Theoretical Background

Namu Kroupa

August 3, 2022

1 Matrix equation

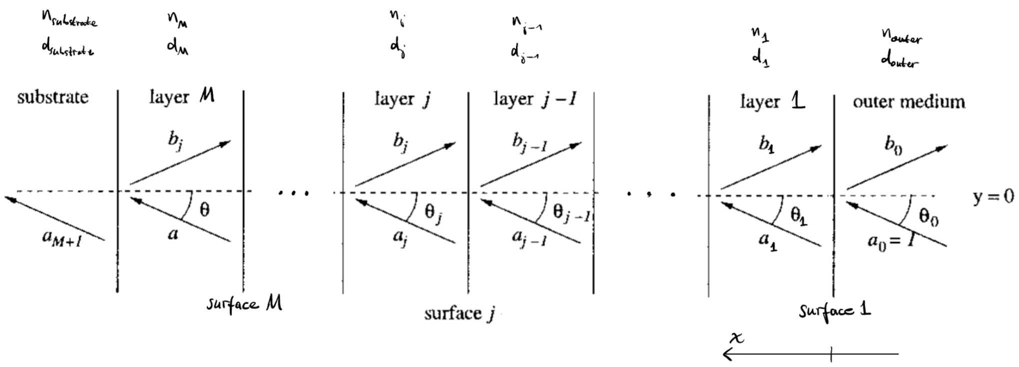

Figure 1

(Notation in this Section: The multilayer stack consists of M layers, numbered from $j = 0$ to $j = M - 1$. The outer medium from which the light is incident is denoted by "outer" and the substrate into which the light exits is denoted by "substrate". See Figure 1.)

To calculate the reflectivity, $R = |b_{\text{outer}}|^2$, the matrix equation

$$\mathbf{Mx} = \mathbf{c} \tag{1}$$

must be solved for $\mathbf{x}$, where

$$\mathbf{x} = (b_{\text{outer}}, a_0, b_0, a_1, b_1, \ldots, a_{M-1}, b_{M-1}, a_{\text{substrate}})^T \tag{2}$$

and

$$\mathbf{c} = (1, 1, 0, 0, \ldots, 0)^T \tag{3}$$

are $(2M + 2)$-dimensional complex vectors.

The matrix $\mathbf{M} \in \mathbb{C}^{(2M+2)\times(2M+2)}$ is[1]

$$\mathbf{M} = \left(\begin{array}{c|c|c|c|c|c|c|c}
\begin{matrix} a \\ b \end{matrix} & \boldsymbol{\beta}_0 & \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} & \begin{matrix} 0 \\ 0 \end{matrix} \\
\hline
\begin{matrix} 0 \\ 0 \end{matrix} & \boldsymbol{\alpha}_1 & \boldsymbol{\beta}_1 & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} & \begin{matrix} 0 \\ 0 \end{matrix} \\
\hline
\begin{matrix} 0 \\ 0 \end{matrix} & \mathbf{0} & \boldsymbol{\alpha}_2 & \boldsymbol{\beta}_2 & \mathbf{0} & \cdots & \mathbf{0} & \begin{matrix} 0 \\ 0 \end{matrix} \\
\hline
\begin{matrix} 0 \\ 0 \end{matrix} & \mathbf{0} & \mathbf{0} & \boldsymbol{\alpha}_3 & \boldsymbol{\beta}_3 & \cdots & \mathbf{0} & \begin{matrix} 0 \\ 0 \end{matrix} \\
\hline
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \boldsymbol{\beta}_{M-1} & \begin{matrix} 0 \\ 0 \end{matrix} \\
\hline
\begin{matrix} 0 \\ 0 \end{matrix} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \boldsymbol{\alpha}_M & \begin{matrix} c \\ d \end{matrix}
\end{array}\right), \tag{4}$$

where

$$\mathbf{0} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}. \tag{5}$$

[1] The horizontal lines are for readability.

To solve Equation 1 efficiently, its "band-storage form" $\mathbf{M}_{\text{band}} \in \mathbb{C}^{5\times(2M+2)}$ is used:

$$\mathbf{M}_{\text{band}} = \begin{pmatrix} 0 & & & & & 0 \\ 0 & & & & & c \\ a & \boldsymbol{c}_0 & \boldsymbol{c}_1 & \cdots & \boldsymbol{c}_{M-1} & d \\ b & & & & & 0 \\ 0 & & & & & 0 \end{pmatrix} \tag{6}$$

where

$$\boldsymbol{c}_i = \begin{pmatrix} 0 & (\boldsymbol{\beta}_i)_{01} \\ (\boldsymbol{\beta}_i)_{00} & (\boldsymbol{\beta}_i)_{11} \\ (\boldsymbol{\beta}_i)_{10} & (\boldsymbol{\alpha}_{i+1})_{01} \\ (\boldsymbol{\alpha}_{i+1})_{00} & (\boldsymbol{\alpha}_{i+1})_{11} \\ (\boldsymbol{\alpha}_{i+1})_{10} & 0 \end{pmatrix} \qquad \text{for} \quad i = 0, \ldots, M-1 \tag{7}$$

For s-polarisation,

$$a = -1 \tag{8}$$
$$b = 1 \tag{9}$$
$$c = 1 \tag{10}$$
$$d = n_{\text{substrate}} \cos\theta_{\text{substrate}} \tag{11}$$
$$\boldsymbol{\alpha}_j = \begin{pmatrix} -e^{i\phi_{j-1}} & -1 \\ -e^{i\phi_{j-1}} n_{j-1}\cos\theta_{j-1} & n_{j-1}\cos\theta_{j-1} \end{pmatrix} \qquad \text{for} \quad j = 1, \ldots, M \tag{12}$$
$$\boldsymbol{\beta}_j = \begin{cases} \begin{pmatrix} 1 & e^{i\phi_0} \\ \frac{n_0\cos\theta_0}{n_{\text{outer}}\cos\theta_{\text{outer}}} & -\frac{n_0\cos\theta_0}{n_{\text{outer}}\cos\theta_{\text{outer}}} e^{i\phi_0} \end{pmatrix} & \text{for} \quad j = 0 \\ \begin{pmatrix} 1 & e^{i\phi_j} \\ n_j\cos\theta_j & -n_j\cos\theta_j e^{i\phi_j} \end{pmatrix} & \text{for} \quad j = 1, \ldots, M-1 \end{cases}. \tag{13}$$

For p-polarisation,

$$a = -1 \tag{14}$$
$$b = 1 \tag{15}$$
$$c = \cos\theta_{\text{substrate}} \tag{16}$$
$$d = n_{\text{substrate}} \tag{17}$$
$$\boldsymbol{\alpha}_j = \begin{pmatrix} -e^{i\phi_{j-1}}\cos\theta_{j-1} & -\cos\theta_{j-1} \\ -e^{i\phi_{j-1}} n_{j-1} & n_{j-1} \end{pmatrix} \qquad \text{for} \quad j = 1, \ldots, M \tag{18}$$
$$\boldsymbol{\beta}_j = \begin{cases} \begin{pmatrix} \frac{\cos\theta_0}{\cos\theta_{\text{outer}}} & e^{i\phi_0}\frac{\cos\theta_0}{\cos\theta_{\text{outer}}} \\ \frac{n_0}{n_{\text{outer}}} & -e^{i\phi_0}\frac{n_0}{n_{\text{outer}}} \end{pmatrix} & \text{for} \quad j = 0 \\ \begin{pmatrix} \cos\theta_j & e^{i\phi_j}\cos\theta_j \\ n_j & -e^{i\phi_j} n_j \end{pmatrix} & \text{for} \quad j = 1, \ldots, M-1 \end{cases}. \tag{19}$$

where

$$\phi_j = k_{\text{outer}} d_j \frac{n_j}{n_{\text{outer}}} \cos\theta_j \tag{20}$$
$$\cos\theta_j = \sqrt{1 - \left(\frac{n_{\text{outer}}\sin\theta_{\text{outer}}}{n_j}\right)^2}. \tag{21}$$

2 Fabry-Perot interferometer

As a test case, the Fabry-Perot interferometer is considered, which consists of a single layer of refractive index n_{layer} and thickness d in a medium of refractive index n_{outer} and whose complex reflected amplitude, $b_{0,\text{FP}}$, at a wavelength λ_{vac} (in vacuum) and incident angle θ_{outer} is given by[2,3]

$$b_{0,\text{FP}} = \frac{r(1 - e^{2i\phi_0})}{1 - r^2 e^{2i\phi_0}} \tag{22}$$

[2]The sign in the complex exponential can be positive or negative depending on the convention. But it must be positive here to be consistent with Equation 1.

[3]This expression allows r and ϕ_0 to become complex, as occurs in total internal reflection, as opposed to the commonly found expression for the reflectivity, which assumes that r is real.

where[4]

$$\phi_0 = \frac{2\pi}{\lambda_{\text{vac}}} n_{\text{layer}} d \cos\theta_{\text{layer}} \tag{23}$$

$$r = \begin{cases} \dfrac{n_{\text{outer}}\cos\theta_{\text{outer}} - n_{\text{layer}}\cos\theta_{\text{layer}}}{n_{\text{outer}}\cos\theta_{\text{outer}} + n_{\text{layer}}\cos\theta_{\text{layer}}} & \text{for s-polarisation,} \\ \dfrac{n_{\text{outer}}\cos\theta_{\text{layer}} - n_{\text{layer}}\cos\theta_{\text{outer}}}{n_{\text{layer}}\cos\theta_{\text{outer}} + n_{\text{outer}}\cos\theta_{\text{layer}}} & \text{for p-polarisation} \end{cases}. \tag{24}$$

The angle θ_{layer} is the angle of the light ray inside the layer. Its cosine is given by

$$\cos\theta_{\text{layer}} = \sqrt{1 - \left(\frac{n_{\text{outer}}\sin\theta_{\text{outer}}}{n_{\text{layer}}}\right)^2}. \tag{25}$$

In the case of total internal refraction, $\cos\theta_{\text{layer}}$ becomes imaginary and the above equations for R, ϕ_0 and r continue to hold.

3 Transfer-matrix method

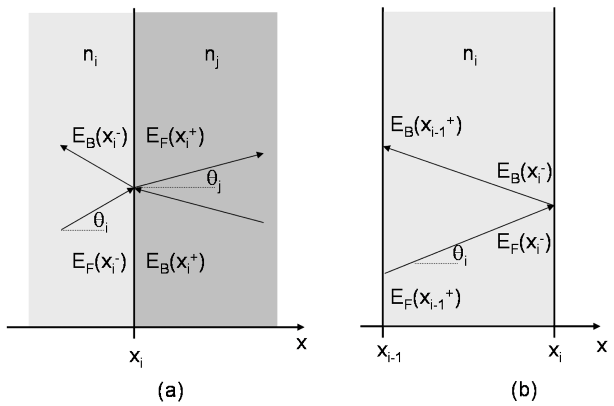

Figure 2

(Notation in this Section: The outer medium has index 0, the first and last layer of the multilayer stack have index 1 and M, respectively, and the substrate has index $M+1$.)

An alternative approach to calculate b_0 is the transfer-matrix method. It can be shown that, at interface i at position x_i between layers i and j ($i < j$), the electric field amplitudes of the forward (F) and backward (B) travelling waves on the left (x_i^-) and right (x_i^+), where $x_i^- < x_i^+$, (Figure 2) are related by

$$\begin{pmatrix} E_F(x_j^-) \\ E_B(x_j^-) \end{pmatrix} = \mathbf{T}_{ij} \begin{pmatrix} E_F(x_j^+) \\ E_B(x_j^+) \end{pmatrix} \tag{26}$$

where

$$\mathbf{T}_{ij} = \frac{1}{t_{ij}} \begin{pmatrix} 1 & r_{ij} \\ r_{ij} & 1 \end{pmatrix}. \tag{27}$$

Furthermore, within layer i, the electric field amplitudes on the left and right are related by complex exponentials such that

$$\begin{pmatrix} E_F(x_{i-1}^+) \\ E_B(x_{i-1}^+) \end{pmatrix} = \mathbf{T}_i \begin{pmatrix} E_F(x_i^-) \\ E_B(x_i^-) \end{pmatrix} \tag{28}$$

where

$$\mathbf{T}_i = \begin{pmatrix} e^{-i\Phi_i} & 0 \\ 0 & e^{i\Phi_i} \end{pmatrix} \tag{29}$$

and

$$\Phi_i = \frac{2\pi}{\lambda_{\text{vac}}} n_i d_i \cos\theta_i. \tag{30}$$

[4]The sign of r_p depends on convention, specifically if the electric field amplitudes were initially chosen to be parallel or antiparallel in the derivation of $r_{s/p}$. For example, Hecht and Wikipedia give the negative of the expression used in this text. For consistency with Equation 1, r_p must be chosen as presented here.

The Fresnel equations are

$$r_{ij} = \begin{cases} \dfrac{n_i \cos\theta_i - n_j \cos\theta_j}{n_i \cos\theta_i + n_j \cos\theta_j} & \text{for s-polarisation} \\ \dfrac{n_i \cos\theta_j - n_j \cos\theta_i}{n_j \cos\theta_i + n_i \cos\theta_j} & \text{for p-polarisation} \end{cases} \tag{31}$$

$$t_{ij} = \begin{cases} \dfrac{2n_i \cos\theta_i}{n_i \cos\theta_i + n_j \cos\theta_j} & \text{for s-polarisation} \\ \dfrac{2n_i \cos\theta_i}{n_j \cos\theta_i + n_i \cos\theta_j} & \text{for p-polarisation} \end{cases}. \tag{32}$$

Hence, the equation relating the incident, $(1, b_0)^T$, to the transmitted field amplitudes, $(a_{M+1}, 0)^T$, are

$$\begin{pmatrix} 1 \\ b_0 \end{pmatrix} = \mathbf{T} \begin{pmatrix} a_{M+1} \\ 0 \end{pmatrix} \tag{33}$$

where the transfer matrix, $\mathbf{T}$, is defined as[5]

$$\mathbf{T} = \mathbf{T}_{01}\mathbf{T}_1\mathbf{T}_{12}\mathbf{T}_2 \ldots \mathbf{T}_M \mathbf{T}_{M(M+1)}. \tag{34}$$

Thus, the reflected amplitude, b_0, is related to the transfer matrix components by

$$b_0 = \frac{(\mathbf{T})_{10}}{(\mathbf{T})_{00}}. \tag{35}$$

[5]Reminder: "Layer" 0 is the outer medium, layers 1 and M are the first and last layers on the multilayer stack, respectively, and "layer" $M + 1$ is the substrate.