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The effect of melting on the electrostatic coherence length of nematic liquid crystals

N. J. Mottram*and S. J. Hogan[†]

Department of Mathematics, University of Strathclyde, Livingstone Tower, 26 Richmond St,

Glasgow G1 1XH, UK.

† *Department of Engineering Mathematics, University of Bristol, Queen's Building*

University Walk, Bristol BS8 1TR, UK.

Abstract

We examine the effects of electric field-induced changes in molecular order on the director structure within a nematic liquid crystal cell. Specifically, we investigate the boundary layer between the cell substrate and the bulk nematic material when strong anchoring forces the nematic director in a different direction to that of an applied field. We find that at low field strengths the classical picture of liquid crystal/electric field interaction occurs, that is, the director orientation is governed by the surface alignment until a transition occurs as the classic electrostatic coherence length ζ becomes comparable to the cell thickness and the director changes orientation so as to align with the electric field. However, at high field strengths, we find that a field-induced change of the molecular order close to the cell boundary causes a significant reduction, to $O(\zeta^2)$, in the effective electrostatic coherence length, i.e. the characteristic length of the director distortion.

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*Author to whom correspondence should be addressed, email: nigel.mottram@strath.ac.uk

I. INTRODUCTION

The behaviour of liquid crystalline materials near to solid substrates is an important factor in liquid crystal displays since it is the competition between the surface alignment forces and the torque due to an applied electric field that governs the switching of such a device. Of particular importance are the stability of the molecular anchoring at the substrate, the temperature dependence of this anchoring and the behaviour of the liquid crystal material in the region close to the surface when an electric field is applied. Much research, both experimental and theoretical, has been conducted into the properties of many different alignment techniques, particularly into weak and bistable anchoring [1–4]. However, almost all previous theoretical work has employed the Oseen-Frank theory [5,6] when dealing with static problems and the Leslie-Ericksen theory [7,8] when dealing with dynamic flow problems. Whilst such theories have been extremely successful in modelling the behaviour of nematic liquid crystal materials at a fixed temperature, well within the nematic phase, they are unable to model the behaviour close to the isotropic-nematic transition point, where external forces may cause a change in the molecular order. At such temperatures it is necessary to describe a nematic material in terms of the average molecular direction at a point, the director $\mathbf{n}$, *and* a measure of how ordered the molecules are with respect to the director.

The common measure for the amount of ordering in a uniaxial nematic liquid crystal is the scalar order parameter S [9]. At a fixed temperature within the nematic phase S can usually be assumed to be constant and therefore any theory of the phase needs only to consider variations in the director orientation. However, near to the isotropic-nematic phase transition the order parameter may vary considerably throughout the material and thus an accurate theory of the system must allow for such variations. A more detailed explanation of such a description of a nematic material will be given in the next section.

Changes in S can occur in the nematic phase when the material undergoes a high amount of distortion. For instance, near to the core of defects, a region of high elastic stress, S can be significantly reduced from its equilibrium value [10] in other words the liquid crystal partially melts. Other work has shown that a change in S may occur close to surfaces which induce an ordering different to the bulk nematic material [11,12].

The application of an electric field can cause either an increase or a decrease in the order parameter. For a positive dielectric material ($\epsilon_a > 0$) the application of an electric field leads to an induced molecular dipole and thus alignment of the major molecular axis with the electric field direction. With the nematic director aligned in the field direction the enhanced orientation of the molecules increases S. However, when the director is constrained to be in a different direction to the field, a disordering effect may occur and thus reduce S [13]. This

field ordering/disordering effect has been previously demonstrated numerically [14] and, in this paper, we intend to provide analytical solutions of the liquid crystal behaviour near to the surfaces.

Such behaviour demonstrates one of the most fundamental processes used in liquid crystal devices, that is the competition between an aligning surface and an applied electric field. With no electric field, the surface alignment forces determine the configuration of the director within a liquid crystal cell. When an electric field is applied, such that the field direction is in a direction perpendicular to the surface alignment direction, a competition of forces is produced. At high enough field strengths the electric field forces will dominate and the director will align with the electric field. This phenomenon, first investigated by Freedericksz and Zolina [15], enables nematic liquid crystal cells to be used as display devices. The electrical control of the director orientation, and consequently the optical characteristics, gives a method of switching from a dark state to a light state and vice-versa.

At sufficiently high field strengths the bulk of the liquid crystal is aligned with the applied field and there exists narrow regions, next to the cell surfaces, where the director realigns from the field direction to the surface alignment direction. Within these *boundary layers* there may occur a high degree of elastic distortion and consequently a significant reduction in the value of the order parameter. It is this phenomenon which we investigate in this paper.

Using a uniaxial order parameter tensor and a Landau-Ginzburg formulation of the free energy, the governing equations for the director orientation and the scalar order parameter are found from the minimization of the free energy. We solve these equations using matched asymptotic expansions in two situations, at low and high field strengths. At low field strengths the classical picture [16] of liquid crystal/electric field interaction occurs, the director angle varies over a length scale equal to the electrostatic coherence length ζ. When the field strength is below the critical Freedericksz value this electrostatic coherence length is larger than the cell thickness and the director is unchanged by the field. As the field increases the electrostatic coherence length tends towards the cell thickness, the torques due to the electric field and surface alignment become comparable and at a critical field strength the director reorients to align with the field direction. At high field strengths the high distortions of the director cause a significant reduction in the order parameter which in turn causes a significant reduction in the characteristic length of the director distortion to a length of order ζ^2.

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II. CONTINUUM THEORY

The uniaxial nematic liquid crystal is a mesomorphic state that occurs in a temperature range between the liquid and the solid (crystalline) phases. In this intermediate state the molecules tend to align along a preferred direction with a measure of order. Such a state may be described by the second order tensor

$$\mathbf{Q} = S\left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}\right), \tag{1}$$

where $\mathbf{I}$ is the identity matrix and the ij^{th} element of the product $\mathbf{n} \otimes \mathbf{n}$ is $\mathbf{n}_i\mathbf{n}_j$.

The *order parameter tensor* $\mathbf{Q}$ describes the orientational order inherent in the liquid crystalline state in terms of the director, $\mathbf{n}$ (Fig. 1), representing the locally averaged direction of the molecules at a point in the material. The order parameter S, which is a measure of the molecular alignment with respect to this average direction vector, is defined as

$$S = \frac{1}{2} < (3\cos^2\psi - 1) >, \tag{2}$$

where ψ is the angle between a molecule and the director and $<>$ denotes a thermal average [9]. When $S = 0$ the molecules are oriented in a random fashion and the material is isotropic and when $S = 1$ the molecules are perfectly ordered with the director and the material is crystalline.

A more accurate description of the liquid crystalline state would be in terms of a biaxial order tensor. For a biaxial nematic state there exists not only an ordering of the long axis of the molecule (as in Fig. 1) but a secondary ordering of the short molecular axis. Although such a biaxial state has never been found to exist in a bulk sample of a thermotropic liquid crystalline material there are certain regions, such as in the core of a defect, within which biaxial states exist over short length scales. However, within a defect core biaxiality is present due to certain topological constraints whereas in the situation presented in this paper there are no such constraints and biaxiality plays a minor rôle in this phenomenon. The biaxial nematic order parameter tensor is also more complicated than the uniaxial case and includes an additional director (associated with the average direction of the molecular short axis) as well as an additional scalar order parameter (associated with the ordering of the short molecular axis about the secondary director). A corresponding biaxial theory is therefore more complicated and for simplicity we neglect biaxiality and concentrate on changes to the uniaxial order parameter and as a result we are able to obtain analytic solutions to the equations.

A continuum theory for uniaxial nematic liquid crystals can be derived using the order parameter tensor $\mathbf{Q}$ by constructing a physically realistic free energy for which minimizing

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solutions are sought. The free energy is approximated by an expansion in powers of $\mathbf{Q}$ and $\nabla \mathbf{Q}$ which satisfies the inherent symmetry of the nematic liquid crystal material and may be written as [17]

$$\mathcal{F} = \int_0^d L \operatorname{tr}(\nabla \mathbf{Q})^2 + \alpha \operatorname{tr}\mathbf{Q}^2 + \frac{2}{3}\beta \operatorname{tr}\mathbf{Q}^3 + \frac{1}{2}\gamma(\operatorname{tr}\mathbf{Q}^2)^2 - \operatorname{tr}(\mathbf{Q}\,\mathcal{E})\,dz, \tag{3}$$

where d is the cell thickness; L is a coefficient of elasticity associated with distortions of the order parameter tensor; α, β and γ are the first three coefficients in the Landau expansion of the thermodynamic potential energy; and the electric field tensor $\mathcal{E}$ is defined in terms of the permitivity of free space, ϵ_0, the dielectric anisotropy of the material, ϵ_a, and the electric field $\mathbf{E}$ as

$$\mathcal{E} = \frac{\epsilon_0 \epsilon_a}{4\pi}\mathbf{E} \otimes \mathbf{E}. \tag{4}$$

Using this theory we will model in-plane switching of a nematic cell in which the director remains in the plane of the surfaces when an electric field, applied in a direction contained in the same plane, switches the director (Fig. 2). Such a switching mechanism was one of the basic modes of switching proposed by Freedericksz and has recently been utilized in the device developed by Hitachi [18] which benefits from the advantageous optical characteristics, specifically an improved viewing angle, of such in-plane director configurations.

For this display we can assume that the director remains in-plane (in the xy-plane) and is strongly anchored in the y direction at the surfaces, the director and order parameter depend only on the coordinate through the cell (the z coordinate) and the electric field is in the direction parallel to the cell surfaces but perpendicular to the director at the surfaces (see Fig. 2). Therefore, we take $\mathbf{n} = (\sin\theta, \cos\theta, 0)$, $S = S(z)$, $\theta = \theta(z)$ and $\mathbf{E} = (E_1,\, 0,\, 0)$. The director must therefore *twist* in order to orient itself with the applied electric field. With these assumptions the free energy (3) becomes

$$\begin{aligned}
\mathcal{F} = \int_0^d \Bigg\{ &L\left(\frac{2}{3}\left(\frac{dS(z)}{dz}\right)^2 + 2\,(S(z))^2\left(\frac{d\theta(z)}{dz}\right)^2\right) \\
&+ \frac{\epsilon_0 \epsilon_a}{4\pi}S(z)E_1^{\,2}\left(\cos^2\theta(z) - \frac{2}{3}\right) \\
&+ \frac{2}{3}\alpha S(z)^2 + \frac{4}{27}\beta S(z)^3 + \frac{2}{9}\gamma S(z)^4\Bigg\}\,dz.
\end{aligned} \tag{5}$$

Minimization of this energy with respect to $S(z)$ and $\theta(z)$ leads to the Euler-Lagrange equations

$$0 = L\left(\frac{d^2 S(z)}{dz^2} - 3S(z)\left(\frac{d\theta(z)}{dz}\right)^2\right) + \frac{\epsilon_0 \epsilon_a}{8\pi}E_1^2\left(1 - \frac{3}{2}\cos^2\theta(z)\right)$$

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$$-\alpha S(z) - \frac{1}{3}\beta S(z)^2 - \frac{2}{3}\gamma S(z)^3, \tag{6a}$$

$$0 = 2L\left(S(z)\left(\frac{d^2\theta(z)}{dz^2}\right) + 2\frac{dS(z)}{dz}\frac{d\theta(z)}{dz}\right) + \frac{\epsilon_0\epsilon_a}{4\pi}E_1^2\sin(\theta(z))\cos(\theta(z)), \tag{6b}$$

which govern the behaviour of the director and scalar order parameter within the cell. At the cell surfaces we assume that an alignment layer not only strongly anchors the director in a fixed direction, the y direction, but also fixes the scalar order parameter to a constant value S_w. The boundary conditions may be written as

$$S(0) = S_w, \tag{7a}$$

$$S(d) = S_w, \tag{7b}$$

$$\theta(0) = 0, \tag{7c}$$

$$\theta(d) = 0. \tag{7d}$$

Thus the wall is orienting the director along the y-axis whilst the field is attempting to orient the director along the x-axis. When the field force is sufficiently strong the bulk of the cell will orient along the field direction whilst close to the surfaces boundary layers will form where the director reorients to satisfy the boundary conditions near to the wall. In such a region of large director distortion a corresponding reduction in the order parameter S is expected.

Reducing the number of parameters in Eqs. (6a) and (6b) by with the nondimensionalisation $z = d\,Z$, $A = \alpha/L$, $B = \beta/L$, $C = \gamma/L$, $\zeta = \sqrt{(4\pi L)/(\epsilon_0\epsilon_a E_1{}^2)}$ the governing equations become,

$$0 = \left(\frac{d^2S}{dZ^2}\right) - 3S\left(\frac{d\theta}{dZ}\right)^2 + \left(\frac{d}{\zeta}\right)^2\left(\frac{1}{2} - \frac{3}{4}\cos^2\theta\right)$$
$$-d^2\left(AS + \frac{1}{3}BS^2 + \frac{2}{3}CS^3\right), \tag{8a}$$

$$0 = 2S\left(\frac{d^2\theta}{dZ^2}\right) + 4\left(\frac{dS}{dZ}\right)\left(\frac{d\theta}{dZ}\right) + \left(\frac{d}{\zeta}\right)^2\sin(\theta)\cos(\theta), \tag{8b}$$

and the boundary conditions are

$$S(0) = S_w, \tag{9a}$$

$$S(1) = S_w, \tag{9b}$$

$$\theta(0) = 0, \tag{9c}$$

$$\theta(1) = 0. \tag{9d}$$

The quantity ζ, which has the dimensions of length, is usually called the *electrostatic coherence length* [9].

We will now solve the above equations in two distinct situations. In §III we solve for low electric field values and show that the director distortion occurs over a length scale equal to the electrostatic coherence length, ζ which at low fields is larger than the cell thickness and thus the surface orientation dominates. The scalar order parameter smoothly changes from the bulk thermotropic equilibrium value S_{eq} to the surface value S_w.

In §IV we consider the system at high electric field values. We show that in this case the order parameter and director orientation vary over different length scales. The director orientation varies over a length scale which is significantly shorter than the electrostatic coherence length. In fact the director reorients over a distance of order ζ^2.

Using asymptotic expansions within different regions of the cell, specified by the order of magnitude of the spatial dimension Z, we find solutions to Eqs. (8a, 8b). By matching the solutions asymptotically between these regions a full solution is found. In each of the cases, low and high electric field strengths, solutions are found in the bulk of the cell where $Z = O(1)$ and close to the surface where $Z = O(\eta^q)$ where η is a small parameter and the index q is determined through a Principle of Least Degeneracy [19]. In fact we see in the high field case that this method fails to produce an analytic asymptotic solution and an alternative ordering is needed to investigate the behaviour close to the cell surface.

III. LOW FIELD STRENGTH SOLUTION

In the low field case we assume that the field strength E_1 is small enough such that $\delta \equiv (d/\zeta)^2 \ll 1$, i.e. the coherence length is much larger than the cell thickness. The parameters d^2A, d^2B and d^2C will be assumed to be large (i.e. $d^2A = O(1/\delta)$ etc). These parameters depend only on cell and material properties and not on the electric field strength and so will be assumed to be fixed and of the same value in both this case and the high field case. Denoting $d^2A = \tilde{A}/\delta$, $d^2B = \tilde{B}/\delta$ and $d^2C = \tilde{C}/\delta$, where $\tilde{A} = O(1)$, $\tilde{B} = O(1)$ and $\tilde{C} = O(1)$, the governing equations (8a, 8b) are

$$0 = \left(\frac{d^2S}{dZ^2}\right) - 3S\left(\frac{d\theta}{dZ}\right)^2 + \delta\left(\frac{1}{2} - \frac{3}{4}\cos^2\theta\right) - \frac{1}{\delta}\left(\tilde{A}S + \frac{1}{3}\tilde{B}S^2 + \frac{2}{3}\tilde{C}S^3\right), \tag{10a}$$

$$0 = 2S\left(\frac{d^2\theta}{dZ^2}\right) + 4\left(\frac{dS}{dZ}\right)\left(\frac{d\theta}{dZ}\right) + \delta\sin\theta\cos\theta. \tag{10b}$$

A. Low field: Outer solution

We firstly consider the solution in the region where $Z = O(1)$ or in dimensional variables $z = O(d)$, i.e. in the bulk of the cell, and use the expansions

$$S = S_0^{out} + \delta S_1^{out} + \delta^2 S_2^{out} + O(\delta^3), \tag{11a}$$

$$\theta = \theta_0^{out} + \delta \theta_1^{out} + \delta^2 \theta_2^{out} + O(\delta^3), \tag{11b}$$

so from Eqs. (10a, 10b) the leading order equations are

$$0 = \left(\tilde{A} S_0^{out} + \frac{1}{3} \tilde{B} S_0^{out\,2} + \frac{2}{3} \tilde{C} S_0^{out\,3} \right), \tag{12a}$$

$$0 = 2S \left(\frac{d^2 \theta_0^{out}}{dZ^2} \right) + 4 \left(\frac{dS_0^{out}}{dZ} \right) \left(\frac{d\theta_0^{out}}{dZ} \right). \tag{12b}$$

Equation (12a) gives the solution $S_0^{out} = S_{eq}$ where S_{eq} is the thermodynamic equilibrium value of the order parameter associated with the non-zero minimum value of the entropic potential, $\alpha \mathrm{tr} \mathbf{Q}^2 + \frac{2}{3} \beta \mathrm{tr} \mathbf{Q}^3 + \frac{1}{2} \gamma (\mathrm{tr} \mathbf{Q}^2)^2$. Therefore, in the bulk of the cell the order parameter is constant and independent of the electric field value. Substituting this solution into the second equation (12b) leads to

$$0 = 2S_{eq} \left(\frac{d^2 \theta_0^{out}}{dZ^2} \right). \tag{13}$$

Directly integrating this equation gives the solution $\theta_0^{out} = a_1 Z + a_2$ where a_1 and a_2 are constants. The symmetry of the cell about the midpoint $[\theta(Z) = \theta(d - Z)]$ ensures that $a_1 = 0$ and thus $\theta_0^{out} = a_2$. The value of a_2 will be calculated through a matching condition with the inner solution.

B. Low field: Inner solution

Near to the cell surface at $Z = 0$, the order parameter will change from the bulk equilibrium value S_{eq} to the surface value S_w and the director angle changes from the bulk solution $\theta_0^{out} = a_2$ to the boundary condition $\theta(0) = 0$.

By the Principle of Least Degeneracy described above, the relevant ordering near to the surface is $Z = O(\sqrt{\delta})$ or in dimensional terms $z = O(d^2/\zeta)$. We therefore set $Z = Z_{in} \sqrt{\delta}$, where $Z_{in} = O(1)$, then use the expansions

$$S = S_0^{in} + \delta S_1^{in} + \delta^2 S_2^{in} + O(\delta^3), \tag{14a}$$

$$\theta = \theta_0^{in} + \delta \theta_1^{in} + \delta^2 \theta_2^{in} + O(\delta^3), \tag{14b}$$

and from Eqs. (10a, 10b) the leading order equations are

$$0 = \left(\frac{d^2 S_0^{in}}{dZ_{in}^2} \right) - 3 S_0^{in} \left(\frac{d\theta_0^{in}}{dZ_{in}} \right)^2 - \left(\tilde{A} S_0^{in} + \frac{1}{3} \tilde{B} S_0^{in\,2} + \frac{2}{3} \tilde{C} S_0^{in\,3} \right), \tag{15a}$$

$$0 = 2 S_0^{in} \left(\frac{d^2 \theta_0^{in}}{dZ_{in}^2} \right) + 4 \left(\frac{dS_0^{in}}{dZ_{in}} \right) \left(\frac{d\theta_0^{in}}{dZ_{in}} \right). \tag{15b}$$

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We may again directly integrate the equation for θ_0^{in} and, from knowing the asymptotic behaviour of the system, show that the solution which satisfies the boundary condition at $Z = 0$ is $\theta_0^{in} = 0$. Equation (15a) then becomes

$$0 = \left(\frac{d^2 S_0^{in}}{dZ_{in}^2} \right) - \left(\tilde{A} S_0^{in} + \frac{1}{3} \tilde{B} S_0^{in^2} + \frac{2}{3} \tilde{C} S_0^{in^3} \right), \tag{16}$$

which may be solved analytically in terms of two unknown integration constants one of which is determined by the boundary condition $S_0^{in}(0) = S_w$.

In order to determine the two remaining unknown constants, one in the solution for θ_0^{out} and one in the solution for S_0^{in}, we must apply a condition which ensures that the inner and outer solutions match asymptotically. This matching condition [19] is,

$$\lim_{Z \to \infty} S_0^{in}(Z) = \lim_{Z_{in} \to 0} S_0^{out}(Z_{in}) \tag{17a}$$

$$\lim_{Z \to \infty} \theta_0^{in}(Z) = \lim_{Z_{in} \to 0} \theta_0^{out}(Z_{in}) \tag{17b}$$

which leads to the solution $\theta_0^{out} = 0$ and specifies that $S_0^{in} \to S_{eq}$ as $Z_{in} \to \infty$. Equation (16) can now be solved explicitly and the solution for S_0^{in}, which varies from a bulk equilibrium value to a fixed surface value, can now be conveniently written as,

$$S_0^{in} = S_{eq} - \frac{4a_4 \exp\left(-\sqrt{\frac{\tilde{C}a_4}{3}} Z_{in} + a_5 \right)}{4a_4 - \left(\exp\left(-\sqrt{\frac{\tilde{C}a_4}{3}} Z_{in} + a_5 \right) - a_3 \right)^2}, \tag{18}$$

where $a_3 = (2\tilde{B})/(3\tilde{C}) + 2S_{eq}$, $a_4 = 3S_{eq}^2 + (2S_{eq}\tilde{B})/(3\tilde{C}) + 3\tilde{A}/\tilde{C}$ and from the boundary condition $S_0^{in}(0) = S_w$,

$$a_5 = -\ln\left(\frac{2a_4 + a_3\tilde{S} + 2\sqrt{a_4}\sqrt{\tilde{S}^2 + a_3\tilde{S} + a_4}}{\tilde{S}} \right) / \sqrt{a_4}, \tag{19}$$

where for simplicity we have written $\tilde{S} = S_0^{in} - S_{eq}$. This solution is shown in Fig. 3 using the parameters $\tilde{A} = 0.14$, $\tilde{B} = -2.7$, $\tilde{C} = 1.5$ (which have been chosen to give $S_{eq} = 0.7$) and $S_w = 0.6$. Such an equation for the scalar order parameter (16) has previously been considered numerically and, in a simplified form, analytically by Barberi & Durand [11] and Barbero & Durand [12].

C. Low field: Electrostatic coherence length scale

Although the electrostatic coherence length is larger than the cell thickness it is useful to consider such a length scale in order to relate this work to the classic model of the

Freedericksz transition [9]. On this length scale $z = O(\zeta)$ or in nondimensional parameters, $Z = O(1/\sqrt{\delta})$. We set $Z = Z_{ec}/\sqrt{\delta}$, where $Z_{ec} = O(1)$, then use the expansions

$$S = S_0^{ec} + \delta S_1^{ec} + \delta^2 S_2^{ec} + O(\delta^3), \tag{20a}$$

$$\theta = \theta_0^{ec} + \delta\theta_1^{ec} + \delta^2\theta_2^{ec} + O(\delta^3), \tag{20b}$$

and from equations (10a, 10b) the leading order equations are

$$0 = \left(\tilde{A}S_0^{ec} + \frac{1}{3}\tilde{B}S_0^{ec2} + \frac{2}{3}\tilde{C}S_0^{ec3}\right), \tag{21a}$$

$$0 = 2S_0^{ec}\left(\frac{d^2\theta_0^{ec}}{dZ_{ec}^2}\right) + 4\left(\frac{dS_0^{ec}}{dZ_{ec}}\right)\left(\frac{d\theta_0^{ec}}{dZ_{ec}}\right) + \sin\theta_0^{ec}\cos\theta_0^{ec}. \tag{21b}$$

Equation (21a) gives the solution $S_0^{ec} = S_{eq}$ and substituting this into the second equation (21b) leads to

$$0 = 2S_{eq}\left(\frac{d^2\theta_0^{ec}}{dZ_{ec}^2}\right) + \sin\theta_0^{ec}\cos\theta_0^{ec}. \tag{22}$$

This is exactly the equation presented in de Gennes & Prost [9] and we see that for the first time the electric field term is present in the governing equations. Below a critical field strength $E_1 = \dfrac{1}{d}\sqrt{\dfrac{8\pi L S_{eq}}{\epsilon_0\epsilon_a}}$ (in the notation of this paper) the trivial solution $\theta_0^{ec} = 0$ is stable. However, above this critical field strength the director configuration distorts in order to align with the field.

Thus director distortions occur on a length scale equal to the electrostatic coherence length ζ. When the electrostatic coherence length approaches the cell thickness the electric field force becomes comparable to the surface alignment force and the Freedericksz transition occurs. The cell then switches from the low field strength solution $\theta = 0$ through a continuous transition to a non-zero director orientation. At such intermediate field strengths $d/\zeta = O(1)$, the governing equations (8a, 8b) do not simplify and little analytic progress can be made. This is not the case at sufficiently high field strengths.

IV. HIGH FIELD STRENGTH SOLUTION

In the high field strength situation we assume that the field strength E_1 is large enough to ensure that $(d/\zeta)^2 \gg 1$ and we will therefore take $(\zeta/d)^2 = \epsilon$ as our small parameter for subsequent solution expansions. We will assume that ϵ is of the same order as δ used in the previous section and therefore, the parameters d^2A, d^2B and d^2C will be assumed to be large and of order $1/\epsilon$. Using the scaled parameters $d^2A = A^*/\epsilon$, $d^2B = B^*/\epsilon$ and

$d^2C = C^*/\epsilon$, where $A^* = O(1)$, $B^* = O(1)$ and $C^* = O(1)$, the governing equations (8a, 8b) become

$$0 = \epsilon\left(\frac{d^2S}{dZ^2}\right) - 3\epsilon S\left(\frac{d\theta}{dZ}\right)^2 + \left(\frac{1}{2} - \frac{3}{4}\cos^2\theta\right) - \left(A^*S + \frac{1}{3}B^*S^2 + \frac{2}{3}C^*S^3\right), \qquad (23a)$$

$$0 = 2\epsilon S\left(\frac{d^2\theta}{dZ^2}\right) + 4\epsilon\left(\frac{dS}{dZ}\right)\left(\frac{d\theta}{dZ}\right) + \sin\theta\cos\theta. \qquad (23b)$$

As in the low field case we will solve these equations in two different regions of the cell. Within the bulk of the cell there will not be large gradients in the variables, θ and S, so we may take $Z = O(1)$ and close to the cell surface $Z = 0$ the Principle of Least Degeneracy specifies an ordering $Z = O(\sqrt{\epsilon})$. However, the inner ordering does not simplify the governing equations and no analytic solution is found. We find an alternative ordering, closer to the cell surface, $Z = O(\epsilon)$ where we find a non-asymptotic analytic solution.

A. High field: Outer solution

In the bulk of the liquid crystal cell $Z = O(1)$ and since we have chosen $(d/\zeta)^2 = 1/\epsilon \gg 1$ the electric field energy term will dominate the elastic distortion term in equation (23a). Therefore the field term will determine the director structure within the bulk whilst the order parameter behaviour will be determined by the entropic energy term, modified by the presence of the field. By assuming $Z = O(1)$ and using the expansions

$$S = S_0^{out} + \epsilon S_1^{out} + \epsilon^2 S_2^{out} + O(\epsilon^3), \qquad (24a)$$

$$\theta = \theta_0^{out} + \epsilon\theta_1^{out} + \epsilon^2\theta_2^{out} + O(\epsilon^3). \qquad (24b)$$

the $O(1)$ equations, from (23a) and (23b), are then

$$0 = \left(\frac{1}{2} - \frac{3}{4}\cos^2\theta_0^{out}\right) - \left(A^*S_0^{out} + \frac{1}{3}B^*S_0^{out2} + \frac{2}{3}C^*S_0^{out3}\right), \qquad (25a)$$

$$0 = \sin(\theta_0^{out})\cos(\theta_0^{out}). \qquad (25b)$$

The relevant stable solution of Eq. (25b) is $\theta_0^{out} = \pi/2$, i.e. the director is aligned with the electric field, and Eq. (25a) then simplifies to

$$0 = \frac{1}{2} - \left(A^*S_0^{out} + \frac{1}{3}B^*S_0^{out2} + \frac{2}{3}C^*S_0^{out3}\right), \qquad (26)$$

or in dimensional variables

$$0 = \frac{\epsilon_0\epsilon_a E_1^2}{8\pi} - \left(\alpha S_0^{out} + \frac{1}{3}\beta S_0^{out2} + \frac{2}{3}\gamma S_0^{out3}\right), \qquad (27)$$

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so that $S_0^{out} = V^{-1}\left(\dfrac{\epsilon_0 \epsilon_a E_1{}^2}{8\pi}\right)$ where the polynomial V is $V(S) = \alpha S + \frac{1}{3}\beta S^2 + \frac{2}{3}\gamma S^3$. There are clearly three roots of this cubic equation. However, within the temperature range in which the nematic phase is stable the relevant solution is the largest positive real stable solution as indicated by the graphical solution in Fig. 4. This solution is the bulk equilibrium value, S_{eq}, modified by the non-zero electric field. As the field strength E_1 increases S_0^{out} will increase (see Fig. 4). Therefore, as expected, in the bulk of the liquid crystal cell the director orients with the electric field (in the x direction) and causes the molecules to increases their alignment with the director and thus increases the order parameter.

B. High field: Inner Solution

Near to the cell surface the strong anchoring of the molecules in the y direction (i.e. $\theta = 0$) is now in competition with the bulk orientation (i.e. $\theta = \pi/2$). There will therefore be a region of reorientation close to the surface in which the director rotates from the x direction to the y direction. Since we have taken $(d/\zeta)^2 \gg 1$, the field term is dominant in most of the cell and this region of reorientation will be small. As mentioned above, the Principle of Least Degeneracy leads to the ordering, $Z = \sqrt{\epsilon}Z_{in}$ where $Z_{in} = O(1)$. With the expansion

$$S = S_0^{in} + \epsilon S_1^{in} + \epsilon^2 S_2^{in} + O(\epsilon^3). \tag{28a}$$

$$\theta = \theta_0^{in} + \epsilon S_1^{in} + \epsilon^2 S_2^{in} + O(\epsilon^3). \tag{28b}$$

The highest order equations from (23a, 23b) become

$$0 = \left(\frac{d^2 S_0^{in}}{dZ_{in}{}^2}\right) - 3S_0^{in}\left(\frac{d\theta_0^{in}}{dZ_{in}}\right)^2 + \left(\frac{1}{2} - \frac{3}{4}\cos^2\theta_0^{in}\right) - \left(A^* S_0^{in} + \frac{1}{3}B^* S_0^{in\,2} + \frac{2}{3}C^* S_0^{in\,3}\right), \tag{29a}$$

$$0 = 2S_0^{in}\left(\frac{d^2\theta_0^{in}}{dZ_{in}^2}\right) + 4\left(\frac{dS_0^{in}}{dZ_{in}}\right)\left(\frac{d\theta_0^{in}}{dZ_{in}}\right) + \sin\theta_0^{in}\cos\theta_0^{in}. \tag{29b}$$

The equations have clearly not been simplified with the use of the above expansion and no analytic solutions to Eqs. (29a) and (29b) are forthcoming. However, there *is* a length scale for which we may solve the equations analytically as detailed in the following section.

C. High field: Boundary solution

At length scales smaller than the preceding section an expansion may be employed to solve the equations and match the boundary condition at $Z = 0$. We concentrate on the region $Z = O(\epsilon)$ close to $Z = 0$. We set $Z = \epsilon Z_{bs}$ where $Z_{bs} = O(1)$ and use the expansions

$$S = S_0^{bs} + \epsilon S_1^{bs} + \epsilon^2 S_2^{bs} + O(\epsilon^3), \tag{30a}$$

$$\theta = \theta_0^{bs} + \epsilon \theta_1^{bs} + \epsilon^2 \theta_2^{bs} + O(\epsilon^3). \tag{30b}$$

From (23a) and (23b) the highest order equations are,

$$0 = \left(\frac{d^2 S_0^{bs}}{dZ_{bs}^2} \right) - 3 S_0^{bs} \left(\frac{d\theta_0^{bs}}{dZ_{bs}} \right)^2, \tag{31a}$$

$$0 = 2 S_0^{bs} \left(\frac{d^2 \theta_0^{bs}}{dZ_{bs}^2} \right) + 4 \left(\frac{dS_0^{bs}}{dZ_{bs}} \right) \left(\frac{d\theta_0^{bs}}{dZ_{bs}} \right). \tag{31b}$$

Equation (31b) may be directly integrated to give

$$\left(\frac{d\theta_0^{bs}}{dZ_{bs}} \right) = \frac{k_1}{S_0^{bs2}}, \tag{32}$$

where k_1 is an integration constant. Substituting in Eq. (31a) gives

$$0 = \left(\frac{d^2 S_0^{bs}}{dZ_{bs}^2} \right) - 3 \frac{k_1^2}{S_0^{bs3}}, \tag{33}$$

and integrating this equation gives

$$0 = \left(\frac{dS_0^{bs}}{dZ_{bs}} \right)^2 + 3 \left(\frac{k_1^2}{S_0^{bs2}} - k_2^2 \right), \tag{34}$$

where k_2 is an integration constant. The solution of (34) is

$$S_0^{bs2} = 3 k_2^2 (Z_{bs} + k_3)^2 + \frac{k_1^2}{k_2^2}, \tag{35}$$

where k_3 is an integration constant. The boundary condition (9a) gives $S_w^2 = 3 k_2^2 k_3^2 + k_1^2 / k_2^2$ which implies $k_3^2 = (S_w^2 k_2^2 - k_1^2)/3 k_2^4$. We can therefore calculate the integration constant k_3 in terms of k_1 and k_2.

Substituting into the θ_0^{bs} Eq. (31b) leads to

$$\left(\frac{d\theta_0^{bs}}{dZ_{bs}} \right) = \frac{k_1}{3 k_2^2 (Z_{bs} + k_3)^2 + k_1^2 / k_2^2}, \tag{36}$$

the solution of which is

$$\theta_0^{bs} = \frac{1}{\sqrt{3}} \tan^{-1} \left(\frac{\sqrt{3} k_2^2}{k_1} (Z_{bs} + k_3) \right) + k_4, \tag{37}$$

where k_4 is an integration constant. The boundary condition (9c) gives

$$k_4 = -\frac{1}{\sqrt{3}} \tan^{-1} \left(\frac{\sqrt{3} k_2^2}{k_1} k_3 \right). \tag{38}$$

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which gives the integration constant k_4 in terms of k_1 and k_2 (Since we know k_3 in terms of k_1 and k_2).

Therefore, the leading order inner solutions S_0^{bs} and θ_0^{bs} only depend on the unknown constants k_1 and k_2,

$$S_0^{bs^2} = 3k_2{}^2 \left(Z_{bs} - \sqrt{(S_w{}^2 k_2{}^2 - k_1{}^2)/3k_2{}^4} \right)^2 + \frac{k_1{}^2}{k_2{}^2}, \tag{39a}$$

$$\theta_0^{bs} = \frac{1}{\sqrt{3}} \tan^{-1} \left(\frac{\sqrt{3}k_2{}^2}{k_1} Z_{bs} - \sqrt{(S_w{}^2 k_2{}^2 - k_1{}^2)/k_1{}^2} \right) +$$
$$\frac{1}{\sqrt{3}} \tan^{-1} \left(\sqrt{(S_w{}^2 k_2{}^2 - k_1{}^2)/k_1{}^2} \right). \tag{39b}$$

It is possible to determine at least one of these unknown constants from the asymptotic value of θ. From the above solution (39b) we see that as $Z_{bs} \to \infty$ the director angle solution asymptotes to a fixed value. This asymptotic value must be the bulk value $\theta = \pi/2$ and so $k_2 = k_1 S_w / \sin(\sqrt{3}\pi/2)$. Thus the number of unknown constants is reduced to one. The remaining constant must be determined by solving Eq. (29a) numerically.

Solutions for θ_0^{bs} and S_0^{bs} are shown in Fig. 5 for which we have used the parameters $S_w = 0.6$ and $k_1 = 2.0$. The crucial aspect of the scalar order parameter (39a) solution is that S_{bs} initially decreases from its boundary value S_w to a minimum value $S_{min} = \sin(\sqrt{3}\pi/2)S_w \approx 0.409 S_w$ and then increases towards the bulk of the cell [Fig. 5(b)]. Thus the high director distortion close to the boundary [as seen in Fig. 5(a)] has caused a partial melting of the liquid crystal.

Even without the full asymptotic solution the behaviour of the boundary solution above is interesting. We have shown that when the order parameter is allowed to vary, the director angle θ changes from the boundary value to the bulk value within a region of length scale ϵ or in dimensional terms ζ^2. Thus the director distortion occurs not over a length scale equal to the electrostatic coherence length but over a length scale equal to the electrostatic coherence length *squared*. It is the reduction in S, i.e. a partial melting, near to the boundary that more readily allows changes in director orientation. The scalar order parameter does not asymptote to the bulk value within the region $Z = O(\epsilon)$ but over a larger length scales. It can be verified numerically that S varies over a length scale comparable to the classic electrostatic coherence length ζ.

V. DISCUSSION

We have shown that, in the low field case, the equations for director angle and order parameter effectively decouple. In the bulk the director angle is zero and the order parameter

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remains constant at its equilibrium value whereas, in a region close to the cell surface, the order parameter varies to satisfy the boundary condition. However, in the high field case the bulk order parameter is increased from its equilibrium value due to the effect of the orienting field. In a region close to the surface the high amount of director distortion causes a significant reduction in the order parameter, to less than half of the value at the substrate, since the elastic stress energy can be reduced by a certain amount of melting. We have shown that this director distortion occurs in a region of length scale *much smaller* than the electrostatic coherence length. In classical elastic theory such distortions are expected to occur over lengths comparable to ζ whereas, when the order parameter is allowed to vary, director distortions to occur over a length scale of ζ^2, a much smaller distance than ζ since $\zeta \ll 1$, when the field strength is large. This effect could have a significant effect on the optical characteristics of such a cell and should be experimentally observable.

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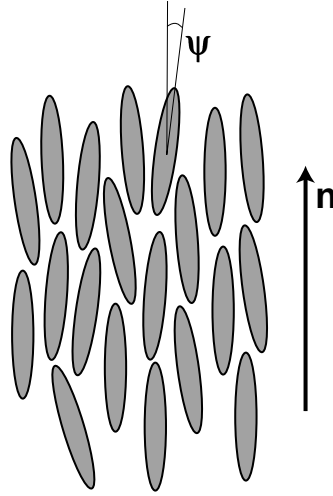[20] I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series and Products* (Academic Press, 1965).

FIG. 1. The macroscopic variables describing the nematic state: The average direction vector of the molecular long axis, the director **n**; The scalar order parameter defined by an average of the angle of deviation of the molecular long axis from the director, $S = \frac{1}{2} < (3\cos^2\psi - 1) >$.
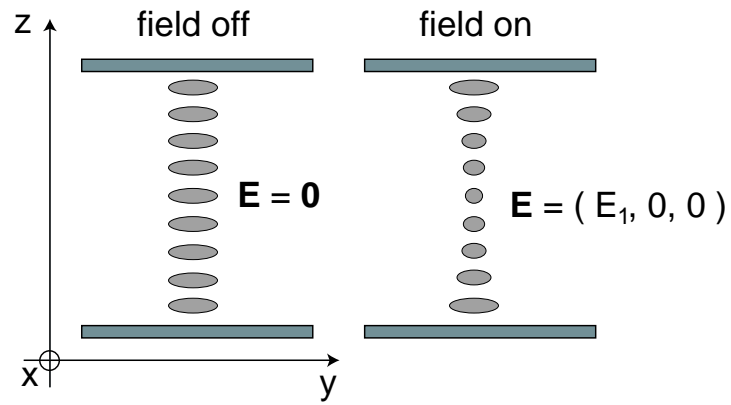
FIG. 2. The In-Plane Switching cell. The nematic director is anchored in the y direction at the cell surfaces and, at sufficiently high field strengths, an electric field applied in the x direction switches the bulk of the cell.
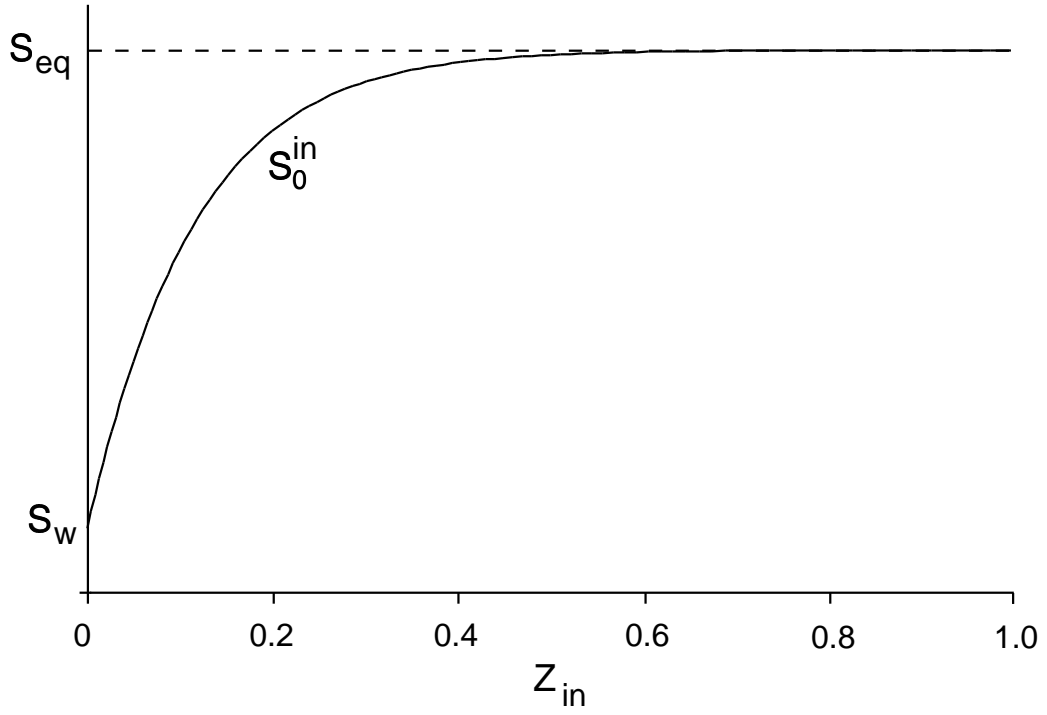
FIG. 3. Scalar order parameter solution at low fields. The order parameter varies from the fixed surface value S_w to the bulk value S_{eq}.
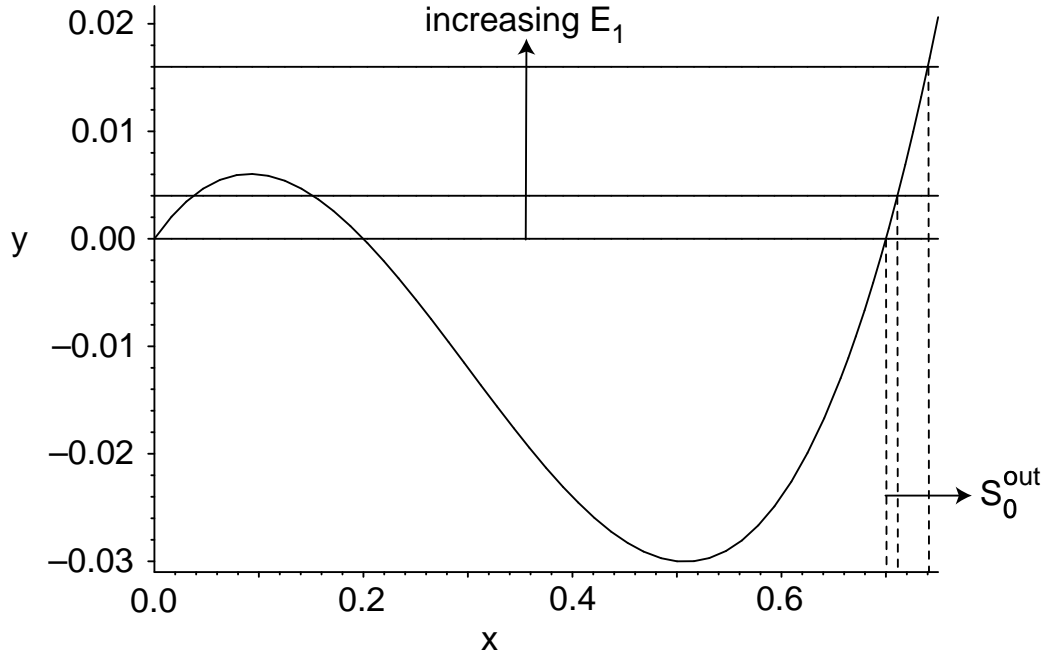
FIG. 4. Graphical solution of Eq. (27): The intersection of the two functions $y = \epsilon_0 \epsilon_a E_1{}^2/(8\pi)$ and $y = \alpha x + \frac{1}{3}\beta x^2 + \frac{2}{3}\gamma x^3$ (α, β and γ have been chosen to give roots of the second equation at $x = 0$, 0.2 and 0.7 as in §III). As E_1 increases the bulk scalar order parameter solution, S_0^{out}, increases.
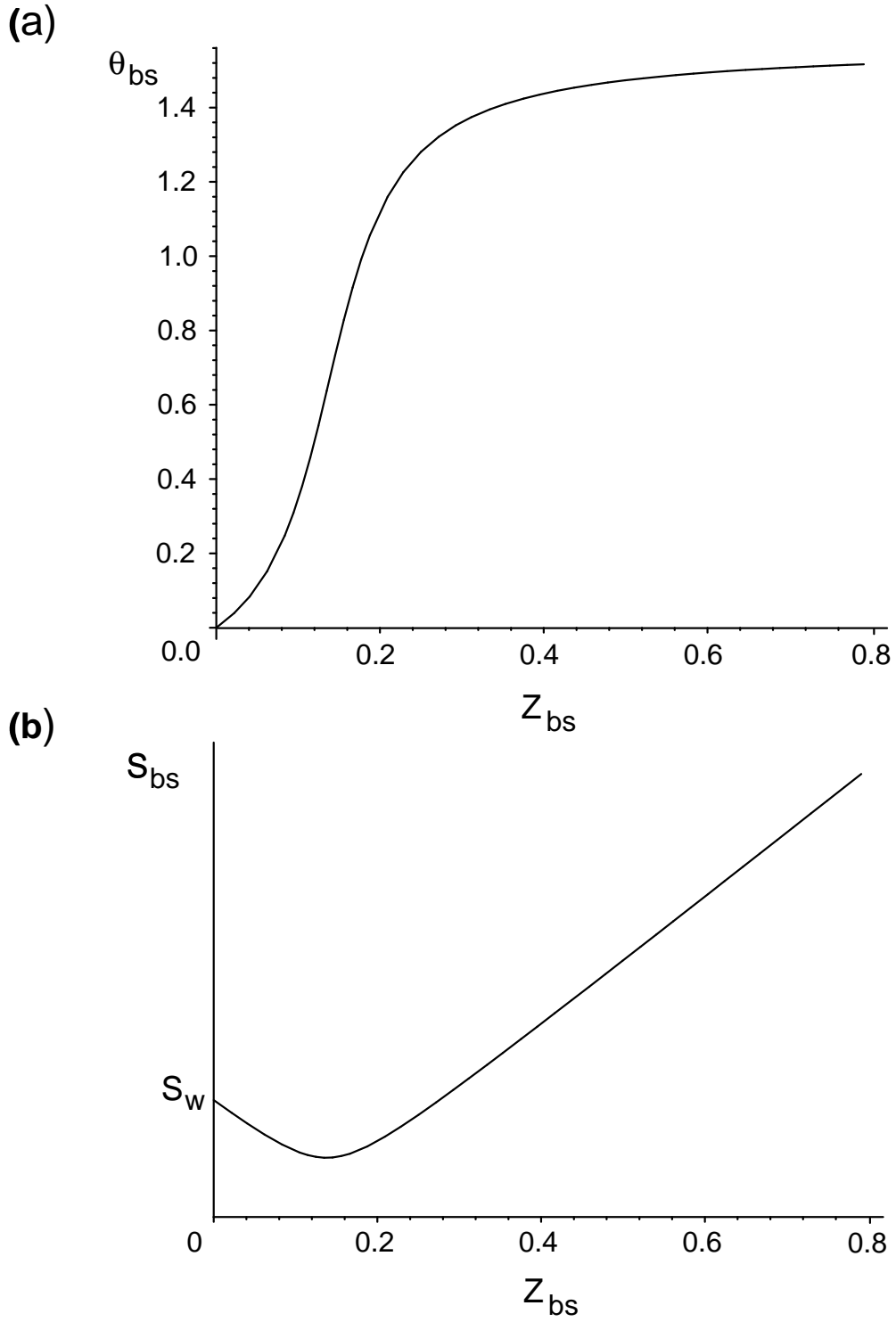
FIG. 5. High field solutions for the director angle θ and the scalar order parameter S. (a) The director angle varies from the fixed surface value $\theta = 0$ to the bulk switched value $\theta = \pi/2$. (b) The scalar order parameter shows a decrease in the region of high director distortion.

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