

Chapter 2

Theoretical analysis of the electrooptic response of a hybrid aligned nematic (HAN) cell

In this Chapter we will analyse theoretically the dynamic response of a hybrid aligned nematic cell under the action of an AC electric field. An AC field applied to a hybrid aligned nematic cell (described later) gives rise to an electrooptic response. This in turn can be used to describe the dynamical response of the director in such a cell.

The orientation of nematic liquid crystals by solid interfaces is of considerable interest. The surface interaction is usually characterised by two parameters, the easy axis at the interface and the anchoring energy. Easy axis is the direction of $\mathbf{n}$ which minimises the energy of the surface layers of nematic in the absence of external torques.

As discussed in chapter 1, in the case of a planar director field the strength of the anchoring is in general expressed by the anisotropic part of the interfacial free energy density F_s .

$$F_s(\theta) = \frac{1}{2}W_\theta \sin^2(\theta - \theta_o) \quad (2.1)$$

where θ and θ_o are the polar angles made by the director $\mathbf{n}$ and the easy axis

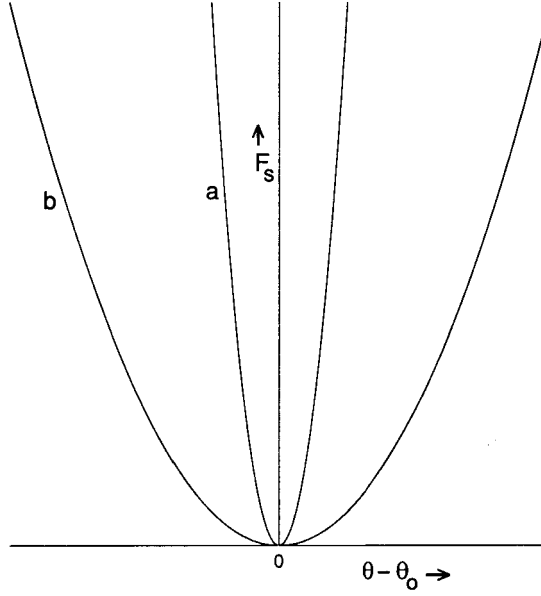


Fig. 2.1: Energy density is shown as ω function of $\theta - \theta_0$ in the case of a) strong anchoring b) weak anchoring.

direction with the surface normal respectively. W_θ is the anchoring energy for the tilt orientation of the director.

The extrapolation length(L) is defined as K_{ii}/W [1], the ratio of an appropriate elastic constant and anchoring energies. The anchoring is strong when the extrapolation length is of the order of 'molecular dimensions. On the other hand when the extrapolation length is much larger than the molecular dimensions the anchoring is weak. In the case of weak anchoring there is a competition between surface and bulk torques, and strong bulk forces can change the surface alignment. The energy density has a shallower minimum when the anchoring is weak as shown in Fig. 2.1

The nematic medium does not exhibit spontaneous polarisation. As described in Chapter 1 however, if the $\mathbf{n}$ field has a splay or bend type of distortion, a flexoelectric polarisation $\mathbf{P}_f$ can result [4]:

$$\mathbf{P}_f = e_1 \mathbf{n} (\nabla \cdot \mathbf{n}) + e_3 (\nabla \times \mathbf{n}) \times \mathbf{n}. \quad (2.2)$$

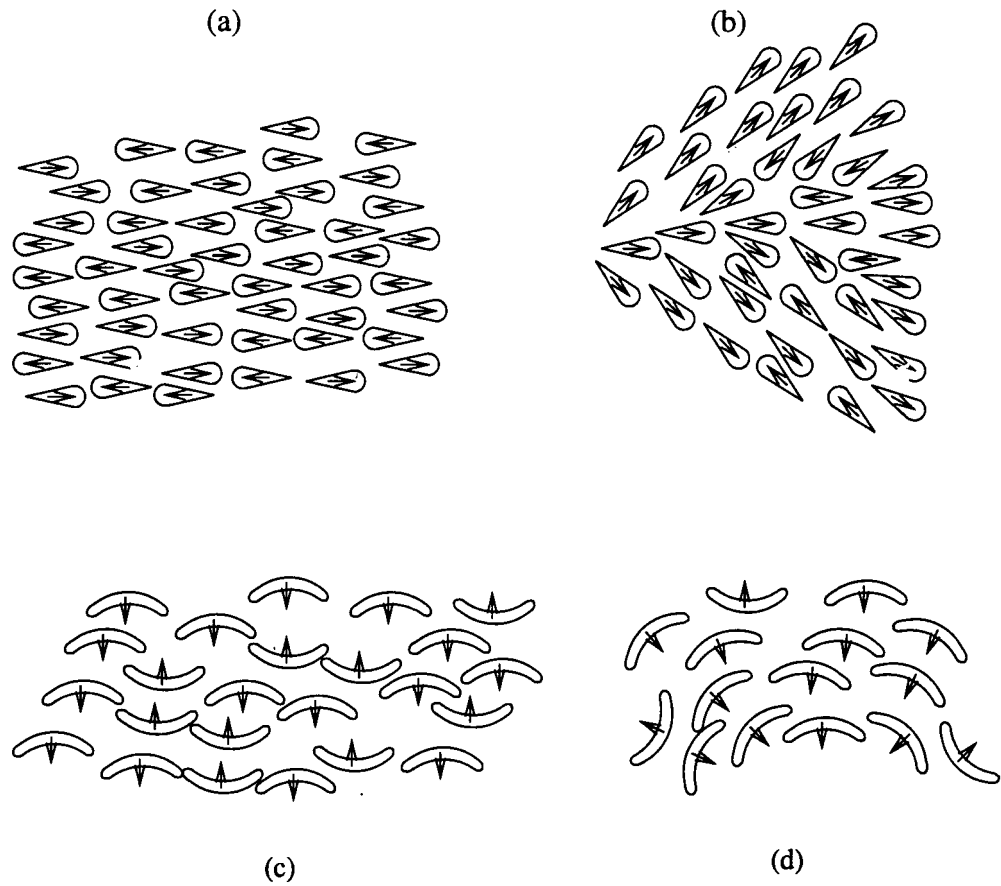


Fig. 2.2: Meyer's model of flexoelectricity. The nematic composed of asymmetric polar molecules has no net polarisation in the undeformed state (a) and (c), but develops a polarisation under splay (b) and bend (d) deformations.

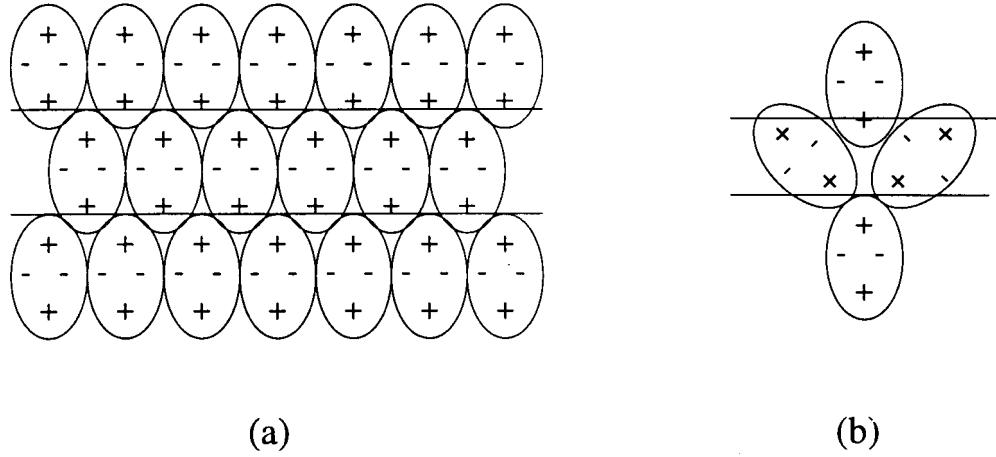


Fig. 2.3: (a) In the undeformed state there is no net polarisation due to the symmetry of the stacking of quadrupoles. (b) The structure becomes polarised when subjected to a splay distortion.

In the absence of an external field the distribution of the dipoles in an undistorted nematic liquid crystal has a non-polar cylindrical symmetry and there is no net polarisation (Fig. 2.2a) and (Fig. 2.2c), but develops a polarisation on splay (Fig. 2.2b) or bend (Fig. 2.2d) deformation. There is no net polarisation in the undistorted state because of equal probability of opposite orientations of the dipole moments of the molecules. However a polarisation arises when subjected to a splay deformation, even in the case of non-polar molecules from the quadrupolar moments [11] of the molecules (see Fig. 2.3a and 2.3b).

In analysing dynamical responses, the viscous torque which opposes the director rotation has to be included. Rotational viscosity is one of the important parameters involved in electrooptical effects. The dynamics of nematic liquid crystals can be described by the director field $\mathbf{n}(\mathbf{r},t)$ and by the velocities of the centre of masses of the molecules $\mathbf{v}(\mathbf{r},t)$. The viscous stress tensor derived by Leslie [12] is given by

$$\begin{aligned} \sigma'_{ki} = & \alpha_1 n_k n_i A_{pq} n_p n_q + \alpha_2 n_k N_i + \alpha_3 n_i N_k + \alpha_4 A_{ki} \\ & + \alpha_5 n_k n_m A_{mi} + \alpha_6 A_{km} n_m n_i \end{aligned} \quad (2.3)$$

where $A_{ij} = \frac{1}{2}(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i})$ and $N = \left[\frac{\partial \mathbf{n}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{n} \right] - \left[\left(\frac{1}{2} \text{curl} \mathbf{v} \right) \times \mathbf{n} \right]$. N represents the rate of change of the director with respect to the background fluid. α_i are the Leslie coefficients. The rotational viscosity is given by $\gamma_1 = \alpha_3 - \alpha_2$.

2.1 Hybrid aligned nematic (HAN)

The orientation of the director in a nematic liquid crystal cell can be controlled by the bounding surfaces treated appropriately as discussed in section 1.8. In a hybrid aligned nematic (HAN) cell one of the glass plates is treated with long ODSE molecules for homeotropic alignment and the director aligns perpendicular to the glass plates. The other glass plate is treated with polyimide and rubbed for homogeneous alignment and the director aligns parallel to the glass plates. In the case of HAN cell the orientation of the director in the bulk will be tilted. The director field is given by $\mathbf{n} = (\sin \theta, 0, \cos \theta)$. The director distribution will depend on the thickness as well as the anchoring strengths of the two surfaces. The director profile in a hybrid aligned nematic cell can have two types of domains as shown Fig. 2.4 as both are energetically equivalent.

2.2 Molecular field

In the absence of external fields, the condition for equilibrium can be obtained by minimising the free energy density (F) with respect to all variations of the director field $\mathbf{n}$. A relevant 'molecular field' is given by [1]

$$h_\beta = -\frac{\partial F}{\partial n_\beta} + \partial_\alpha \left(\frac{\partial F}{\partial g_{\alpha\beta}} \right) \quad (2.4)$$

where the gradient $g_{\alpha\beta} = \partial_\alpha n_\beta$. In equilibrium the director must be parallel to the molecular field at each point. When $\mathbf{n}$ and $\mathbf{h}$ are not parallel, the director experiences

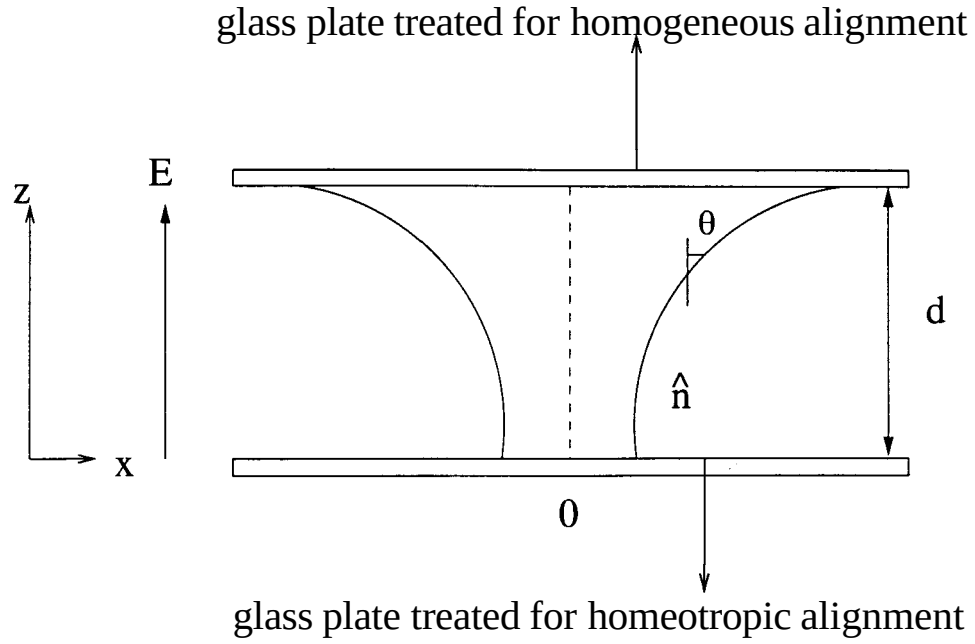


Fig. 2.4: Schematic representation of the director profile in an hybrid aligned nematic cell. Two types of domains are possible in a HAN cell.

a torque which tends to make them collinear. The torque density is given by

$$\mathbf{\Gamma} = \mathbf{n} \times \mathbf{h} \quad (2.5)$$

The various torques arising in a HAN cell are: a) the anchoring torque at both the surfaces, b) the flexoelectric torque acting mainly on the surfaces, c) the viscous torque in the bulk of the medium, d) the dielectric torque in the bulk of the medium and e) the elastic torque acting in the bulk as well as on the surface. The dissipative viscous torque is equated to the rest of the reactive torques acting in the bulk to find the equations of motion of the director.

2.3 Theoretical Analysis

The AC response of a HAN cell gives rise to an 'f' signal at the frequency of the applied voltage and a '2f' signal at twice that frequency. The flexoelectric coupling

depends linearly on the electric field and hence gives rise to the f signal whereas the dielectric coupling depends quadratically on the electric field and produces the $2f$ signal. In the present work we are interested only in the flexoelectric effect and hence in the f signal. We now describe the equations for the various contributions to the bulk torque on the director.

Hydrodynamic torque:

In calculating the hydrodynamic torque, we have ignored the backflow effects as the amplitude of oscillations of polar angle θ (defined in Fig. 2.4) is quite small. The molecular field due to hydrodynamic dissipation is given by

$$h_i^{hy} = \gamma_1 \frac{\partial n_i}{\partial t} \quad (2.6)$$

where γ_1 is the rotational viscosity coefficient. The components of molecular field are

$$h_x^{hy} = \gamma_1 \cos \theta \frac{\partial \theta}{\partial t}, \quad (2.7)$$

$$h_z^{hy} = -\gamma_1 \sin \theta \frac{\partial \theta}{\partial t}. \quad (2.8)$$

The hydrodynamic torque is given by

$$\Gamma^{hy} = \gamma_1 \frac{\partial \theta}{\partial t}. \quad (2.9)$$

Elastic torque:

In the present geometry, there is no twist of the director. The elastic free energy density is given by

$$f^{el} = \frac{K_{11}}{2} (\text{div } \mathbf{n})^2 + \frac{K_{33}}{2} (\mathbf{n} \times \text{curl } \mathbf{n})^2. \quad (2.10)$$

The components of the molecular field are

$$h_z^{el} = K_{11} \frac{\partial^2 n_z}{\partial z^2}. \quad (2.11)$$

$$h_x^{el} = K_{33} \frac{\partial^2 n_x}{\partial z^2}. \quad (2.12)$$

Writing in terms of polar angle θ , the components of the molecular field are given

$$h_z^{el} = -K_{11} \left[\sin \theta \frac{\partial^2 \theta}{\partial z^2} + \cos \theta \left(\frac{\partial \theta}{\partial z} \right)^2 \right]. \quad (2.13)$$

$$h_x^{el} = K_{33} \left[\cos \theta \frac{\partial^2 \theta}{\partial z^2} - \sin \theta \left(\frac{\partial \theta}{\partial z} \right)^2 \right]. \quad (2.14)$$

The elastic torque is given by

$$\Gamma^{el} = (K_{11} - K_{33}) \sin 2\theta \left(\frac{\partial \theta}{\partial z} \right)^2 + (K_{11} \sin^2 \theta + K_{33} \cos^2 \theta) \frac{\partial^2 \theta}{\partial z^2}. \quad (2.15)$$

Dielectric torque:

Assuming the electric field has a component only along the z-direction, the dielectric free energy density is given by

$$f^{diel} = -\frac{\Delta\epsilon}{8\pi} E^2(z) n_z^2. \quad (2.16)$$

The components of the molecular field are given by

$$h_z^{diel} = \frac{\Delta\epsilon}{4\pi} E^2(z) n_z, \quad (2.17)$$

$$h_x^{diel} = 0. \quad (2.18)$$

Expressing h_z^{diel} in terms of polar angle θ we get

$$h_z^{diel} = \frac{\Delta\epsilon}{4\pi} E^2(z) \cos \theta. \quad (2.19)$$

The dielectric torque is given by

$$\Gamma^{diel} = -\frac{\Delta\epsilon}{8\pi} E^2 \sin 2\theta. \quad (2.20)$$

Flexoelectric torque:

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The flexoelectric free energy density is given by

$$f^{fl} = -\mathbf{P}_f \cdot \mathbf{E} \quad (2.21)$$

The component of the flexoelectric polarisation along the z direction is given by

$$P_f(z) = e_1 n_z \frac{\partial n_z}{\partial z} - e_3 n_x \frac{\partial n_x}{\partial z}. \quad (2.22)$$

The components of the molecular field are given by

$$h_z^{fl} = -e_1 n_z \frac{\partial E(z)}{\partial z}, \quad (2.23)$$

$$h_x^{fl} = e_3 n_x \frac{\partial E(z)}{\partial z}. \quad (2.24)$$

The components of the molecular field in terms of polar angle θ are given by

$$h_z^{fl} = -e_l \cos \theta \frac{\partial E(z)}{\partial z}, \quad (2.25)$$

$$h_x^{fl} = e_3 \sin \theta \frac{\partial E(z)}{\partial z}. \quad (2.26)$$

The flexoelectric torque is given by

$$\Gamma^{fl} = \frac{(e_1 + e_3)}{2} \frac{\partial E}{\partial z} \sin 2\theta. \quad (2.27)$$

2.4 Insulating nematic

Bulk torque balance equation:

For the sake of simplicity we ignore the ionic contributions to the conductivity of the nematic liquid crystal. We assume the nematic to be an insulator. The torque balance equation in the bulk in this case is given by

$$\begin{aligned} \gamma_1 \frac{\partial \theta}{\partial t} = & \frac{(K_{11} - K_{33})}{2} \sin 2\theta \left(\frac{\partial \theta}{\partial z} \right)^2 + (K_{11} \sin^2 \theta + K_{33} \cos^2 \theta) \frac{\partial^2 \theta}{\partial z^2} \\ & - \frac{\Delta \epsilon}{8\pi} E^2 \sin 2\theta + \frac{(e_1 + e_3)}{2} \frac{\partial E}{\partial z} \sin 2\theta \end{aligned} \quad (2.28)$$

where γ_1 is the rotational viscosity coefficient, $\Delta\epsilon$ the dielectric anisotropy, K_{11} the splay elastic constant and K_{33} the bend elastic constant. In the present section we assume that the nematic is an insulator which turns out to be a reasonable approximation when the temperature is not too high. Hence from the Maxwell equation $\nabla \cdot \mathbf{D} = 0$ and as all the variations are only along the z -direction the z component of the displacement vector D_z is a constant. Note that the flexoelectric effect does not contribute to the bulk torque, when the electric field is uniform (see equation 2.28). The applied voltage $V = V_o \sin \omega t$ is given by

$$V = \int_0^d E dz. \quad (2.29)$$

$$\begin{aligned} D_z &= (\epsilon_{\perp} \sin^2 \theta + \epsilon_{\parallel} \cos^2 \theta) E(z) + 4\pi P_f(z) \\ &= \text{constant} \end{aligned} \quad (2.30)$$

where $\epsilon_{\perp}$ and $\epsilon_{\parallel}$ are the dielectric constants parallel and perpendicular to the director. The z dependent local electric field is given by

$$E(z, t) = \frac{D, \sin \omega t}{\epsilon_{\perp} + \Delta\epsilon \cos^2 \theta(z, t)} - \frac{4\pi P_f(z, t)}{\epsilon_{\perp} + \Delta\epsilon \cos^2 \theta(z, t)} \quad (2.31)$$

where the flexoelectric polarisation

$$P_f = -\frac{(e_1 + e_3)}{2} \sin 2\theta \frac{\partial \theta}{\partial z}. \quad (2.32)$$

Surface torque balance equation:

The surface torque due to anchoring is given by

$$-\frac{\partial F_s(\theta)}{\partial \theta} = -W_s \sin \theta, \cos \theta_s \quad (2.33)$$

where s stands for either surface and W_s is the corresponding anchoring energy.

The elastic torque at the surface is given by

$$\frac{\partial f^{el}}{\partial (\frac{\partial \theta}{\partial z})} = (K_{11} \sin^2 \theta_s + K_{33} \cos^2 \theta_s) \left(\frac{\partial \theta}{\partial z} \right)_s \quad (2.34)$$

The flexoelectric torque at the surface is given by

$$\frac{\partial f^{fl}}{\partial(\frac{\partial\theta}{\partial z})} = \frac{(e_1 + e_3)}{2} E \sin 2\theta_s \quad (2.35)$$

The net surface torque balance equation is written as

$$\frac{W_s}{2} \sin 2\theta_s - (K_{11} \sin^2 \theta_s + K_{33} \cos^2 \theta_s) \left(\frac{\partial\theta}{\partial z} \right)_s - \frac{(e_1 + e_3)}{2} E \sin 2\theta_s = 0. \quad (2.36)$$

The polar angle θ can be written as

$$\theta(z, t) = \theta_o(z) + \theta_t(z, t) \quad (2.37)$$

where θ_o is the time independent part and θ_t the time dependent part. As we are only interested in the signal due to flexoelectric coupling at the frequency of the applied field we write

$$\theta_t(z, t) = \theta_1(z) \sin \omega t + \theta_2(z) \cos \omega t. \quad (2.38)$$

As the ω signal is very small θ_t has a small amplitude. Hence we expand θ dependent functions in equations 2.28, 2.31, 2.32 and 2.36 to the first power in θ_t . It is useful to define

$$\epsilon_{eff} = \epsilon_{\perp} + \Delta\epsilon \cos^2 \theta_o \quad (2.39)$$

and

$$E_o = \frac{D_z + 2\pi(e_1 + e_3) \left(\sin 2\theta_o \frac{\partial\theta_1}{\partial z} + 2 \cos 2\theta_o \frac{\partial\theta_2}{\partial z} \theta_1 \right)}{\epsilon_{eff}} \quad (2.40)$$

Time independent part:

The time independent part of the surface torque balance equation is given by

$$(K_{11} \sin^2 \theta_{os} + K_{33} \cos^2 \theta_{os}) \left(\frac{\partial\theta_o}{\partial z} \right)_s = \frac{W_s}{2} \sin 2\theta_{os}. \quad (2.41)$$

The time independent part of the bulk torque balance equation is given by

$$\begin{aligned} (K_{11} \sin^2 \theta_o + K_{33} \cos^2 \theta_o) \frac{\partial^2 \theta_o}{\partial z^2} &= \frac{\Delta\epsilon \sin(2\theta_o) D_z^2}{16\pi \epsilon_{eff}^2} \\ &\quad - \frac{(K_{11} - K_{33})}{2} \sin 2\theta_o \left(\frac{\partial\theta_o}{\partial z} \right)^2. \end{aligned} \quad (2.42)$$

Time dependent part:

The in phase component (i.e. $\sin\omega t$ -dependent part) of the surface torque balance equation is given by

$$\begin{aligned} \left\{ K_{11} \sin^2 \theta_{os} + K_{33} \cos^2 \theta_{os} + (e_1 + e_3)^2 \pi \sin^2(2\theta_{os})/\epsilon_{eff} \right\} \left(\frac{\partial \theta_1}{\partial z} \right)_s = \\ W_s \cos(2\theta_{os}) \theta_{1s} - (K_{11} - K_{33}) \sin(2\theta_{os}) \theta_{1s} \left(\frac{\partial \theta_o}{\partial z} \right)_s \\ - \frac{(e_1 + e_3)}{2\epsilon_{eff}} \sin 2\theta_{os} \left\{ D_z + 4\pi (e_1 + e_3) \cos 2\theta_{os} \left(\frac{\partial \theta_o}{\partial z} \right)_s \theta_{1s} \right\}. \end{aligned} \quad (2.43)$$

The out of phase component of the surface torque balance equation is given by

$$\begin{aligned} (K_{11} \sin^2 \theta_{os} + K_{33} \cos^2 \theta_{os}) \left(\frac{\partial \theta_2}{\partial z} \right)_s = W_s \cos(2\theta_{os}) \theta_{2s} \\ - (K_{11} - K_{33}) \sin(2\theta_{os}) \theta_{2s} \left(\frac{\partial \theta_o}{\partial z} \right)_s. \end{aligned} \quad (2.44)$$

The in phase component of the bulk torque balance equation is given by

$$\begin{aligned} \left\{ K_{11} \sin^2 \theta_o + K_{33} \cos^2 \theta_o + (e_1 + e_3)^2 \pi \sin^2(2\theta_o)/\epsilon_{eff} \right\} \frac{\partial^2 \theta_1}{\partial z^2} = \\ -\gamma_1 \omega \theta_2 - (K_{11} - K_{33}) \left\{ \sin 2\theta_o \frac{\partial \theta_1}{\partial z} \frac{\partial \theta_o}{\partial z} + \cos(2\theta_o) \theta_1 \left(\frac{\partial \theta_o}{\partial z} \right)^2 + \sin(2\theta_o) \theta_1 \frac{\partial^2 \theta_o}{\partial z^2} \right\} \\ + \frac{3\Delta\epsilon \cos(2\theta_o) \theta_1 D_z^2}{16\pi\epsilon_e^2} - \frac{(e_1 + e_3)^2 \pi}{\epsilon_{eff}} \left\{ 2 \sin 4\theta_o \frac{\partial \theta_o}{\partial z} \frac{\partial \theta_1}{\partial z} \right. \\ \left. - 4 \sin^2(2\theta_o) \left(\frac{\partial \theta_o}{\partial z} \right)^2 \theta_1 + \sin(4\theta_o) \theta_1 \frac{\partial^2 \theta_o}{\partial z^2} \right\} \\ - \frac{(e_1 + e_3)}{2\epsilon_{eff}} \sin^2(2\theta_o) E_o \Delta\epsilon \frac{\partial \theta_o}{\partial z}. \end{aligned} \quad (2.45)$$

The out of phase component of the bulk torque balance equation is given by

$$\begin{aligned} (K_{11} \sin^2 \theta_o + K_{33} \cos^2 \theta_o) \frac{\partial^2 \theta_2}{\partial z^2} = \\ \gamma_1 \omega \theta_1 - (K_{11} - K_{33}) \left\{ \sin 2\theta_o \frac{\partial \theta_2}{\partial z} \frac{\partial \theta_o}{\partial z} + \cos(2\theta_o) \theta_2 \left(\frac{\partial \theta_o}{\partial z} \right)^2 + \sin(2\theta_o) \theta_2 \frac{\partial^2 \theta_o}{\partial z^2} \right\} \\ + \frac{\Delta\epsilon \cos(2\theta_o) \theta_2 D_z^2}{16\pi\epsilon_{eff}^2} \end{aligned} \quad (2.46)$$

In the above equations the physical parameters involved are the surface anchoring energies W_l (l stands for lower surface) and W_u (u stands for upper surface), the flexoelectric coefficient $(e_1 + e_3)$, the rotational viscosity γ_1 , the elastic constants K_{11} and K_{33} and the dielectric constants $\epsilon_\perp$ and $\Delta\epsilon$. For the compound chosen the last four parameters have been measured. W_l , W_u , $(e_1 + e_3)$ and γ_1 are treated as unknown parameters and for an assumed set of the unknown parameters the director profile is theoretically computed using the following procedure.

The Bulirsch Stoer [13] method was used for solving the differential equations. It is an excellent method for solving differential equations containing smooth functions. When the step size is small the round off error increases. Each step involves an error which gets added up when the number of iterations become large. But the truncation error increases if a large step size is used. Most of the true solutions require infinite number of iterations. However the solutions are computed using finite number of iterations which increases the truncation error. The method used tries to strike a balance between the round off errors and truncation errors as it is an extrapolation method which uses a variable stepsize to evolve from one boundary to the other. It gives very accurate solutions to ordinary differential equations with minimal computational effort. In Bulirsch Stoer method the integrations are performed using the modified midpoint method. The modified midpoint method which is an ordinary differential equation integrator method advances a vector of dependent variables $y(x)$ from a point x to a point $x+H$ by a sequence of n substeps each of size h ($h=H/n$). A single Bulirsch Stoer step which consists of many substeps of modified midpoint method, is then extrapolated to zero stepsize using Richardson extrapolation. Richardson extrapolation uses the idea of extrapolating a computed result that would have been obtained if the stepsize had been very much smaller than the actual step size. A large interval H is spanned by different sequences of finer

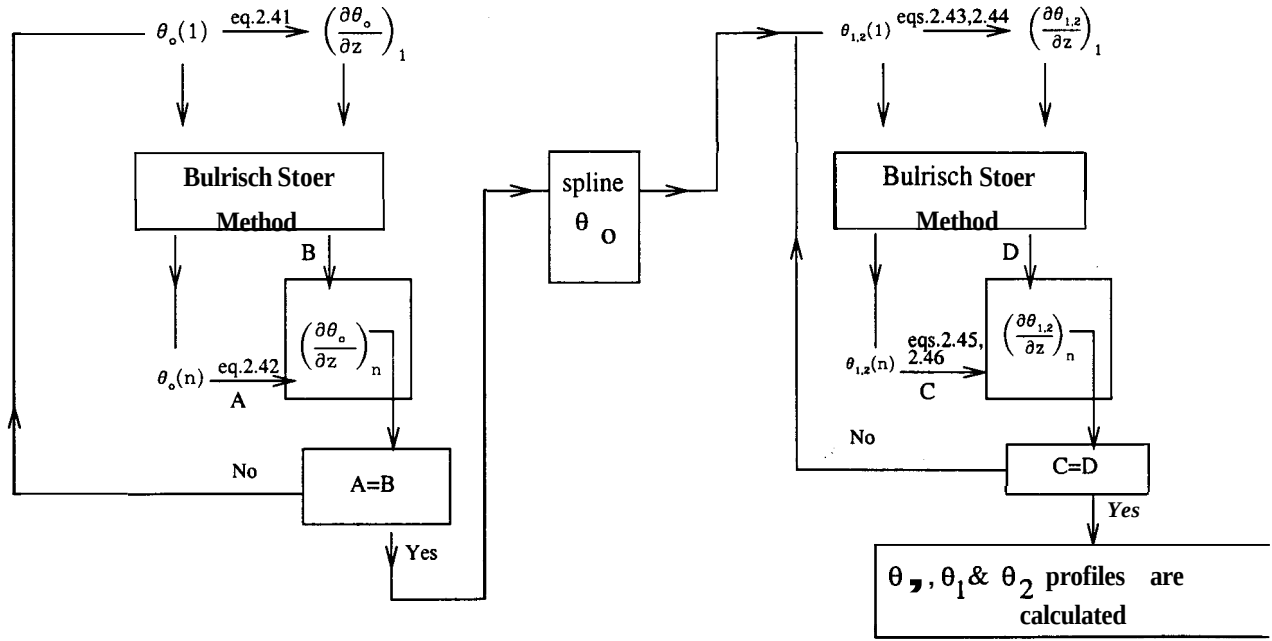


Fig. 2.5: The flow chart of the algorithm used for obtaining the profiles of θ_o , θ_1 and θ_2 .

and finer substeps. Their results are extrapolated to an answer that is supposed to correspond to infinitely fine substeps or in other words extrapolation to zero stepsize is the desired goal. Error control is enforced by monitoring internal consistency and adapting stepsize to match a prescribed bound on the local truncation error.

To solve equation 2.42 we use the above mentioned Bulrich Stoer method. We have found that the accuracy of the resulting θ_o profile is quite adequate for further calculations. For a given value of D_z , we use some reasonable θ_o at the lower plate (i.e. θ_{ol}) as an initial guess. Using the boundary condition given by equation 2.41 the derivative $\partial\theta_o/\partial z$ at the lower plate (i.e. $(\partial\theta_o/\partial z)_l$) is calculated. The Bulrich Stoer procedure leads to the values of θ_o and $\partial\theta_o/\partial z$ at the upper plate (i.e. θ_{ou} and $(\partial\theta_o/\partial z)_u$). $(\partial\theta_o/\partial z)_u$ at the upper plate is also calculated from θ_{ou} using equation 2.41. The value of θ_{ol} is adjusted such that the two values of $(\partial\theta_o/\partial z)_u$ are equal. Hence the θ_o profile is obtained for a given value of D_z , i.e.

for a given voltage. This θ_o profile is used in equations 2.43-2.46 to calculate the profiles of θ_1 and θ_2 . Equations 2.45 and 2.46 are solved numerically using the Bulirsch Stoer method adjusting the values of both θ_1 and θ_2 at the lower surface so that the boundary conditions given by equations 2.43 and 2.44 are satisfied simultaneously. Since equations 2.45 and 2.46 are coupled differential equations involving both θ_1 and θ_2 , a globally convergent Newton Raphson method [13] is used to solve them simultaneously. The flow chart of the algorithm used for obtaining the profiles of θ_o , θ_1 and θ_2 is shown in Fig. 2.5. The resulting profiles of θ_o , θ_1 and θ_2 for a given value of D_z are used in equation 2.29 to calculate the voltage across the cell.

The intensity of the transmitted light beam which propagates in a uniaxial medium between crossed polarisers is given by

$$I_t = I_o \sin^2 2\psi \left(\frac{1 - \cos \Delta\phi}{2} \right) \quad (2.47)$$

where $A\#$ the optical phase difference introduced by the sample, I_o the incident intensity, and ψ the azimuthal angle made by the effective optic axis with the plane of polarisation of the incident beam. The intensity is maximum when the angle made by the effective optic axis with the plane of polarisation of the incident beam is 45° . In this setting the transmission coefficient is given by

$$I = \frac{1 - \cos A\#}{2} \quad (2.48)$$

where I is the normalised intensity with respect to the incident intensity I_o .

The optical phase difference is due to the different propagating speeds of the extraordinary and the ordinary rays in the LC medium and is given by

$$\Delta\phi = \frac{2\pi}{\lambda} \int_0^d (n_{ef}(z) - n_o) dz \quad (2.49)$$

where $n_{ef} = n_o / \sqrt{1 - R \sin^2 \theta(z)}$, $R = (n_e^2 - n_o^2) / n_e^2$ and n_e and n_o are the extraordinary and ordinary refractive indices of the nematic which are available in the

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literature [14] for the compound studied. $\Delta\phi$ can be written as

$$\Delta\phi = \Delta\phi_o + \Delta\phi_t \quad (2.50)$$

where $\Delta\phi_o \gg \Delta\phi_t = \Delta\phi_1 \sin \omega t + \Delta\phi_2 \cos \omega t$. The time independent phase difference is given by

$$\Delta\phi_o = \frac{2\pi n_o}{\lambda} \int_0^d \left(\frac{1}{\sqrt{1 - R \sin^2 \theta_o}} - 1 \right) dz. \quad (2.51)$$

The time dependent phase differences are given by

$$\Delta\phi_i = \frac{\pi n_o}{\lambda} \int_0^d \frac{R \sin 2\theta_o \theta_i}{(1 - R \sin^2 \theta_o)^{\frac{3}{2}}} dz \quad (2.52)$$

where $i=1$ and 2 for the in phase component and the out of phase component respectively. The DC transmission coefficient is given by

$$I_{DC} = \frac{1 - \cos \Delta\phi_o}{2} \quad (2.53)$$

The amplitude of the normalised AC optical signal is given by

$$I_{AC} = \frac{\sin \Delta\phi_o \sqrt{\Delta\phi_1^2 + \Delta\phi_2^2}}{2} \quad (2.54)$$

The phase of the AC optical signal is given by

$$\phi_{AC} = \tan^{-1} \frac{\Delta\phi_1}{\Delta\phi_2}. \quad (2.55)$$

From equations 2.51 and 2.52 the phase differences can be calculated using θ_o , θ_1 and θ_2 profiles for a given voltage. Hence by using equation 2.53 to equation 2.55, the normalised DC optical intensity and the magnitude as well as the phase of the AC optical signal are calculated. The value of D_z is increased in steps so that the calculations are repeated for different voltages. As a result we obtain the intensity profiles for a given set of assumed parameters.

2.5 Conducting nematic

In the present section, the nematic is treated as a conductor. From Maxwell's equations

$$\text{div}\mathbf{D} = \rho \quad (2.56)$$

where ρ is the total charge density.

$$\text{curl}\mathbf{H} = \mathbf{j} + \frac{\partial\mathbf{D}}{\partial t}. \quad (2.57)$$

Hence

$$\text{div}(\mathbf{j} + \frac{\partial\mathbf{D}}{\partial t}) = 0 \quad (2.58)$$

as the divergence of the curl of a vector is zero. The total current density $\mathbf{J} = \mathbf{j} + \frac{\partial\mathbf{D}}{\partial t}$ is a constant. As all the variations of the director are along the z -direction only:

$$\frac{\partial}{\partial z}(j_z + \frac{\partial D_z}{\partial t}) = 0. \quad (2.59)$$

$$\text{i.e. } J_z = j_z + \frac{\partial D_z}{\partial t} = \text{constant for all } z, \text{ at any given time.} \quad (2.60)$$

The z component of the displacement vector can be written as

$$D_z(z,t) = D_0(z) + D_1(z)\sin \omega t + D_2(z)\cos \omega t. \quad (2.61)$$

where ω is the frequency of the applied voltage across the HAN cell. As we assume that the ionic charges screen the flexoelectric polarisation $D_0=0$. The z component of the current density vector can be written as

$$j_z(z, t) = j_o(z) + j_1(z) \sin \omega t + j_2(z) \cos \omega t. \quad (2.62)$$

The z component of the total current density vector can be written as

$$J_z(t) = J_o + J_1 \sin \omega t + J_2 \cos \omega t. \quad (2.63)$$

Substituting equation 2.61-2.63 in equation 2.60 we get

$$J_o = j_o, \quad (2.64)$$

$$J_1 = j_1(z) - \omega D_2(z), \quad (2.65)$$

$$J_2 = j_2(z) + \omega D_1(z). \quad (2.66)$$

As the current density can be related to the electric field

$$j_1(z) = \sigma E_1(z) \quad (2.67)$$

$$j_2(z) = \sigma E_2(z) \quad (2.68)$$

It is useful to define

$$\epsilon_{eff} = \epsilon_{\perp} + \Delta \epsilon \cos^2 \theta_o \quad (2.69)$$

$$\sigma_{eff} = \sigma_{\perp} + \Delta \sigma \cos^2 \theta_o \quad (2.70)$$

where the conductivity anisotropy $\Delta \sigma$ is given by

$$\Delta \sigma = \sigma_{\parallel} - \sigma_{\perp}. \quad (2.71)$$

$\sigma_{\perp}$ and $\sigma_{\parallel}$ are the perpendicular and the parallel components of conductivity respectively. From equation 2.31 the inphase and out of phase components of the local electric field are given by

$$E_i(z) = \frac{D_i(z) - 4\pi P_i(z)}{\epsilon_{eff}} \quad (2.72)$$

where $i=1, 2$ for the inphase component and out of phase component respectively. P_1, P_2 are the inphase component and the out of phase components of flexoelectric polarisation P_f . From 2.32 we get

$$P_1 = 2\pi (e_1 + e_3) \left(\sin 2\theta_o \frac{\partial \theta_1}{\partial z} + 2 \cos 2\theta_o \frac{\partial \theta_o}{\partial z} \theta_1 \right). \quad (2.73)$$

$$P_2 = 2\pi (e_1 + e_3) \left(\sin 2\theta_o \frac{\partial \theta_2}{\partial z} + 2 \cos 2\theta_o \frac{\partial \theta_o}{\partial z} \theta_2 \right). \quad (2.74)$$

Using equations 2.72-2.74 and equations 2.64-2.68, we get the inphase(E_1) and out of phase (E_2) components of the local electric field as

$$\begin{aligned} E_1 = & \left\{ J_1 \sigma_{eff} + J_2 \omega \epsilon_{eff} + 2\pi (e_1 + e_3) \omega^2 \epsilon_{eff} \sin 2\theta_o \frac{\partial \theta_1}{\partial z} \right. \\ & + 4\pi (e_1 + e_3) \omega^2 \epsilon_{eff} \cos 2\theta_o \frac{\partial \theta_o}{\partial z} \theta_1 - 2\pi (e_1 + e_3) \omega \sigma_{eff} \sin 2\theta_o \frac{\partial \theta_2}{\partial z} \\ & \left. - 4\pi (e_1 + e_3) \omega \sigma_{eff} \cos 2\theta_o \frac{\partial \theta_o}{\partial z} \theta_2 \right\} / (\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2). \end{aligned} \quad (2.75)$$

and

$$\begin{aligned} E_2 = & \left\{ J_2 \sigma_{eff} - J_1 \omega \epsilon_{eff} + 2\pi (e_1 + e_3) \omega^2 \epsilon_{eff} \sin 2\theta_o \frac{\partial \theta_2}{\partial z} \right. \\ & + 4\pi (e_1 + e_3) \omega^2 \epsilon_{eff} \cos 2\theta_o \frac{\partial \theta_o}{\partial z} \theta_2 + 2\pi (e_1 + e_3) \omega \sigma_{eff} \sin 2\theta_o \frac{\partial \theta_1}{\partial z} \\ & \left. + 4\pi (e_1 + e_3) \omega \sigma_{eff} \cos 2\theta_o \frac{\partial \theta_o}{\partial z} \theta_1 \right\} / (\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2). \end{aligned} \quad (2.76)$$

Chapter 2

The applied voltage $V = V_o \sin wt$ is given by

$$\int_0^d E_1 dz = V. \quad (2.77)$$

When a sine wave voltage is applied across the cell

$$\int_0^d E_2 dz = 0. \quad (2.78)$$

Time independent part:

The time independent part of the surface torque balance equation is given by

$$\left(K_{11} \sin^2 \theta_{os} + K_{33} \cos^2 \theta_{os} \right) \frac{\partial \theta_{os}}{\partial z} = \frac{W_s}{2} \sin 2\theta_{os}. \quad (2.79)$$

The time independent part of the bulk torque balance equation is given by

$$\begin{aligned} \left(K_{11} \sin^2 \theta_o + K_{33} \cos^2 \theta_o \right) \frac{\partial^2 \theta_o}{\partial z^2} &= \left\{ \Delta \epsilon \sin 2\theta_o \left(J_1^2 + J_2^2 \right) \right\} / 16\pi \left(\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2 \right) \\ &\quad - \left(K_{11} - K_{33} \right) \sin 2\theta_o \left(\frac{\partial \theta_o}{\partial z} \right)^2. \end{aligned} \quad (2.80)$$

Time dependent part:

The in phase component of the surface torque balance equation is given by

$$\begin{aligned} &\left\{ K_{11} \sin^2 \theta_{os} + K_{33} \cos^2 \theta_{os} + (e_1 + e_3)^2 \pi \omega^2 \epsilon_{eff} \sin^2(2\theta_{os}) / \left(\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2 \right) \right\} \frac{\partial \theta_{1s}}{\partial z} \\ &\quad - \left\{ \pi \omega (e_1 + e_3)^2 \sin^2 2\theta_{os} \sigma_{eff} / \left(\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2 \right) \right\} \frac{\partial \theta_{2s}}{\partial z} = \\ &\quad W_s \cos 2\theta_{os} \theta_{1s} - (K_{11} - K_{33}) \sin 2\theta_{os} \theta_{1s} \frac{\partial \theta_{os}}{\partial z} \\ &\quad - (e_1 + e_3) \sin 2\theta_{os} \left\{ J_1 \sigma_{eff} + J_2 \omega \epsilon_{eff} \right. \\ &\quad \left. + 4\pi (e_1 + e_3) \omega^2 \epsilon_{eff} \cos 2\theta_{os} \frac{\partial \theta_{os}}{\partial z} \theta_{1s} \right. \\ &\quad \left. - 4\pi (e_1 + e_3) \omega \sigma_{eff} \cos 2\theta_{os} \frac{\partial \theta_{os}}{\partial z} \theta_{2s} \right\} / 2 \left(\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2 \right). \end{aligned} \quad (2.81)$$

The out of phase component of the surface torque balance equation is given by

$$\begin{aligned}
& \left\{ K_{11} \sin^2 \theta_{os} + K_{33} \cos^2 \theta_{os} + (e_1 + e_3)^2 \pi \omega^2 \epsilon_{eff} \sin^2(2\theta_{os}) / (\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2) \right\} \frac{\partial \theta_{2s}}{\partial z} \\
& - \{ TW (e_1 + e_3)^2 \sin^2 2\theta_{os} \sigma_{eff} / (\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2) \} \frac{\partial \theta_{1s}}{\partial z} = \\
& W_s \cos 2\theta_{os} \theta_{2s} - (K_{11} - K_{33}) \sin 2\theta_{os} \theta_{2s} \frac{\partial \theta_{os}}{\partial z} \\
& - (e_1 + e_3) \sin 2\theta_{os} \left\{ J_2 \sigma_{eff} - J_1 \omega \epsilon_{eff} \right. \\
& + 4\pi (e_1 + e_3) \omega^2 \epsilon_{eff} \cos 2\theta_{os} \frac{\partial \theta_{os}}{\partial z} \theta_{2s} \\
& \left. + 4\pi (e_1 + e_3) \omega \sigma_{eff} \cos 2\theta_{os} \frac{\partial \theta_{os}}{\partial z} \theta_{1s} \right\} / 2 (\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2) \quad (2.82)
\end{aligned}$$

The in phase component of the bulk torque balance equation is given by

$$\begin{aligned}
& \left\{ K_{11} \sin^2 \theta_o + K_{33} \cos^2 \theta_o + (e_1 + e_3)^2 \pi \omega^2 \epsilon_{eff} \sin^2(2\theta_o) / (\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2) \right\} \frac{\partial^2 \theta_1}{\partial z^2} \\
& - \left\{ \pi \omega (e_1 + e_3)^2 \sin^2 2\theta_o \sigma_{eff} / (\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2) \right\} \frac{\partial^2 \theta_2}{\partial z^2} = \\
& - \gamma_1 \omega \theta_2 - (K_{11} - K_{33}) \left\{ \sin 2\theta_o \frac{\partial \theta_1}{\partial z} \frac{\partial \theta_o}{\partial z} + \cos 2\theta_o \theta_1 \left(\frac{\partial \theta_o}{\partial z} \right)^2 + \sin 2\theta_o \theta_1 \frac{\partial^2 \theta_o}{\partial z^2} \right\} \\
& + \Delta \epsilon \cos 2\theta_o \left[\theta_2 J_1 J_2 (\sigma_{eff}^2 - \omega^2 \epsilon_{eff}^2) + \theta_2 \sigma_{eff} \omega \epsilon_{eff} (J_2^2 - J_1^2) \right. \\
& + \left. \left\{ (3J_1^2 + J_2^2) \sigma_{eff}^2 + (3J_2^2 + J_1^2) \omega^2 \epsilon_{eff}^2 + 4J_1 J_2 \sigma_{eff} \omega \epsilon_{eff} \right\} \frac{\theta_1}{2} \right] / 8\pi (\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2)^2 \\
& + \left\{ (e_1 + e_3) \sin^2(2\theta_o) \frac{\partial \theta_o}{\partial z} (A \omega J_1 + \omega \Delta \epsilon J_2) \right\} / 2 (\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2) \\
& + \left\{ - (e_1 + e_3)^2 2\pi \omega \sin(4\theta_o) \frac{\partial \theta_o}{\partial z} \left(\omega \epsilon_{eff} \frac{\partial \theta_1}{\partial z} - \sigma_{eff} \frac{\partial \theta_2}{\partial z} \right) \right. \\
& + (e_1 + e_3)^2 \pi \omega \sin^3(2\theta_o) \frac{\partial \theta_o}{\partial z} \left(\Delta \epsilon \omega \frac{\partial \theta_1}{\partial z} - \Delta \sigma \frac{\partial \theta_2}{\partial z} \right) \\
& + (e_1 + e_3)^2 4\pi \omega \sin^2(2\theta_o) \left(\frac{\partial \theta_o}{\partial z} \right)^2 (\omega \epsilon_{eff} \theta_1 - \sigma_{eff} \theta_2) \\
& - (e_1 + e_3)^2 \pi \omega \sin(4\theta_o) \frac{\partial^2 \theta_o}{\partial z^2} (\omega \epsilon_{eff} \theta_1 - \sigma_{eff} \theta_2) \\
& + (e_1 + e_3)^2 \pi \omega \sin(4\theta_o) \sin(2\theta_o) \left(\frac{\partial \theta_o}{\partial z} \right)^2 (\Delta \epsilon \omega \theta_1 - \Delta \sigma \theta_2) \\
& \left. - \sin^2(2\theta_o) \frac{\partial \theta_o}{\partial z} (e_1 + e_3) (\Delta \sigma \sigma_{eff} + \omega^2 \Delta \epsilon \epsilon_{eff}) E_1 \right\} / (\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2). \quad (2.83)
\end{aligned}$$

The out of phase component of the bulk torque balance equation is given by

$$\begin{aligned}
& \left\{ K_{11} \sin^2 \theta_o + K_{33} \cos^2 \theta_o + (e_1 + e_3)^2 \pi \omega^2 \epsilon_{eff} \sin^2(2\theta_o) / (\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2) \right\} \frac{d^2 \theta_2}{dz^2} \\
& + \left\{ a_w (e_1 + e_3)^2 \sin^2 2\theta_o \sigma_{eff} / (\sigma_{eff}^2 + \epsilon_{eff}^2) \right\} \frac{\partial^2 \theta_2}{\partial z^2} = \\
& \gamma_1 \omega \theta_1 - (K_{11} - K_{33}) \left\{ \sin 2\theta_o \frac{\partial \theta_2}{\partial z} \frac{\partial \theta_o}{\partial z} + \cos 2\theta_o \theta_2 \left(\frac{\partial \theta_o}{\partial z} \right)^2 + \sin 2\theta_o \theta_2 \frac{\partial^2 \theta_o}{\partial z^2} \right\} \\
& + \Delta \epsilon \cos 2\theta_o \left[\theta_1 J_1 J_2 (\sigma_{eff}^2 - \omega^2 \epsilon_{eff}^2) + \theta_1 \sigma_{eff} \omega \epsilon_{eff} (J_2^2 - J_1^2) \right. \\
& + \left. \left\{ (J_1^2 + 3J_2^2) \sigma_{eff}^2 + (J_2^2 + 3J_1^2) \omega^2 \epsilon_{eff}^2 - 4J_1 J_2 \sigma_{eff} \omega \epsilon_{eff} \right\} \frac{\theta_2}{2} \right] / 8\pi (\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2)^2 \\
& - \left\{ (e_1 + e_3) \sin^2(2\theta_o) \frac{\partial \theta_o}{\partial z} (\omega \Delta \epsilon J_1 - \Delta \sigma J_2) \right\} / 2 (\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2) \\
& + \left\{ - (e_1 + e_3)^2 2\pi \omega \sin(4\theta_o) \frac{\partial \theta_o}{\partial z} \left(\omega \epsilon_{eff} \frac{\partial \theta_2}{\partial z} + \sigma_{eff} \frac{\partial \theta_1}{\partial z} \right) \right. \\
& + (e_1 + e_3)^2 \pi \omega \sin^3(2\theta_o) \frac{\partial \theta_o}{\partial z} \left(\Delta \epsilon \omega \frac{\partial \theta_2}{\partial z} + \Delta \sigma \frac{\partial \theta_1}{\partial z} \right) \\
& + (e_1 + e_3)^2 4\pi \omega \sin^2(2\theta_o) \left(\frac{\partial \theta_o}{\partial z} \right)^2 (\omega \epsilon_{eff} \theta_2 + \sigma_{eff} \theta_1) \\
& - (e_1 + e_3)^2 \pi \omega \sin(4\theta_o) \frac{\partial^2 \theta_o}{\partial z^2} (\omega \epsilon_{eff} \theta_2 + \sigma_{eff} \theta_1) \\
& + (e_1 + e_3)^2 \pi \omega \sin(4\theta_o) \sin(2\theta_o) \left(\frac{\partial \theta_o}{\partial z} \right)^2 (\Delta \epsilon \omega \theta_2 + \Delta \sigma \theta_1) \\
& \left. - \sin^2(2\theta_o) \frac{\partial \theta_o}{\partial z} (e_1 + e_3) (\Delta \sigma \sigma_{eff} + \omega^2 \Delta \epsilon \epsilon_{eff}) E_2 \right\} / (\sigma_{eff}^2 + \omega^2 \epsilon_{eff}^2). \quad (2.84)
\end{aligned}$$

To solve equation 2.80 we use the above mentioned Bulirsch Stoer method. There are two unknowns namely J_1 and J_2 . To start with, their initial values are guessed. Similar to the case of an insulating nematic we use some reasonable θ_o at the lower plate (i.e. θ_{ol}) as an initial guess. Using the boundary condition given by equation 2.79 the derivative $\partial \theta_o / \partial z$ at the lower plate (i.e. $(\partial \theta_o / \partial z)_l$) is calculated. The Bulirsch Stoer procedure leads to the values of θ_o and $\partial \theta_o / \partial z$ at the upper plate (i.e. θ_{ou} and $(\partial \theta_o / \partial z)_u$). $(\partial \theta_o / \partial z)_u$ is also calculated from θ_{ou} using equation 2.79. The value of θ_{ol} is adjusted such that the two values of $(\partial \theta_o / \partial z)_u$ are equal. Hence the θ_o

profile is obtained for a given value of J_1 and J_2 . This θ_o profile is used in equations 2.81-2.84 to calculate the profiles of θ_1 and θ_2 . Equations 2.83 and 2.84 are solved numerically using the Bulirsch Stoer method adjusting the values of both θ_1 and θ_2 at the lower surface so that the boundary conditions given by equations 2.81 and 2.82 are satisfied simultaneously. Since equations 2.83 and 2.84 are coupled differential equations involving both θ_1 and θ_2 a globally convergent Newton Raphson method [13] is used to solve them simultaneously. Using a similar procedure as in the case of the insulating nematic the profiles of θ_o , θ_1 and θ_2 for a given value of J_1 and J_2 are calculated. Equations 2.77 and 2.78 are solved simultaneously using the above mentioned Newton Raphson programme. Each time Newton Raphson method tries to adjust J_1 and J_2 it has to go through the whole procedure of calculating θ_o , θ_1 and θ_2 profiles. Hence the calculations are more computationally involved than in the case of insulating nematic. The profiles of θ_o , θ_1 and θ_2 are used in 2.47 to calculate the intensity of transmitted light using the same procedure as in the case of an insulating nematic: By increasing voltages in steps, the values of J_1 and J_2 are obtained and the transmitted light intensity is calculated for the corresponding values of J_1 and J_2 or *as* a function of voltage.

In the next Chapter we will be describing the experimental setup for measuring the optical signal from a HAN cell. We will also be describing a numerical fitting procedure to obtain the best fit between the theoretical data and the experimental intensity profiles to determine the set of unknown parameters.