\frac{1}{1+\omega\sin^2\theta}+\frac{\chi_a}{\mu_0}B^2\sin^2\theta. \tag{12}$$

Thus, equation (11) is the differential equation of the disturbed solution θ, which is derived from equation (6). It reflects the rate of the spatial change of the director distribution in the disturbed state. Equation (11) can be further transformed into an integral equation

$$\int_{\theta_0}^{\theta_m}\left[\frac{c(\theta_m)-c(\theta)}{k_{11}\left(1+\gamma\sin^2\theta\right)}\right]^{\frac{1}{2}}\mathrm{d}\theta=\frac{l}{2}. \tag{13}$$

The boundary condition (7) can be re-expressed, by using equation (13), as

$$\left[k_{11}\left(1+\gamma\sin^2\theta\right)\right]^{\frac{1}{2}}\left[c(\theta_m)-c(\theta)\right]^{\frac{1}{2}}=A\sin\theta_0\cos\theta_0\left(1+2\zeta\sin^2\theta_0\right). \tag{14}$$

We can see that equilibrium state equation (6) with the boundary condition (7) has three solutions. The uniform solution (8) corresponds to the state in which the director keeps the initial undisturbed spatial distribution. The saturation solution (9) corresponds to the state in which the director aligns completely along the external field. The solution satisfying equations (13) and (14) corresponds to the disturbed distribution of director. When the external field is applied, the alignment of the molecules depends on which solution minimizes the free energy. Denoting the three solutions above by G_0, G_S and G_θ, respectively, equation (5) yields

$$G_0=Sl\left[-\frac{1}{2}\frac{\varepsilon_0\varepsilon_\parallel V^2}{d^2}\right] \tag{15}$$

$$G_S=Sl\left[-\frac{1}{2}\frac{\varepsilon_0\varepsilon_\parallel V^2}{d^2}\frac{1}{1+\omega}-\frac{1}{2}\frac{\chi_a}{\mu_0}\mathbf{B}^2\right]+SA(1+\zeta) \tag{16}$$

$$G_\theta=S\left\{\int_0^l\left[c(\theta_m)-c(\theta)\right]\mathrm{d}z-\frac{1}{2}c(\theta_m)l\right\}+SA\sin^2\theta_0\left(1+\zeta\sin^2\theta_0\right). \tag{17}$$

Generally, when the external magnetic field **B** begins to increase from zero, the value of G_0 will first become the smallest, and solution (8) is the most stable. As **B** increases to some value denoted by $\mathbf{B}_{th}$, G_θ will become the smallest; the director distribution begins to change and the disturbed solution (11) is the most stable. B_{th} is the so-called threshold field. When **B** increases to another special value denoted as $\mathbf{B}_{sat}$, G_S becomes the smallest, and the director distribution will change again and finally reach a saturation state (9); $\mathbf{B}_{sat}$ is the so-called saturation field.

In order to study the saturation behaviour of the cell, we introduce a new parameter and a new variable denoted by u and v, respectively.

$$u=\cos^2\theta_m \tag{18}$$

$$v=\frac{\cos^2\theta_m}{\cos^2\theta}\quad\left(v_0=\frac{\cos^2\theta_m}{\cos^2\theta_0}\right). \tag{19}$$

Furthermore we introduce the reduced anchoring strength α, reduced free energy density g and reduced magnetic field b, where

$$\alpha = \frac{Al}{2k_{11}} \tag{20}$$

$$g = \frac{Gl}{2k_{11}S} \tag{21}$$

$$b = \frac{\mathbf{B}}{\mathbf{B}_c^0}. \tag{22}$$

Here $\mathbf{B}_c^0 = \frac{\pi}{l}\left(\frac{\mu_0 k_{11}}{\chi_a}\right)^{\frac{1}{2}}$ is the threshold magnetic field under strong anchoring. From these equations, and using equation (12) through a complex transformation; the integral equation (13), boundary condition (14) and free energies of the disturbed and saturation solution (17), (16) can be re-expressed using u, as

$$b = \frac{2}{\pi} I_1 \tag{23}$$

$$I_1 = \alpha\, p^{\frac{1}{2}} \left\{ 1 + \frac{1}{4\alpha^2}\left(\frac{l}{d}\right)^2 \frac{q}{p} \right\}^{\frac{1}{2}} \tag{24}$$

$$\begin{aligned} g_\theta = {} & \frac{e}{4\omega}\left[\frac{1}{1+\omega u - \omega u} - \frac{2I_3}{I_1}\right] + \left(I_1^2 - 2I_1 I_2\right) + \alpha(1+\zeta) \\ & - \left[\left(I_1^2 - 2I_1 I_2\right) + \frac{\alpha}{v_0}\left(1 + 2\zeta - \zeta\frac{u}{v_0}\right)\right] \end{aligned} \tag{25}$$

$$g_S = \frac{e}{4\omega(1+\omega)} - I_1^2 + \alpha(1+\zeta) \tag{26}$$

where:

$$p = \frac{v_0 - u}{v_0^2(1-v_0)} \frac{[(1+2\zeta)v_0 - 2\zeta u]^2}{v_0(1+\gamma) - \gamma u} \tag{27}$$

$$q = \frac{e}{(l/d)^2} \frac{v_0}{[(1+\omega) - \omega u)[v_0(1+\omega) - \omega u]} \tag{28}$$

$$e = \frac{\varepsilon_0 \varepsilon_{\parallel} V^2 \omega}{k_{11}} \left(\frac{l}{d}\right)^2 \tag{29}$$

$$I_1 = \int_{v_0}^{1} \frac{1}{2v} \left[\frac{v(1+\gamma) - \gamma u}{(1-v)(v-u)}\right]^{\frac{1}{2}} R^{\frac{1}{2}}\, \mathrm{d}v \tag{30}$$

$$I_2 = \int_{v_0}^{1} \frac{1}{2v^2(1-u)} \left\{\frac{(v-u)[v(1+\gamma) - \gamma u]}{1-v}\right\}^{\frac{1}{2}} R^{\frac{1}{2}}\, \mathrm{d}v, \tag{31}$$

$$I_3 = \int_{v_0}^{1} \frac{1}{2[(1+\omega)v - \omega u]} \left[\frac{v(1+\gamma) - \gamma u}{(1-v)(v-u)}\right]^{\frac{1}{2}} R^{\frac{1}{2}}\, \mathrm{d}v \tag{32}$$

and

$$R = 1 + \frac{\left(\frac{l}{d}\right)^2 q \frac{v[(1+\omega)v_0 - \omega u]}{v_0[(1+\omega)v - \omega u]}}{4\alpha^2 p + \left(\frac{l}{d}\right)^2 q \left\{\frac{u\omega(v - v_0)}{v_0[(1+\omega)v - \omega u]}\right\}} \tag{33}$$

Because foundational functions I_1, p and q are all functions of u and v_0, and from equation (24) we know that v_0 is an implicit function of u, then there is only one independent variable, u, in above equations. In order to discuss the saturation behavour of the cell, the values of the disturbed and saturation solutions must to be compared. Defining the difference of the two reduced free energies by g,

$$\begin{aligned} g = g_\theta - g_S = {} & \frac{e}{4\omega}\left[\frac{1}{1+\omega - \omega u} - \frac{2I_3}{I_1} + \frac{1}{1+\omega}\right] \\ & + 2I_1(I_1 - I_2) - u\left[\left(I_1^2 - 2I_1 I_2\right) + \frac{\alpha}{v_0}\left(1 + 2\zeta - \zeta\frac{u}{v_0}\right)\right]. \end{aligned} \tag{34}$$

Using these equations, we can discuss the saturation behaviour of the cell.

3. The transition at the saturation point

By means of equations (23), (24) and (34) we can study the transition property at the saturation point. Combining equation (23) with (24) gives

$$\alpha p^{\frac{1}{2}} \left\{ 1 + \frac{1}{4\alpha^2}\left(\frac{l}{d}\right)^2 \frac{q}{p} \right\}^{\frac{1}{2}} = \int_{v_0}^{1} \frac{1}{2v} \left[\frac{v(1+\gamma) - \gamma u}{(1-v)(v-u)}\right]^{\frac{1}{2}} R^{\frac{1}{2}}\, \mathrm{d}v \tag{35}$$

which defines the implicit function $v_0(u)$. Substituting $v_0(u)$ into equations (23) and (34) yields functions $b(u)$ and $g(u)$, respectively. Denoting u at the saturation point by u_c, the value of u_c is determined by $g(u_c)=0$. If $u_c=0$ the transition is second order; if $u_c \neq 0$ it is first order.

Taking the liquid crystal material MBBA (4-methoxy-benylidenez-4′-*n*-butylaniline) as an example, the elastic constants are $k_{33}/k_{11} \approx 1.25$; $\varepsilon_{\parallel}=5.54$; $\varepsilon_{\perp}=5.70$. Supposing $e=6.0$, $l/d=0.15$, $\omega=0.2$, $\alpha=2.0$, we study the influence of different anchoring on the transition property. So a set of different anchoring parameters (a) $\zeta=0.2$, (b) $\zeta=0.0$, (c) $\zeta=-0.2$ and (d) $\zeta=-0.3$ are chosen for comparison. The results are illustrated in figures 2–4.

From figures 2–4, we find two different typical transitions at the saturation point, as follows:

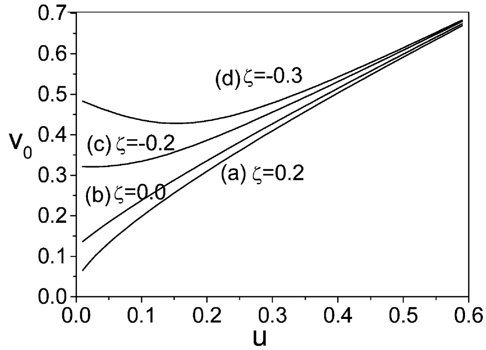

Figure 2. The function $v_0(u)$ for different values of ζ, with parameters $e=6.0$, $l/d=0.15$, $\omega=0.2$. $v_0=\cos^2\theta_m/\cos^2\theta_0$, $u=\cos^2\theta_m$.

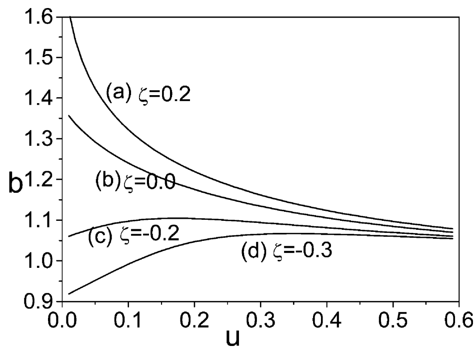

Figure 3. Function $b(u)$ for different values of ζ, with parameters $e=6.0$, $l/d=0.15$, $\omega=0.2$.

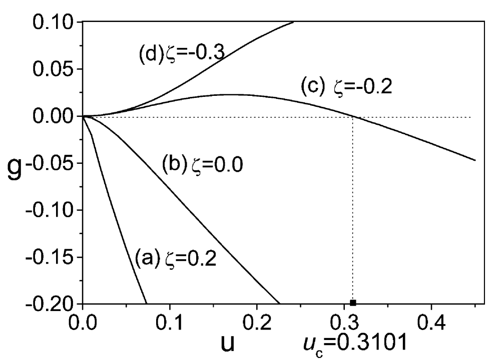

Figure 4. Order parameter u versus reduced Gibbs free energy g for different values of ζ, with parameters $e=6.0$, $l/d=0.15$, $\omega=0.2$.

(1) The normal situation; curves (a) and (b) of figures 2–4 apply to this situation. In figure 2, we see that $v_0(u)$ is a single-valued function and curve (b) is higher than (a) in the diagram, as expected. Figure 3 shows the dependence of magnetic field b on the state parameter u; b decreases monotonically with u and curve (a) becomes higher Figure 4 shows that both curves (a) and (b) are tangential to the horizontal axis $g=0$ at $u=0$, and decrease monotonously with increasing u. This indicates that when $u=0$, $G_0=G_S$, and when $u>0$, $G_0<G_S$. The transition from disturbed state to saturation state occurs at $u=u_c=0$, and the director **n** and its distribution change continuously. So the saturation transition is second order.

(2) The abnormal situation; curves (c) and (d) of figures 2–4 apply to this situation. From figure 2 we see that $v_0(u)$ is increases monotonously at first, but becomes a double-valued function with the decrease of ζ; i.e. one v_0 value may correspond to two different u values. Figure 3 shows that b increases with u, with a difference in curves (a) and (b). From figure 4, we find that curves (c) and (d) are both also tangential to the horizontal axis $g=0$ at $u=0$. But (c) first rises, then falls and finally intersects with the horizontal axis at $u=0.3101$, which implies $g\leqslant 0$ for $u\geqslant 0.3101$. So the saturation transition occurs at $u=u_c=0.3101$. It is a first order transition because $u=u_c\neq 0$. In last case of curve (d), is always greater than zero, which means that the uniform state transforms directly to the saturation state at $u=0$; it is also first order.

From this discussion we see that a first order saturation transition may occur under appropriate conditions. We will now determine these conditions.

4. The condition for the first order saturation transition

Using the Taylor formula, Frisken and Palffy-Muhoray [4] 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 threshold effects of perpendicular electric and magnetic fields on a strong anchoring liquid crystal sample. We similarly adopt $u=\cos^2\theta_m$ as the order parameter. As curves (c) and (d) in figure 4 show, the reduced free energy difference is greater than zero in the vicinity of $u=0$ for the first order transition, but is less than zero for the second order transition. From this, we can obtain the condition for the first order transition. Let us calculate the values of g and its first and second order derivatives at $u=0$ from equation (34). The results are:

$$g|_{u=0}=0 \tag{36}$$

$$\left.\frac{\mathrm{d}g}{\mathrm{d}u}\right|_{u=0}=0 \tag{37}$$

$$
\begin{aligned}
\left.\frac{\mathrm{d}^2 g}{\mathrm{d}u^2}\right|_{u=0} = \left.\frac{\mathrm{d}v_0}{\mathrm{d}u}\right|_{u=0} & \left\{ \frac{e\left[(2R_0+V_0R_0-V_0)[(1+\gamma)(1-V_0)R_0]^{\frac{1}{2}}+I_{1,0}(R_0-1)V_0^2\right]}{4I_{1,0}R_0(1-V_0)V_0^2(1+\omega)^2} \right. \\
& \left. -\frac{I_{1,0}(R_0-1)\left[(2-V_0)[(1+\gamma)(1-V_0)R_0]^{\frac{1}{2}}-I_{1,0}V_0^2\right]}{R_0(1-V_0)V_0^2} \right\} \\
& +\left.\frac{\mathrm{d}I_1}{\mathrm{d}u}\right|_{u=0} \frac{\left\{[(1+\gamma)(1-V_0)R_0]^{\frac{1}{2}}+I_{1,0}V_0\right\}\left[4(1+\omega)^2I_{1,0}^2+e\right]}{2V_0(1+\omega)^2I_{1,0}^2} \\
& +\frac{I_{1,0}}{4V_0^2}\left\{\left[(2-V_0)[(1+\gamma)(1-V_0)R_0]^{\frac{1}{2}}-I_{1,0}V_0^2\right]\left[\frac{\omega(R_0-1)}{1+\omega}+\frac{1}{1+\gamma}\right]\right\} \\
& -\frac{e}{16I_{1,0}(1+\omega)^3V_0^2}\left[\frac{1+3\omega+2\omega\gamma}{1+\gamma}+\omega(R_0-1)\right] \\
& \left\{[(1+\gamma)(1-V_0R_0)]^{\frac{1}{2}}(2+3V_0)+3V_0^2I_{1,0}\right\} \\
& +\frac{R_0-1}{R_0V_0^2}\left[\frac{\omega(1+V_0-R_0)}{(1+\omega)V_0}+\frac{1+6\zeta+4\zeta\gamma}{V_0(1+2)(1+\gamma)}\right] \\
& \times\left\{\left([(1+\gamma)(1-V_0)R_0]^{\frac{1}{2}}+I_{1,0}V_0\right)\left[I_{1,0}-\frac{e}{4I_{1,0}(1+\omega)^2}\right]-2I_{1,0}^2V_0\right\} \\
& +\frac{e\omega}{2(1+\omega)^3}+\frac{2\alpha\zeta}{V_0^2}
\end{aligned} \tag{38}
$$

where V_0, $I_{1,0}$ and $\left.\frac{\mathrm{d}v_0}{\mathrm{d}u}\right|_{u=0}$, $\left.\frac{\mathrm{d}I_1}{\mathrm{d}u}\right|_{u=0}$ are the values of v_0, I_1 and their first order derivatives at $u=0$, respectively. They are determined by the following equations.

Substituting $u=0$ into equations (33), (35) and (30) respectively, yields

$$(1-V_0)^{\frac{1}{2}}\tanh^{-1}(1-V_0)^{\frac{1}{2}}=\frac{\alpha(1+2\zeta)}{(1+\gamma)} \tag{39}$$

$$I_{1,0}=[(1+\gamma)R_0]^{\frac{1}{2}}\tanh^{-1}(1-V_0)^{\frac{1}{2}} \tag{40}$$

where R_0 is the value of R at $u=0$, which can be obtained using equation (33),

$$R_0=1+\frac{e}{4\alpha^2}\frac{(1+\gamma)(1-V_0)}{(1+\omega)^2(1+2\zeta)^2}. \tag{41}$$

Taking the first-order derivative of u in equations (30) and (35) at $u=0$, we obtain

$$
\begin{aligned}
\left.\frac{\mathrm{d}v_0}{\mathrm{d}u}\right|_0 = & \frac{(1-V_0)[\omega(1+\gamma)(R_0-1)+(1+\omega)]}{2(1+\gamma)(1+\omega)} \\
& +\frac{I_{1,0}(1-V_0)}{I_{1,0}V_0[(1+\gamma)(1-V_0)R_0]^{\frac{1}{2}}} \\
& \left[\frac{1+6\zeta+4\zeta\gamma}{(1+\gamma)(1+2\zeta)}-\frac{\omega(R_0-1)}{1+\omega}\right]
\end{aligned} \tag{42}
$$

$$
\begin{aligned}
\left.\frac{\mathrm{d}I_1}{\mathrm{d}u}\right|_0 = & -\frac{1}{2}\left.\frac{\mathrm{d}v_0}{\mathrm{d}u}\right|_0\left\{\frac{[(1+\gamma)R_0]^{\frac{1}{2}}}{V_0(1-V_0)^{\frac{1}{2}}}+\frac{R_0-1}{R_0}\frac{I_{1,0}}{1-V_0}\right\} \\
& +\frac{\left\{[(1+\gamma)(1-V_0)R_0]^{\frac{1}{2}}+I_{1,0}V_0\right\}[(1+\omega)+\omega(1+\gamma)(R_0-1)]}{4V_0(1+\gamma)(1+\omega)} \\
& +\frac{I_{1,0}(R_0-1)}{2R_0V_0}\left[\frac{1+6\zeta+4\zeta\gamma}{(1+2\zeta)(1+\gamma)}+\frac{(V_0+1-R_0)}{1+\omega}\right].
\end{aligned} \tag{43}
$$

When $\left.\frac{\mathrm{d}^2g}{\mathrm{d}u^2}\right|_{u=0}>0$, the value of g is greater than zero in the vicinity of $u=0$ and the first order transition will appear. This the only is condition for the first order transition.

For a given liquid crystal cell, the parameters α, ζ, ω, e are known; V_0, R_0 can be obtained from equations (39) and (41), respectively. Substituting them into (40) (42) (43) we obtain the value of $\left.\frac{\mathrm{d}^2g}{\mathrm{d}u^2}\right|_{u=0}$ and judge the saturation property according to whether or not the value obtained is greater than zero. Taking $\omega=0.2$, $e=6.0$, $\gamma=0.25$ and (a) $\zeta=0.2$, (b) $\zeta=0.0$, (c) $\zeta=-0.2$, (d) $\zeta=-0.3$, for example, the results are as arranged in the table. From this table we can see that the calculated results accord with the conclusions obtained in § 3. One may carry out similar calculations for many other cases, reaching the conclusion that $\zeta<0$ is required for a first order transition at the saturation point.

5. The saturation field strength

The expression of the saturation field strength can now be discussed in detail; there are two situations:

5.1. *The second order transition*

If the transition is second order, it should occur at $u=0$ and the saturation field strength denoted by b_{sat}^0 can

Table. The values of the second order derivative of reduced free energy g for different values of ζ with parameters $e=6.0$, $l/d=0.15$, $\omega=0.2$. The saturation transition property can be judged by the calculation results.

ζ	V_0	R_0	$I_{1,0}$	$\left.\frac{\mathrm{d}v_0}{\mathrm{d}u}\right\|_0$	$\left.\frac{\mathrm{d}I_1}{\mathrm{d}u}\right\|_0$	$\left.\frac{\mathrm{d}^2g}{\mathrm{d}u^2}\right\|_0$	Order conclusion
0.1	0.0716	1.2099	2.4506	2.2243	−13.0631	−248.04<0	second
0.0	0.1230	1.2855	2.1658	1.3548	−3.8106	−45.021<0	second
−0.2	0.3225	1.6126	1.6559	−0.1131	0.9783	5.1647>0	first
−0.3	0.4897	2.0381	1.4301	−0.6926	1.2844	4.8271>0	first

easily be obtained. Substituting $u=0$ into equation (23) we get

$$b^0_{\text{sat}} = \frac{2}{\pi} I_{1,0}. \tag{44}$$

On the other hand, from (24), we have

$$I_{1,0} = \alpha \left\{ \frac{(1+2\zeta)^2}{(1+\gamma)(1-V_0)} + \frac{e}{[2\alpha(1+\omega)]^2} \right\}^{\frac{1}{2}}. \tag{45}$$

Combing equation (44) with (45) and using (40) and (41) results in

$$\coth\left\{ \frac{\left(\frac{\pi}{2} b^0_{\text{sat}}\right)^2 - \left[\frac{e^{\frac{1}{2}}}{2(1+\omega)}\right]^2}{1+\gamma} \right\}^{\frac{1}{2}} = \frac{(1+\gamma)^{\frac{1}{2}}}{\alpha(1+2\zeta)} \left\{ \left(\frac{\pi}{2} b^0_{\text{sat}}\right)^2 - \left[\frac{e^{\frac{1}{2}}}{2(1+\omega)}\right]^2 \right\}^{\frac{1}{2}} \tag{46}$$

This is the only equation which saturation field strength b^0_{S} satisfies. Letting

$$B^0_{\text{sat}} = \left\{ \frac{\left(\frac{\pi}{2} b^0_{\text{sat}}\right)^2 - \left[\frac{e^{\frac{1}{2}}}{2(1+\omega)}\right]^2}{1+\gamma} \right\}^{\frac{1}{2}}$$

we can simplify equation (46) to

$$\coth \mathbf{B}^0_{\text{sat}} = \frac{1+\gamma}{\alpha(1+2\zeta)} \mathbf{B}^0_{\text{sat}}. \tag{47}$$

When the parameters γ, ω, e, α and ζ are known, the saturation field strength for the second order transition can be obtained from equations (46) or (47).

5.2. *The first order transition*

For the first order transition, formula (47) is invalid. The analytic expression of the saturation field strength, b_{sat}, cannot be calculated because $u_c \neq 0$. But we can obtain values of u_c and b_{sat} from the change of Gibbs free energy. From equation (34), we obtain

$$g = u\left[\frac{e}{4\omega u}\left(\frac{1}{1+\omega-\omega u} + \frac{1}{1+\omega}\right) - I_1(I_1 - 2I_2 - 2I_4) - \frac{\alpha}{v_0}\left(1+2\zeta-\zeta\frac{u}{v_0}\right) - \frac{eI_3}{2\omega I_5} \right] \tag{48}$$

where

$$I_4 = \frac{I_1 - I_2}{u} = \int_{v_0}^{1} \frac{1}{2v^2(1-u)} \left\{ \frac{(1-v)[v(1+\gamma)-\gamma u]}{(v-u)} \right\}^{\frac{1}{2}} R^{\frac{1}{2}}\, dv$$

$$I_5 = uI_1 = \int_{v_0}^{1} \frac{u}{2v} \left\{ \frac{v(1+\gamma)-\gamma u}{(1-v)(v-u)} \right\}^{\frac{1}{2}} R^{\frac{1}{2}}\, dv$$

The value of u_c is determined by $g(u_c)=0$; that is

$$\frac{e}{4\omega u_c}\left(\frac{1}{1+\omega-\omega u_c} + \frac{1}{1+\omega}\right) - I_1(I_1 - 2I_2 - 2I_4) - \frac{\alpha}{v_0}\left(1+2\zeta-\zeta\frac{u_c}{v_0}\right) - \frac{eI_3}{2\omega I_5} = 0. \tag{49}$$

Substituting u_c obtained from (49) into equation (23), we may obtain the saturation field strength b_{sat}. We now plot the curve of $g(b)$, which is obtained by eliminating u from the functions $b(u)$ and $g(u)$ obtained in § 3. The results are show in figures 5 and 6.

6. Discussion and conclusion

What have discussed the influence of surface anchoring on the saturation behaviour of a NLC cell under external electric and magnetic fields. The equilibrium

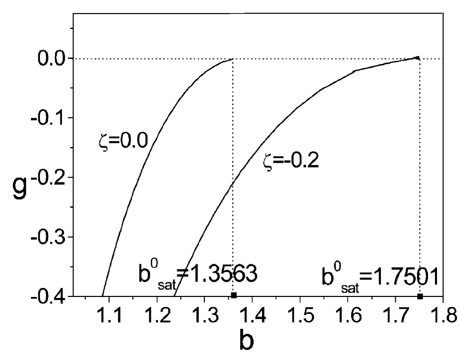

Figure 5. The dependence of g on b for ζ=0.2, 0.0, with parameters e=6.0, l/d=0.15, ω=0.2. It can be seen that $b^0_{\text{sat}}=1.3563$ for ζ=0.0 and $b^0_{\text{sat}}=1.7501$ for ζ=0.2. These values satisfy the formula (46) of second order saturation field strength.

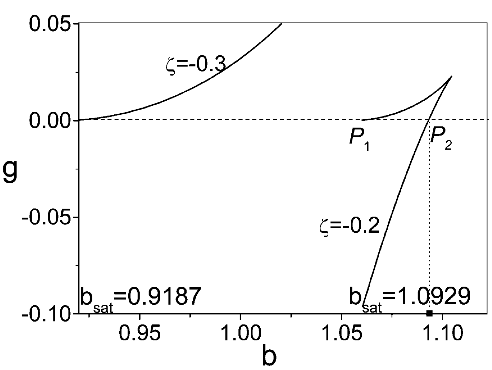

Figure 6. The dependence of g on b for $\zeta=-0.2$, -0.3, with parameters e=6.0, l/d=0.15, ω=0.2. It can be seen that b_{sat}=0.9187 for $\zeta=-0.3$. The curve for $\zeta=-0.2$ intersects the horizontal axis g=0 at two points, P_1 and P_2. Between P_1 and P_2, $g \geqslant 0$; so P_2 corresponds to the saturation point and b_{sat}=1.0929; this leads to the first order saturation transition.

equation and boundary condition of the director have been obtained with the methods of analytical derivation. Results obtained by numerical calculation show that the value of the field strength and the transition property at saturation point are strongly influenced by the anchoring parameters. Apart from the usual second order transition, a first order saturation transition can also be induced by suitable surface anchoring for the investigated system. Methods of calculation of the saturation field strength, related to surface anchoring, are given for both the second order and first order transitions. Conditions for the occurrence of the first order transition are given. It is required that $\zeta<0$ so the fourth order term in θ in the expansion of the surface anchoring energy is necessary to characterize the saturation transition. Whether or not higher order terms reflect some other physical effects entails further clarification, but we believe that a few lower order terms may be significant.

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