1 Light Propagation in Uniaxial Media

We consider here light propagation in uniaxial materials without absorption. Most nematic liquid crystals are effectively in this category. We need to solve Maxwell's equations; specifically, for monochromatic plane waves,

$$\hat{\mathbf{k}} \cdot \mathbf{D} = 0 \tag{1}$$

and v

$$(I - \hat{\mathbf{k}}\hat{\mathbf{k}})\mathbf{E} = \frac{\omega^2 \varepsilon_o \mu_o}{k^2} \varepsilon_r \mathbf{E} \tag{2}$$

We note that ε_r is the relative dielectric constant *tensor*. Usually, the direction of propagation $\hat{\mathbf{k}}$ is known, we are interested in knowing the directions of the eigenvectors $\mathbf{E}$ and the velocity of propagation, or, equivalently, k. First we consider the dielectric constant tensor.

2 The Dielectric Constant Tensor ε_r.

If a polarizable uniaxial liquid crystal molecule with orientation $\hat{l}$ is placed in a field $\mathbf{E}$, the induced polarization $\mathbf{p}$ is given by

$$\mathbf{p} = \alpha_{||}(\hat{\mathbf{l}} \cdot \mathbf{E})\hat{\mathbf{l}} + \alpha_\perp(\mathbf{E} - (\hat{\mathbf{l}} \cdot \mathbf{E})\hat{\mathbf{l}} \tag{3}$$

or, writing this in tensor notation,

$$\mathbf{p} = (\alpha_{||}\hat{\mathbf{l}}\hat{\mathbf{l}} + \alpha_\perp(I - \hat{\mathbf{l}}\hat{\mathbf{l}}))\mathbf{E} \tag{4}$$

The molecular polarizability tensor is thus

$$\alpha = \alpha_\perp I + (\alpha_{||} - \alpha_\perp)\hat{\mathbf{l}}\hat{\mathbf{l}} \tag{5}$$

This can also be written as

$$\alpha = \frac{\alpha_{||} + 2\alpha_\perp}{3} I + \frac{2}{3}(\alpha_{||} - \alpha_\perp)\frac{1}{2}(3\hat{\mathbf{l}}\hat{\mathbf{l}} - I) \tag{6}$$

and averaging this over all molecules (or for a single molecule over time) gives

$$< \alpha > = \frac{\alpha_{||} + 2\alpha_\perp}{3} I + \frac{2}{3}(\alpha_{||} - \alpha_\perp) < \frac{1}{2}(3\hat{\mathbf{l}}\hat{\mathbf{l}} - I) > \tag{7}$$

The quantity $< \frac{1}{2}(3\hat{\mathbf{l}}\hat{\mathbf{l}} - \mathbf{I}) >$ is just the order parameter tensor. For uniaxial materials it can be written as

$$< \frac{1}{2}(3\hat{\mathbf{l}}\hat{\mathbf{l}} - I) > = S\frac{1}{2}(3\hat{\mathbf{n}}\hat{\mathbf{n}} - I) \tag{8}$$

where $\hat{\mathbf{n}}$ is the director and S is the scalar uniaxial order parameter, and

$$< \alpha > = \frac{\alpha_{||} + 2\alpha_\perp}{3} I + \frac{2}{3}(\alpha_{||} - \alpha_\perp) S \frac{1}{2}(3\hat{\mathbf{n}}\hat{\mathbf{n}} - I) \tag{9}$$

The polarization $\mathbf{P}$ is just $\rho\mathbf{p}$ where ρ is the number density; so

$$\mathbf{P} = \boldsymbol{\rho}\mathbf{p} = \boldsymbol{\rho} < \boldsymbol{\alpha} > \mathbf{E} = (\boldsymbol{\rho}\frac{\alpha_{||} + 2\alpha_{\perp}}{3}I + \frac{2}{3}\rho(\alpha_{||} - \alpha_{\perp})S\frac{1}{2}(3\hat{\mathbf{n}}\hat{\mathbf{n}} - I))\mathbf{E} \tag{10}$$

Now we can determine the dielectric constant, since

$$\mathbf{D} = \varepsilon_o\varepsilon_r\mathbf{E} = \varepsilon_o\mathbf{E} + \mathbf{P} \tag{11}$$

and

$$\varepsilon_o\varepsilon_r\mathbf{E} = \varepsilon_o(I + \rho\frac{\alpha_{||} + 2\alpha_{\perp}}{3\varepsilon_o}I + \frac{2}{3\varepsilon_o}\rho(\alpha_{||} - \alpha_{\perp})S\frac{1}{2}(3\hat{\mathbf{n}}\hat{\mathbf{n}} - I))\mathbf{E} \tag{12}$$

and finally we get for uniaxial materials

$$\varepsilon_r = I + \rho\frac{\alpha_{||} + 2\alpha_{\perp}}{3\varepsilon_o}I + \frac{2}{3\varepsilon_o}\rho(\alpha_{||} - \alpha_{\perp})S\frac{1}{2}(3\hat{\mathbf{n}}\hat{\mathbf{n}} - I) \tag{13}$$

We note that the above expression is only approximate, since we did not take into account the fact that the local field acting on a molecule differs from the macroscopic Maxwell field $\mathbf{E}$. We have also ignored permanent contributions from permanent dipoles (this is a good approximation at optical frequencies).

The expression for ε_r is often written as

$$\varepsilon_r = \varepsilon_{\perp}I + (\varepsilon_{||} - \varepsilon_{\perp})\hat{\mathbf{n}}\hat{\mathbf{n}} \tag{14}$$

$\varepsilon_{||} = \rho\alpha_{||}\frac{1}{3}(1 + 2S) + \rho\alpha_{\perp}\frac{2}{3}(1 - S)$ and $\varepsilon_{\perp} = \rho\alpha_{||}\frac{1}{3}(1 - S) + \rho\alpha_{\perp}\frac{2}{3}(1 + \frac{1}{2}S)$. It useful to compute the inverse of ε_r; it is

$$\varepsilon_r^{-1} = \frac{1}{\varepsilon_{\perp}}I + (\frac{1}{\varepsilon_{||}} - \frac{1}{\varepsilon_{\perp}})\hat{\mathbf{n}}\hat{\mathbf{n}} \tag{15}$$

3 Solution of Maxwell's Equation for the Propagating Eigenmodes

Now we solve Maxwell's Equations. We start with

$$(I - \hat{\mathbf{k}}\hat{\mathbf{k}})\mathbf{E} = \frac{\omega^2\varepsilon_o\mu_o}{k^2}\varepsilon_r\mathbf{E} \tag{16}$$

and again we assume that the direction of propagation $\hat{\mathbf{k}}$ and the dielectric tensor ε_r (and its inverse) are known. We note that $\omega^2\varepsilon_o\mu_o = \omega^2/c^2 = (2\pi/\lambda_o)^2$ and $k = 2\pi/\lambda = 2\pi n/\lambda_o$, so $\omega^2\varepsilon_o\mu_o/k^2 = 1/n^2$ where n is the refractive index. The equation

$$\varepsilon_r^{-1}(I - \hat{\mathbf{k}}\hat{\mathbf{k}})\mathbf{E} = \frac{1}{n^2}\mathbf{E} \tag{17}$$

is a standard eigenvalue equation, where the eigenvalues determine the refractive index (and the speed of propagation), and the eigenvectors determine the direction of $\mathbf{E}$ (and $\mathbf{D}$) for the modes. We expect three solutions.

3.1 The Non-propagating Mode

One solution we can obtain at once by inspection: if $\mathbf{E}$ is parallel to $\hat{\mathbf{k}}$, it is an eigenvector, with eigenvalue 0. This is therefore a non-propagating mode, with velocity $v = c/n = 0$.

We now look for the two propagating modes. We write the equation in term of $\mathbf{D}$ (which we know must be perpendicular to $\hat{\mathbf{k}}$), and obtain

$$(I - \hat{\mathbf{k}}\hat{\mathbf{k}})\varepsilon_r^{-1}\mathbf{D} = \frac{1}{n^2}\mathbf{D} \tag{18}$$

Substituting for ε_r^{-1} from Eq. 15 gives

$$\left(\frac{1}{\varepsilon_\perp}I - \frac{1}{\varepsilon_\perp}\hat{\mathbf{k}}\hat{\mathbf{k}} + \left(\frac{1}{\varepsilon_{||}} - \frac{1}{\varepsilon_\perp}\right)\hat{\mathbf{n}}\hat{\mathbf{n}} - \left(\frac{1}{\varepsilon_{||}} - \frac{1}{\varepsilon_\perp}\right)\hat{\mathbf{k}}(\hat{\mathbf{k}}\cdot\hat{\mathbf{n}})\hat{\mathbf{n}}\right)\mathbf{D} = \frac{1}{n^2}\mathbf{D} \tag{19}$$

Since $\hat{\mathbf{k}} \cdot \mathbf{D} = 0$, we can write $\mathbf{D} = a\hat{\mathbf{x}} + b\hat{\mathbf{y}}$, where the unit vectors $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are perpendicular to $\hat{\mathbf{k}}$, and $\hat{\mathbf{y}}$ is perpendicular to $\hat{\mathbf{n}}$ as shown.

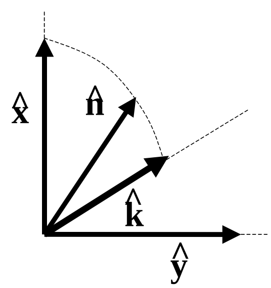

Fig. 1. Illustration of the geometry.

This gives

$$\frac{1}{\varepsilon_\perp}(a\hat{\mathbf{x}} + b\hat{\mathbf{y}}) + \left(\frac{1}{\varepsilon_{||}} - \frac{1}{\varepsilon_\perp}\right)a\hat{\mathbf{n}}(\hat{\mathbf{n}}\cdot\hat{\mathbf{x}}) - \left(\frac{1}{\varepsilon_{||}} - \frac{1}{\varepsilon_\perp}\right)a\hat{\mathbf{k}}(\hat{\mathbf{k}}\cdot\hat{\mathbf{n}})(\hat{\mathbf{n}}\cdot\hat{\mathbf{x}}) = \frac{1}{n^2}(a\hat{\mathbf{x}} + b\hat{\mathbf{y}}) \tag{20}$$

3.2 The Ordinary Wave

One solution is $a = 0$; then $\mathbf{D} = b\hat{\mathbf{y}}$ (for arbitrary b) and $n = \sqrt{\varepsilon_\perp}$ Here $\mathbf{E} = \varepsilon_o^{-1}\varepsilon_r^{-1}\mathbf{D} = \frac{b}{\varepsilon_o\varepsilon_\perp}\hat{\mathbf{y}}$; that is, $\mathbf{E}$ is parallel to $\mathbf{D}$. This is the *ordinary* solution, with the index denoted by $n_o = \sqrt{\varepsilon_\perp}$.

3.3 The Extraordinary Wave

The second solution is obtained if $b = 0$. Then

$$\frac{1}{\varepsilon_\perp}\hat{\mathbf{x}} + \left(\frac{1}{\varepsilon_{||}} - \frac{1}{\varepsilon_\perp}\right)\hat{\mathbf{n}}(\hat{\mathbf{n}}\cdot\hat{\mathbf{x}}) - \left(\frac{1}{\varepsilon_{||}} - \frac{1}{\varepsilon_\perp}\right)\hat{\mathbf{k}}(\hat{\mathbf{k}}\cdot\hat{\mathbf{n}})(\hat{\mathbf{n}}\cdot\hat{\mathbf{x}}) = \frac{1}{n^2}\hat{\mathbf{x}} \tag{21}$$

We note that taking the inner product of both sides with $\hat{\mathbf{k}}$ gives 0. Taking the inner product with $\hat{\mathbf{x}}$ gives

$$\frac{1}{\varepsilon_\perp}+(\frac{1}{\varepsilon_{||}}-\frac{1}{\varepsilon_\perp})(\hat{\mathbf{n}}\cdot\hat{\mathbf{x}})^2=\frac{1}{n^2} \tag{22}$$

This is the *extraordinary* solution. Since $\hat{\mathbf{n}}=(\hat{\mathbf{n}}\cdot\hat{\mathbf{x}})\hat{\mathbf{x}}+(\hat{\mathbf{n}}\cdot\hat{\mathbf{k}})\hat{\mathbf{k}}$, $1=(\hat{\mathbf{n}}\cdot\hat{\mathbf{x}})^2+(\hat{\mathbf{n}}\cdot\hat{\mathbf{k}})^2$ and

$$\frac{1}{\varepsilon_{||}}-(\frac{1}{\varepsilon_{||}}-\frac{1}{\varepsilon_\perp})(\hat{\mathbf{n}}\cdot\hat{\mathbf{k}})^2=\frac{1}{n^2} \tag{23}$$

or

$$n^2=\frac{\varepsilon_{||}\varepsilon_\perp}{\varepsilon_\perp+(\varepsilon_{||}-\varepsilon_\perp)(\hat{\mathbf{n}}\cdot\hat{\mathbf{k}})^2} \tag{24}$$

If we use the notation $n_e=\sqrt{\varepsilon_{||}}$, then

$$n=\frac{n_e n_o}{\sqrt{n_o^2+(n_e^2-n_o^2)(\hat{\mathbf{n}}\cdot\hat{\mathbf{k}})^2}}=\frac{n_e n_o}{\sqrt{n_o^2\sin^2\theta+n_e^2\cos^2\theta}} \tag{25}$$

where $\cos\theta=(\hat{\mathbf{n}}\cdot\hat{\mathbf{k}})$. The direction of the electric field is given by $\mathbf{E}=\varepsilon_o\varepsilon_r^{-1}\mathbf{D}=a\varepsilon_o(\frac{1}{\varepsilon_\perp}\hat{\mathbf{x}}+(\frac{1}{\varepsilon_{||}}-\frac{1}{\varepsilon_\perp})(\hat{\mathbf{n}}\cdot\hat{\mathbf{x}})\hat{\mathbf{n}})$, and if β is the angle between $\mathbf{D}$ and $\mathbf{E}$,

$$\tan\beta=\frac{\mathbf{E}\cdot\hat{\mathbf{k}}}{\mathbf{E}\cdot\hat{\mathbf{x}}}=\frac{(\frac{1}{\varepsilon_{||}}-\frac{1}{\varepsilon_\perp})(\hat{\mathbf{n}}\cdot\hat{\mathbf{x}})(\hat{\mathbf{n}}\cdot\hat{\mathbf{k}})}{\frac{1}{\varepsilon_\perp}+(\frac{1}{\varepsilon_{||}}-\frac{1}{\varepsilon_\perp})(\hat{\mathbf{n}}\cdot\hat{\mathbf{x}})^2} \tag{26}$$

or

$$\tan\beta=\frac{(\frac{1}{\varepsilon_{||}}-\frac{1}{\varepsilon_\perp})(\hat{\mathbf{n}}\cdot\hat{\mathbf{k}})\sqrt{1-(\hat{\mathbf{n}}\cdot\hat{\mathbf{k}})^2}}{\frac{1}{\varepsilon_{||}}-(\frac{1}{\varepsilon_{||}}-\frac{1}{\varepsilon_\perp})(\hat{\mathbf{n}}\cdot\hat{\mathbf{k}})^2}=\frac{(n_o^2-n_e^2)\sin\theta\cos\theta}{n_o^2\sin^2\theta+n_e^2\cos^2\theta} \tag{27}$$