Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713926090

Response of a twisted nematic liquid crystal to any applied potential

T. W. Preist[a]; K. R. Welford[ab]; J. R. Sambles[a]
[a] Department of Physics, University of Exeter, Exeter, Devon, England [b] Royal Signals and Radar Research Establishment, Great Malvern, England

To cite this Article Preist, T. W. , Welford, K. R. and Sambles, J. R.(1989) 'Response of a twisted nematic liquid crystal to any applied potential', Liquid Crystals, 4: 2, 103 — 116
To link to this Article: DOI: 10.1080/02678298908029064
URL: http://dx.doi.org/10.1080/02678298908029064

LIQUID CRYSTALS, 1989, VOL. 4, NO. 2, 103–116

Response of a twisted nematic liquid crystal to any applied potential

by T. W. PREIST, K. R. WELFORD† and J. R. SAMBLES
Department of Physics, University of Exeter, Stocker Road, Exeter, Devon EX4 4QL, England

(*Received 16 February 1988; accepted 9 August 1988*)

The response of a twisted nematic liquid crystal trapped between flat and parallel aligning layers is analysed. Using a recently developed form for the relevant integrals it has been possible to evaluate the twist and tilt of the director for any applied voltage for twists up to a maximum of 90°. It is shown that the equations describing the cell simplify in the high voltage limit and allow an analytic solution. This leads to considerable improvement in the computational procedures and also enables the twist profile to be expressed in a particularly simple algebraic form.

1. Introduction

The theoretical analysis of the response of a twisted nematic liquid crystal to an applied voltage has been well documented in the literature. The early foundation work of Dafermos [1], and Leslie [2, 3], was exploited by Deuling [4, 5] in developing integral representations of the solution to the problem while Berreman [6] developed numerical codes based upon the solution to the Euler–Lagrange equations. The present work follows the former approach with a view to providing a mixture of analytic and numerical methods allowing a rapid computational solution to the problem. The analytic results presented here are particularly pertinent in the limit of high voltages where computational difficulties arise. While the approach is similar in spirit to that of Scheffer [7] his results were limited to very low voltages whereas this paper particularly addresses the problem of how to find a satisfactory solution in the high voltage limit.

Welford and Sambles [8] have shown that, by restructuring the relevant integrals, the response of a parallel aligned nematic liquid crystal layer may be fully evaluated for all applied voltages. They produced a new procedure for extracting the relevant integrals on a computer as well as analytic expressions for the high voltage limit response of the liquid crystal. The purpose of the present article is to examine the twisted cell in a similar manner. Deuling [5] has already presented the necessary starting point for this work with appropriate integral expressions based on the minimization of the free energy of the system. This present study re-expresses the relevant integrals allowing them to be evaluated numerically at all voltages and thereby obtaining full characterization of the tilt and twist profiles through the cell. Further, limiting analytic expressions are obtained for the high voltage response which provide very useful simple forms for the important parameters specifying the director configuration within the cell.

† Present address: Royal Signals and Radar Research Establishment, Great Malvern, England.

In this latter context the work presented here is a natural extension of the results of Thurston [9] who deduced exact solutions for particular liquid crystal configurations. What this paper does is to produce, for all configurations, including arbitrary twist (up to a maximum of $\pi/2$), an exact solution in the limit of high voltage. This solution also proves to be a very good approximation at voltages as low as twice the scale voltage.

2. The basic model

Consider a homogeneously aligned nematic liquid crystal cell in which the cartesian coordinate system is chosen such that the direction normal to the bounding plane surfaces is the z direction. Further suppose that with no applied voltage the director on one aligning plate is parallel to the x axis while on the other it is in a direction rotated by ω_m with respect to the x axis with the constraint that $\omega_m \leqslant \pi/2$. Following Deuling's [5] approach for the minimization of the free energy of this system we end up with two important equations. The first specifies the twist angle $\omega(z)$ within the cell as an integral of the form

$$\omega(z) = \beta \int_0^{\phi(z)} \frac{(1 + k \sin^2 \phi)^{1/2}}{g(\phi) \cos^2 \phi \, (1 + \alpha \sin^2 \phi)} d\phi, \tag{1}$$

where $\phi(z)$ is the tilt of the director which is determined implicitly through

$$\frac{z}{L} = \frac{1}{2} \int_0^{\phi(z)} \frac{(1 + k \sin^2 \phi)^{1/2}}{g(\phi)} d\phi \Bigg/ \int_0^{\phi_m} \frac{(1 + k \sin^2 \phi)^{1/2}}{g(\phi)} d\phi, \tag{2}$$

with L being the thickness of the cell and z being the distance measured from one edge. In these equations $k = (k_{33} - k_{11})/k_{11}$ is a simple function of the relevant elasticities, β is an unknown constant of integration and $g(\phi)$ is a complicated function which depends upon β and ϕ_m (the maximum tilt angle which occurs at $z = L/2$)

$$g(\phi) = \left\{ \frac{\sin^2 \phi_m - \sin^2 \phi}{(1 + \gamma \sin^2 \phi)(1 + \gamma \sin^2 \phi_m)} + \beta^2 \frac{1 + k}{1 + \alpha} \left(\frac{1}{(1 + \alpha \sin^2 \phi_m) \cos^2 \phi_m} - \frac{1}{(1 + \alpha \sin^2 \phi) \cos^2 \phi} \right) \right\}^{1/2}. \tag{3}$$

In the latter $\gamma = (\varepsilon_{\parallel} - \varepsilon_{\perp})/\varepsilon_{\perp}$ where $\varepsilon_{\parallel}$ and $\varepsilon_{\perp}$ are the relevant dielectric constants and $\alpha = (k_{33} - k_{22})/k_{22}$.

In the second important equation the maximum tilt angle ϕ_m is determined by the applied voltage V across the cell through

$$\frac{V}{V_0} = \frac{2}{\pi} \int_0^{\phi_m} \frac{(1 + k \sin^2 \phi)^{1/2}}{(1 + \gamma \sin^2 \phi) g(\phi)} d\phi, \tag{4}$$

where V_0 is a natural unit of voltage given by

$$V_0 = \pi \left\{ \frac{k_{11}}{\varepsilon_0 (\varepsilon_{\parallel} - \varepsilon_{\perp})} \right\}^{1/2}.$$

Noting that $\omega(z) = \omega_m/2$ and $\phi(z) = \phi_m$ when $z = L/2$ equation (1) gives

$$\omega_m = 2\beta \int_0^{\phi_m} \frac{(1 + k \sin^2 \phi)^{1/2}}{g(\phi) \cos^2 \phi \, (1 + \alpha \sin^2 \phi)} d\phi. \tag{5}$$

Thus, given the initial parameters ω_m and V for the cell, equations (4) and (5) need to be solved simultaneously for β and ϕ_m. Since $g(\phi)$ contains β this is best done iteratively:

(i) set $\beta = 0$ in equation (4) and determine $\phi_m(\beta = 0)$ (i.e. ϕ_{mo}); use this value in equation (5) to determine a first approximation β_0 for β;

(ii) next using β_0 as the starting value repeat the procedure and so on until the desired convergence is obtained.

To avoid problems with singularities in the integrals the following substitutions (see Dafermos [1], Leslie [2, 3] and Deuling [4]) are made:

$$\sin\phi = \sin\phi_m \sin\psi, \quad \eta = \sin^2\phi_m.$$

With these substitutions equation (5) becomes

$$\omega_m = 2\beta \int_0^{\pi/2} \left\{ \frac{(1 + \eta k \sin^2\psi)(1 + \eta\gamma \sin^2\psi)(1 + \eta\gamma)}{(1 - \eta \sin^2\psi)^3 (1 + \eta\alpha \sin^2\psi)^2 h(\psi)} \right\}^{1/2} d\psi, \tag{6}$$

where

$$\begin{aligned} h(\psi) &= g^2(\phi) \left[\frac{(1 + \gamma \sin^2\phi)(1 + \gamma \sin^2\phi_m)}{\sin^2\phi_m - \sin^2\phi} \right] \\ &= 1 + \frac{\beta^2}{(1 - \eta)} \left(\frac{1 + k}{1 + \alpha} \right) \left(\frac{1 + \eta\gamma}{1 + \eta\alpha} \right) \left(\frac{1 + \eta\gamma \sin^2\psi}{1 + \eta\alpha \sin^2\psi} \right) \\ &\quad \times \left(\frac{1 - \alpha + \eta\alpha(1 + \sin^2\psi)}{1 - \eta \sin^2\psi} \right) \end{aligned} \tag{7}$$

and equation (4) becomes

$$\frac{V}{V_0} = \frac{2(1 + \eta\gamma)^{1/2}}{\pi} \int_0^{\pi/2} \left\{ \frac{(1 + \eta k \sin^2\psi)}{(1 + \eta\gamma \sin^2\psi)(1 - \eta \sin^2\psi) h(\psi)} \right\}^{1/2} d\psi. \tag{8}$$

These integrals also present a problem when integrating numerically if the applied voltage V is large; consequently it is expedient to consider in some detail the high voltage limit.

3. The high voltage limit

In the limit $V/V_0 \geqslant 4$ an enormous simplification is possible by recognizing that the numerical difficulties arise because the important region of integration occurs when $\psi \approx \pi/2$ due to the near singularity produced by the factor $(1 - \eta \sin^2\psi)$ in the denominator. This means that in this limit it is vital to include the variation of the factor $(1 - \eta \sin^2\psi)$ but all other factors can be replaced by their value at $\psi = \pi/2$ without introducing a significant error.

Equations (6) and (8) have a structure that implies that as $V \to \infty$ and $\eta \to 1$ then β tends to zero like $(1 - \eta)$. Therefore, defining

$$x = \frac{\beta(1 + k)^{1/2}(1 + \gamma)}{(1 - \eta)(1 + \alpha)}$$

and also putting $\eta = 1$ and $\psi = \pi/2$ in all factors where variations from these values can safely be ignored equations (6) and (8) reduce to

$$\frac{\omega_m}{(1-\eta)} \simeq \int_0^{\pi/2} \frac{2x\,d\psi}{[(1-\eta\sin^2\psi)^3 H(\psi)]^{1/2}} \tag{9}$$

and

$$\frac{V}{V_0} \simeq \frac{2}{\pi}(1+k)^{1/2}\left\{\int_0^{\pi/2} \frac{d\psi}{[(1-\eta\sin^2\psi)H(\psi)]^{1/2}} + C_0\right\}, \tag{10}$$

with

$$C_0 = \frac{(1+\gamma)^{1/2}}{(1+k)^{1/2}}\int_0^{\pi/2}\left[\left(\frac{1+k\eta\sin^2\psi}{1+\gamma\eta\sin^2\psi}\right)^{1/2} - \left(\frac{1+k\eta}{1+\gamma\eta}\right)^{1/2}\right] \times \frac{d\psi}{[H(\psi)(1-\eta\sin^2\psi)]^{1/2}}$$

and

$$\begin{aligned} H(\psi) &= 1 + \frac{(1-\eta)x^2}{1-\eta\sin^2\psi} \\ &= \frac{1+x^2(1-\eta)-\eta\sin^2\psi}{1-\eta\sin^2\psi} \\ &= [1+x^2(1-\eta)]\frac{(1-\eta'\sin^2\psi}{(1-\eta\sin^2\psi)}, \end{aligned}$$

where

$$\eta' = \frac{\eta}{1+x^2(1-\eta)}.$$

In the following it will be important to note that

$$1-\eta' = \frac{1+x^2(1-\eta)-\eta}{1+x^2(1-\eta)} \xrightarrow[\eta\to 1]{} (1+x^2)(1-\eta).$$

C_0 contains no singularity and is readily evaluated numerically at all voltages. There is, of course, a similar correction term in equation (9) but it is of less importance since the integral in this equation depends upon $(1-\eta)^{-1}$ whereas in equation (10) the integral depends upon $\log(1-\eta)$. Consequently equations (9) and (10) become

$$\frac{\omega_m}{2x(1-\eta)} \simeq \int_0^{\pi/2} \frac{d\psi}{(1-\eta\sin^2\psi)(1-\eta'\sin^2\psi)^{1/2}} \tag{11}$$

and

$$\frac{V}{V_0} \simeq \frac{2(1+k)^{1/2}}{\pi}\left\{\int_0^{\pi/2}\frac{d\psi}{(1-\eta'\sin^2\psi)^{1/2}} + C_0\right\}. \tag{12}$$

The expression in equation (12) is a standard elliptic integral of the first kind [10] giving, as $\eta' \to 1$,

$$\begin{aligned} \frac{V}{V_0} &\simeq \frac{2(1+k)^{1/2}}{\pi}[-\tfrac{1}{2}\ln(1-\eta') + \ln 4 + C_0] \\ &\simeq \frac{2(1+k)^{1/2}}{\pi}\{-\tfrac{1}{2}\ln((1+x^2)(1-\eta)) + \ln 4 + C_0\}. \end{aligned} \tag{13}$$

The expression in equation (11) is also an elliptic integral—of the third kind—whose leading term [10] in the limit $\eta \rightarrow 1$ gives

$$\frac{\omega_m}{2} = \frac{\pi}{2} - \sin^{-1}\left(\frac{1-\eta}{1-\eta'}\right)^{1/2}.$$

That is

$$\frac{\omega_m}{2} = \frac{\pi}{2} - \sin^{-1}(1 + x^2)^{-1/2}$$

or

$$x = \tan\left(\frac{\omega_m}{2}\right)$$

so that

$$\beta \simeq \frac{(1+\alpha)(1-\eta)}{(1+\gamma)(1+k)^{1/2}}\tan\left(\frac{\omega_m}{2}\right). \tag{14}$$

Recalling that $\eta = \sin^2\phi_m$ then equation (13) gives

$$\frac{V}{V_0} \simeq \frac{(1+k)^{1/2}}{\pi}\left\{\ln(1 + \tan^2\phi_m) - \ln\left(1 + \tan^2\frac{\omega_m}{2}\right) + 2\ln 4 + 2C_0\right\}. \tag{15}$$

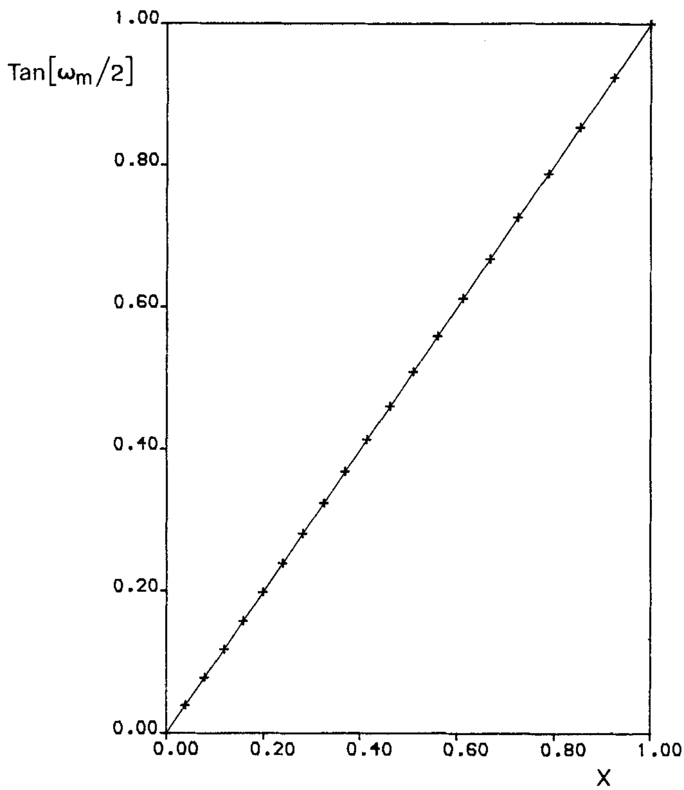

Figure 1. Plot of iteratively calculated values of x for various twist angles ω_m at $V/V_0 = 5{\cdot}0$. These calculated values are shown as crosses on a plot of $\tan(\omega_m/2)$ versus x. The 'analytic' solution is represented by the solid straight line.

This expression is the analogous result for the twisted cell to that obtained by Welford and Sambles for the zero twist case. In the limiting situation of $\omega_m = \pi/2$, $\tan^2(\omega_m/2) = 1$, then

$$\frac{V}{V_0} \simeq \frac{(1+k)^{1/2}}{\pi}\left\{\ln\left(\frac{1+\tan^2\phi_m}{2}\right) + 2\ln 4 + 2C_0\right\}.$$

In general, for a given voltage $V(\gg V_0)$ across the twisted cell, with a total twist angle of ω_m, it will have a maximum tilt angle given by

$$\tan^2\phi_m \simeq \left(1 + \tan^2\frac{\omega_m}{2}\right)\tan^2\phi_{mo}, \tag{16}$$

where ϕ_{mo} is the maximum tilt angle for zero twist at the same voltage.

Thus we have obtained analytic expressions for the important constants in the integral for the limit of high voltages, that is, both β given by equation (14), and ϕ_m given by equation (15). To establish that these expressions are valid we have computed both β and $\tan^2\phi_m$ for a range of ω_m values at a voltage of 5 V_0. The graph of x against $\tan(\omega_m/2)$ is shown in figure 1 and confirms the expression (14), while figure 2 shows a graph of $\tan^2\phi_m$ against $(1 + \tan^2\omega_m/2)$ which also confirms equation (16) and hence equation (15). All these calculations have been performed using the nematic

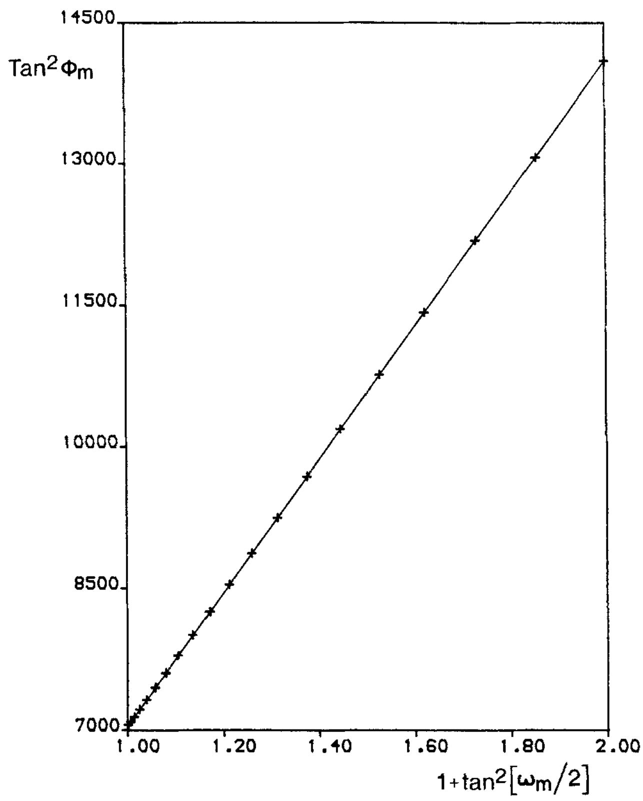

Figure 2. Plot of iteratively calculated values of ϕ_m for various values of ω_m at $V/V_0 = 5{\cdot}0$. These calculated values are shown as crosses on a plot of $\tan^2\phi_m$ versus $(1 + \tan^2(\omega_m/2))$. The analytic solution is again represented by the solid straight line.

Parameters for the liquid crystal mixture E7 (BDH Chemicals Ltd) modelled in the calculations presented in this paper.

Parameter	Symbol	Value
Parallel relative permittivity	$\varepsilon_{\parallel}$	20·25
Perpendicular relative permittivity	$\varepsilon_{\perp}$	5·355
Splay elastic constant	k_{11}	$1{\cdot}111 \times 10^{-11}$ N
Twist elastic constant	k_{22}	$1{\cdot}713 \times 10^{-11}$ N
Bend elastic constant	k_{33}	$1{\cdot}8 \times 10^{-11}$ N
Layer thickness	L	5 μm
Wavelength of incident radiation	λ	$632{\cdot}8 \times 10^{-9}$ m

mixture E7 as a model liquid crystal for which the relevant parameters used are listed in the table.

4. The director profile in the high voltage limit

In the limit of high voltage the tilt angle rises rapidly at the edges of the cell to a value very close to 90° and is then effectively constant across the cell. The twist angle on the other hand varies rapidly in the centre of the cell rising from a value close to zero to one close to ω_m. In both cases the rapidity of the change depends markedly upon the voltage V and since these features can readily be investigated in the high voltage limit it is instructive to do so.

The differential forms of equations (1) and (2) are

$$\frac{d\omega}{dz} = \frac{A\beta}{(1 + \alpha \sin^2\phi)\cos^2\phi} \tag{17}$$

and

$$\frac{d\phi}{dz} = \frac{Ag(\phi)}{(1 + k\sin^2\phi)^{1/2}}, \tag{18}$$

with $A = D_z(k_{11}\varepsilon_0\varepsilon_{\perp}/\gamma)^{-1/2}$, D_z being the electric displacement produced by the applied voltage V. The voltage across the cell is

$$\begin{aligned} V &= \int_0^L E dz \\ &= D_z \int_0^L \frac{dz}{\varepsilon_0\varepsilon_{\perp}(1 + \gamma \sin^2\phi)} \end{aligned} \tag{19}$$

so that

$$\begin{aligned} A &= \frac{D_z}{(k_{11}\varepsilon_0\varepsilon_{\perp}/\gamma)^{1/2}} = \frac{\pi V}{V_0}\Big/\int_0^L \frac{dz}{[1 + \gamma\sin^2\phi]} \\ &= \frac{\pi V}{L V_0}(1 + \gamma)/\xi, \end{aligned} \tag{20}$$

where

$$\xi = \frac{1}{L}\int_0^L \frac{(1 + \gamma)\, dz}{1 + \gamma \sin^2\phi}. \tag{21}$$

In the high voltage limit $\xi \to 1$ but as V decreases ξ progressively increases and in the limit $V \to V_0$, $\xi \to (1 + \gamma)$. Details of this variation which are relevant to the shape of both the twist and tilt profile are given in the Appendix. Writing $\phi = \phi_m - \delta$ and assuming that δ is small (for a region near the centre of the cell)

$$\begin{aligned} \cos\phi &= \cos\phi_m \cos\delta + \sin\phi_m \sin\delta \\ &= (1 - \eta)^{1/2}(1 - \delta^2/2) + \eta^{1/2}\delta. \end{aligned}$$

It then follows that in the limit $\eta \to 1$ that

$$\begin{aligned} \cos^2\phi &= (1 - \eta) + \delta^2 + 2(1 - \eta)^{1/2}\delta \\ &= (1 - \eta)(1 + P)^2 \end{aligned}$$

and

$$g(\phi) = \frac{(1 - \eta)^{1/2}}{1 + \gamma}(P^2 + 2P)^{1/2}\left[1 + \frac{x^2}{(1 + P)^2}\right]^{1/2}, \tag{22}$$

where

$$P = \frac{\delta}{(1 - \eta)^{1/2}}.$$

(Terms higher than δ^2 have been consistently neglected.) Using these latter three results together with equation (14) we see that equation (17) reduces to

$$\frac{d\omega}{dz} = \frac{\pi}{L}\frac{V}{V_0\xi}\frac{1}{(1 + k)^{1/2}}\frac{x}{(1 + P)^2} \tag{23}$$

and equation (18) becomes

$$\frac{d\phi}{dz} = (1 - \eta)^{1/2}\frac{dP}{dz} = \frac{\pi(1 + \gamma)}{L\xi}\frac{V}{V_0}\frac{(1 - \eta)^{1/2}}{(1 + \gamma)}\frac{(P^2 + 2P)^{1/2}}{(1 + k)^{1/2}}\left[1 + \frac{x^2}{(1 + P)^2}\right]^{1/2}$$

so that

$$\frac{dP}{dz} = \frac{\pi}{L}\frac{V}{V_0}\frac{(P^2 + 2P)^{1/2}}{(1 + k)^{1/2}\xi}\left[1 + \frac{x^2}{(1 + P)^2}\right]^{1/2}. \tag{24}$$

Equations (23) and (24) then give

$$\frac{d\omega}{dP} = \frac{x}{(1 + P)^2(P^2 + 2P)^{1/2}}\left[1 + \frac{x^2}{(1 + P)^2}\right]^{-1/2}. \tag{25}$$

The sharpness of the resulting profiles depends upon a scale length L_0 defined by

$$L_0 = \frac{2L}{\pi}\frac{V_0}{V}(1 + k)^{1/2}\xi$$

since equation (24) becomes

$$\frac{dP}{dz} = \frac{2}{L_0}[P^2 + 2P]^{1/2}\left[1 + \frac{x^2}{(1 + P)^2}\right]^{1/2}$$

and so

$$\frac{dz}{L_0} = \frac{dP}{2[P^2 + 2P]^{1/2}}\left[1 + \frac{x^2}{(1 + P)^2}\right]^{-1/2}.$$

The substitution $(1 + P) = 1/\sin u$ and the boundary condition $P = 0$ at $z = L/2$ readily reduces the integral to the standard form

$$2s \equiv \frac{2(L/2 - z)}{L_0} = \int_u^{\pi/2} \frac{du}{\sin u\,(1 + x^2\sin^2 u)^{1/2}}$$
$$= \tfrac{1}{2}\log\left(\frac{(1 + x^2\sin^2 u)^{1/2} + \cos u}{(1 + x^2\sin^2 u)^{1/2} - \cos u}\right).$$

After some algebraic manipulation it follows that

$$(1 + P)^2 = \frac{1 + x^2\tanh^2 2s}{1 - \tanh^2 2s}. \tag{26}$$

Integrating equation (25) gives

$$\omega(P) - \frac{\omega_m}{2} = \pm\int_0^P \frac{x\,dP}{(1 + P)^2(P^2 + 2P)^{1/2}}\left[1 + \frac{x^2}{(1 + P)^2}\right]^{-1/2}, \tag{27}$$

where the $\pm$ is chosen according as $z \gtrless L/2$. The substitution $y = (1 + P)^{-2}$ reduces the integral to the form

$$\pm\frac{x}{2}\int_y^1 \frac{dy}{[(1 - y)(1 + x^2 y)]^{1/2}}$$

which simplifies to a simple trigonometric integral giving

$$\omega = \frac{\omega_m}{2} \pm \frac{1}{2}\left[\frac{\pi}{2} - \Xi\right],$$

where

$$\sin\Xi = \left(1 - x^2 + \frac{2x^2}{(1 + P)^2}\right)(1 + x^2)^{-1}.$$

Using equation (26) and noting that

$$\cos\Phi \equiv \cos(\pi/2 - \Xi) = \sin\Xi = \frac{1 - x^2T^2}{1 + x^2T^2}$$

(where $T = \tanh 2s$) it follows that $\Phi/2 = \tan^{-1}(x\tanh 2s)$ since

$$\cos\Phi = \frac{1 - \tan^2\Phi/2}{1 + \tan^2\Phi/2}.$$

Consequently

$$\omega(z) = \frac{\omega_m}{2} + \tan^{-1}\left(\tan\frac{\omega_m}{2}\tanh 2s\right) \tag{28}$$

recalling that $s = (L/2 - z)/L_0$.

The expressions (26) and (28) are correct provided δ is small enough for the small angle approximation to be valid and so hold in the centre of the cell. The sharpness of the variation in the twist profile is enhanced by both increasing the voltage and increasing the twist angle. The agreement between the analytic form (28) and the computer generated solution is illustrated in figure 3 for the voltage ratio, $V/V_0 = 4$.

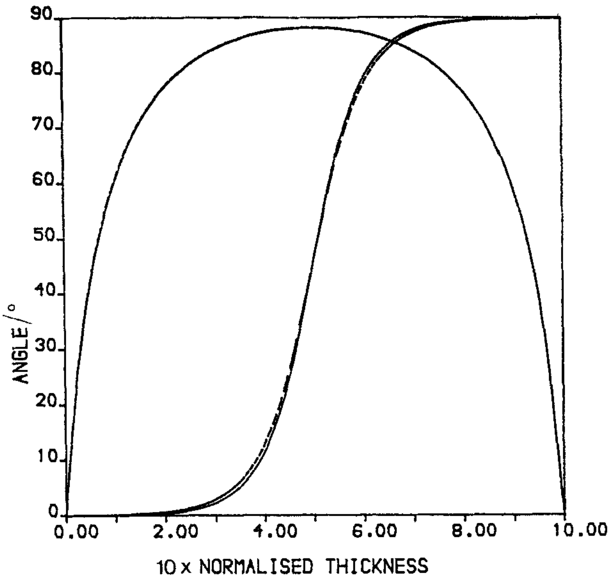

Figure 3. Comparison at $V/V_0 = 4$ of the exact twist profile (solid line) with the analytic expression of equation (28) (dotted line).

At the edges of the cell the tilt angle increases linearly with z with a gradient

$$\left.\frac{d\Phi}{dz}\right|_{\text{edge}} = \pm A/(1 + \gamma)^{1/2}$$

$$= \pm \frac{2}{L_0}(1 + \gamma)^{1/2}(1 + k)^{1/2}.$$

Consequently near $z = 0$

$$\phi(z) = \frac{2z}{L_0}(1 + k)^{1/2}(1 + \gamma)^{1/2}$$

with an analogous expression valid near $z = L$. In the centre of the cell

$$\cos\phi = (1 - \eta)^{1/2}(1 + P)$$

$$= (1 - \eta)^{1/2}(\cosh^2 2s + x^2 \sinh^2 2s)^{1/2},$$

where

$$s = (L/2 - z)/L_0.$$

We have found no simple analytical form for $\phi(z)$ in the critical turn-over region.

5. Computation of full tilt and twist profiles

Expressions (2) and (1) may be used with our knowledge of β and ϕ_m to evaluate $\phi(z)$ and $\omega(z)$ for all voltages. However, as pointed out in the previous study [8] the variable ϕ_m is better replaced by $\tan^2\phi_m$ and the expressions suitably recast in the new variable to allow the small changes in ϕ_m ($\approx 90°$) found for high voltages to influence the integrals and hence the distribution of $\phi(z)$ and $\omega(z)$ appropriately. Using this type of integral expression together with the high voltage analytic expressions for

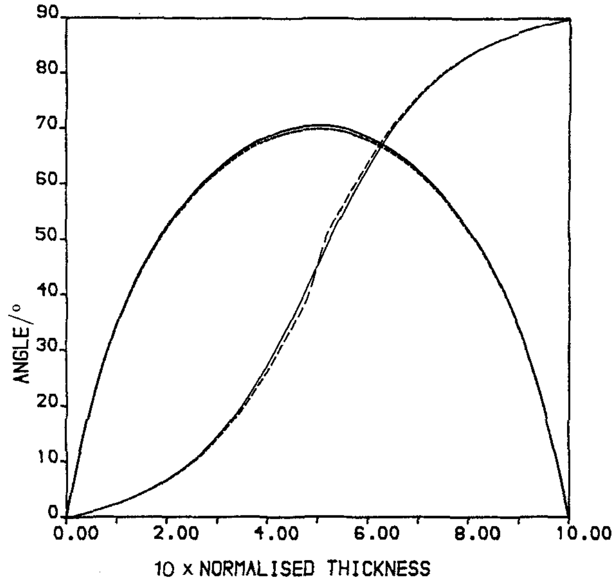

Figure 4. Comparison for $V/V_0 = 2$ and $\omega_m = \pi/2$ of the profiles generated using the iterated values of β and ϕ_m (full curves) and the analytic expressions for these constants (dotted curves).

the coefficient β and $\tan^2\phi_m$ allows the computation of twist and tilt profiles for all voltages. Figure 4 shows the twist and tilt profiles determined numerically at $V/V_0 = 2$ using expressions (1) and (2); the full curves use the parameters β and ϕ_m obtained iteratively from equations (4) and (5) whereas the dotted curves use the

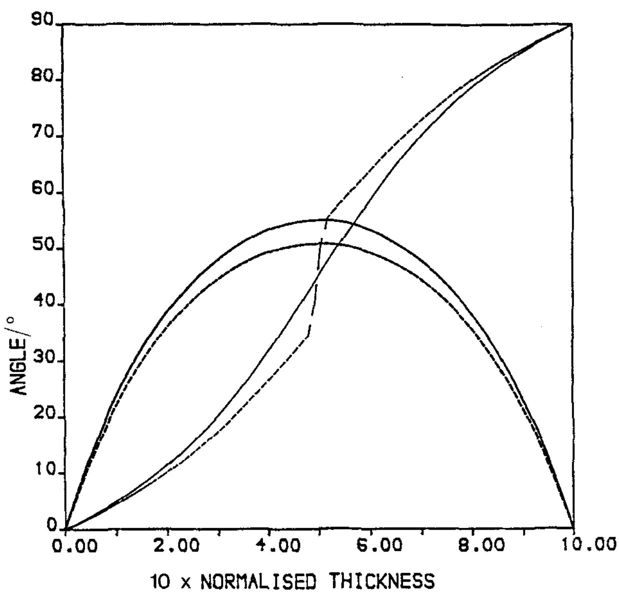

Figure 5. Comparison for $V/V_0 = 1{\cdot}5$ and $\omega_m = \pi/2$ of the profiles generated using the iterated values of β and ϕ_m (full curves) and the analytic expressions for these constants (dotted curves).

analytic expressions for β and ϕ_m (obtained from those for x and η) determined in this paper. The differences in the profiles even at this low voltage are less than 1 per cent and at $V/V_0 = 4$ the full and dotted curves are indistinguishable. Figure 5 shows a similar comparison carried out a $V/V_0 = 1{\cdot}5$ where, as might be expected, the differences are becoming significant.

Because the analytic solutions avoid the necessity of iteratively solving two equations requiring numerical integration the execution time in obtaining the dotted curve is considerably less than that required to generate the full curve. Consequently it is desirable to extend the analytic solution to as low a voltage as possible commensurate with the desired degree of accuracy. An immediate significant improvement can be obtained by simply using the analytic solution *at any voltage* to determine the starting values of β and ϕ_m for an iterative numerical solution.

6. Summary

The focal point for the genesis of the results presented here were difficulties in the numerical modelling of the optical properties of a liquid crystal cell using the integral formulation [5]. The coupled integral expressions require iterative solutions for the unknown parameters ϕ_m and β contained in their definition and it is not surprising that considerable computation time is necessary since each iteration involves two integrations and it is necessary to carry out calculations at a sufficient number of points across the cell to calculate the director profiles. More particularly at high voltages the significant region of integration shrinks towards one of the end points producing computational difficulties unless special care is taken. Analysis of this aspect shows however that in this apparently difficult limit the integrals simplify considerably and may be evaluated analytically to an accuracy of 1 part in $\sec^2\phi_m$. Since ϕ_m is approaching $\pi/2$ this accuracy is typically better than 1 in 1000 for $V/V_0 > 4$ and comparison with numerical solutions for $V/V_0 = 2$ show that here the expressions are accurate to 1 per cent. The use of these analytic expressions at lower voltages can provide a very effective first approximation leading to an improvement of a factor of more than ten in the execution times for computer generated solutions, the simplification in the integrals also allows the director twist profile to be expressed in a concise analytic form which reproduces the computed curves with remarkable accuracy.

Dr K. R. Welford would like to thank the University of Exeter Research Fund for the provision of a Postdoctoral Research Assistantship during which this work was undertaken. The authors would also like to thank Dr K. Harrison for supplying information on E7.

Appendix

The scale factor ξ is simply expressed in the form

$$\xi = \frac{(1+\gamma)}{L}\int_0^L \frac{dz}{1+\gamma\sin^2\phi}$$

$$= \frac{2(1+\gamma)}{L}\int_0^{L/2} \frac{dz}{1+\gamma\sin^2\phi}.$$

Since its variation is considerable (in the present case from 1·0 to 3·55) as the voltage, and hence the tilt profile $\phi(z)$, changes it is important to have a reasonable estimate of its value. A precise result can only be determined after $\phi(z)$ is known but a suitable approximation to the profile can give a satisfactory estimate as we now outline.

At $z = 0$ the initial slope is

$$\left(\frac{d\phi}{dz}\right)_0 = A/(1 + \gamma)$$

and as z increases the slope decreases monotonically to zero at $z = L/2$. The profile is approximated by

(i) a straight line of slope $\frac{1}{2}(d\phi/dz)_0$ until ϕ reaches ϕ_m (at $z = z_0$).

(ii) a constant value of $\phi = \phi_m$ for $z_0 \leqslant z \leqslant L/2$.

This trapezoidal approximation underestimates in one part of the region of integration and overestimates in the other. Hence

$$\xi = \frac{2(1 + \gamma)}{L} \int_0^{z_0} \frac{dz}{1 + \gamma \sin^2\left(\frac{z}{z_0}\phi_m\right)} + \frac{(L/2 - z_0)}{1 + \gamma \sin^2 \phi_m} \frac{2(1 + \gamma)}{L},$$

where

$$z_0 = \frac{\phi_m}{A} 2(1 + \gamma)^{1/2}$$

$$= \frac{V_0 L}{\pi V} \frac{2\phi_m}{(1 + \gamma)^{1/2}} \xi$$

so that

$$\xi = \frac{(1 + \gamma)}{1 + \gamma \sin^2 \phi_m} D,$$

where

$$D = 1 - 4(1 + \gamma)^{1/2} \frac{V_0 \phi_m}{\pi V} \left(F(\phi_m) - \frac{1}{1 + \gamma \sin^2 \phi_m}\right)$$

with

$$F(\phi_m) = \frac{1}{\phi_m (1 + \gamma)^{1/2}} \tan^{-1}((1 + \gamma)^{1/2} \tan \phi_m).$$

For the nematic modelled here at $V/V_0 = 4$, $\xi = 1{\cdot}35$ and at $V/V_0 = 2$, $\xi = 1{\cdot}90$.

References

[1] Dafermos, C. M., 1968, *SIAM J. appl. Math.*, **16**, 1305.
[2] Leslie, F. M., 1970, *J. Phys.* D, **3**, 889.
[3] Leslie, F. M., 1970, *Molec. Crystals liq. Crystals*, **12**, 57.
[4] Deuling, H. J., 1972, *Molec. Crystals liq. Crystals*, **19**, 123.
[5] Deuling, H. J., 1974, *Molec. Crystals liq. Crystals*, **27**, 81.
[6] Berreman, D. W., 1983, *Phil. Trans. R. Soc.* A, **309**, 203.

[7] SHEFFER, T. J., 1980, *Advances in Liquid Crystal Research and Applications*, edited by L. Bata (Pergamon Press), p. 1145.
[8] WELFORD, K. R., and SAMBLES, J. R., 1987, *Molec. Crystals liq. Crystals*, **147**, 25.
[9] THURSTON, R. N., 1983, *J. appl. Phys.*, **54**, 4966.
[10] ABRAMOWITZ, M., and STEGUN, I. A., 1965, *Handbook of Mathematical Functions* (Dover Publications).