# Matrix methods for the calculation of reflection amplitudes 

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#### Abstract

Improved numerical techniques for the calculation of the reflection of electromagnetic waves by an arbitrary stratified inhomogeneity are derived and assessed. The inhomogeneity is sectioned into thin layers, in each of which the dielectric function is taken to vary linearly, or cubically, with depth. The matrices representing each layer are calculated to third order in layer thickness. Some general properties of the matrices used in these calculations are also presented.


## 1. INTRODUCTION

We present improved matrix methods for the numerical evaluation of reflection amplitudes for $s$ and $p$ polarizations for an arbitrary planar stratified transition between two uniform media. The reflection amplitudes $r_{s}$ and $r_{p}$ give the reflectances $R_{s}=\left|r_{s}\right|^{2}$ and $R_{p}=\left|r_{p}\right|^{2}$ and the ellipsometric ratio $r_{p} / r_{s}$. Matrix methods are reviewed and extended in Chaps. 12 and 13 of a recent monograph (Ref. 1, hereafter referred to as TR). All matrix methods approximate the stratified inhomogeneous region by a set of $N$ uniform or nonuniform layers; the reflection properties are then obtained from the product of $N$ two-by-two layer matrices or $N+1$ two-by-two boundary matrices. In the conventional approach, matrices relate the mutually perpendicular components of the electric and magnetic fields from layer to neighboring layer. ${ }^{2}$ Here we use layer matrices introduced in TR, which relate the fields and their derivatives. In the absence of absorption, the matrix elements are all real. The standard approach leads to imaginary off-diagonal matrix elements, complicating the process of taking matrix products. Figure 1 illustrates how an inhomogeneous transition between uniform media of dielectric constants $\epsilon_{a}$ and $\epsilon_{b}$ is approximated by a set of layers in each of which the dielectric function varies linearly with depth.

For the $s$ polarization, $\mathbf{E}=\{0, \exp [i(K x-\omega t)] E(z), 0\}$, where $K$ is the $x$ component of the wave vector and is a constant of the motion. At $z_{n}$ and $z_{n+1}, E(z)$ takes the values $E_{n}$ and $E_{n+1}$, its derivative $D=\mathrm{d} E / \mathrm{d} z$ takes the values $D_{n}$ and $D_{n+1}$, and these two pairs are linked by the matrix $M_{n}=$ $\left\{m_{i j}\right\}$ :

$$
\left[\begin{array}{l}
E_{n+1}  \tag{1}\\
D_{n+1}
\end{array}\right]=\left[\begin{array}{ll}
m_{11} & m_{12} \\
m_{21} & m_{22}
\end{array}\right]\left[\begin{array}{l}
E_{n} \\
D_{n}
\end{array}\right]
$$

If the uniform media on either side of the inhomogeneity are labeled $a$ and $b$, and the wave is incident from medium $a$, $E(z)$ has the limiting forms

$$
\begin{array}{ll}
E=\exp \left(i q_{a} z\right)+r_{s} \exp \left(-i q_{a} z\right) & \left(z \leq z_{1}\right) \\
E=t_{s} \exp \left(i q_{b} z\right) & \left(z \geq z_{N+1}\right) \tag{2}
\end{array}
$$

Here $q_{a}$ and $q_{b}$ are the $z$ components of the wave vector in media $a$ and $b$. If $s_{i j}$ are the matrix elements of
$M_{N} M_{N-1} \ldots M_{n} \ldots M_{2} M_{1}$, the $s$ reflection amplitude is given by

$$
\begin{equation*}
r_{s}=\exp \left(2 i q_{a} z_{1}\right) \frac{q_{a} q_{b} s_{12}+s_{21}+i q_{a} s_{22}-i q_{b} s_{11}}{q_{a} q_{b} s_{12}-s_{21}+i q_{a} s_{22}+i q_{b} s_{11}} \tag{3}
\end{equation*}
$$

For the $p$ polarization, $\mathbf{B}=\{0, \exp [i(K x-\omega t)] B(z), 0\}$, and the matrix $M_{n}$ relates the values of $B$ and $C=\mathrm{d} B / \epsilon \mathrm{d} z$ at $z_{n}$ and $z_{n+1} ; \epsilon(z)$ is the dielectric function. If now $p_{i j}$ are the elements of $M_{N} \ldots M_{n} \ldots M_{1}$, the $p$ reflection amplitude is given by

$$
\begin{equation*}
-r_{p}=\exp \left(2 i q_{a} z_{1}\right) \frac{Q_{a} Q_{b} p_{12}+p_{21}+i Q_{a} p_{22}-i Q_{b} p_{11}}{Q_{a} Q_{a} p_{12}-p_{21}+i Q_{a} p_{22}+i Q_{b} p_{11}} \tag{4}
\end{equation*}
$$

where $Q_{a}=q_{a} / \epsilon_{a}$ and $Q_{b}=q_{b} / \epsilon_{b}$. (With the definition of $r_{p}$ used in TR and here, $r_{p}=r_{s}$ at normal incidence, when there is no physical distinction between the two polarizations.)

The simplest approximation replaces $\epsilon(z)$ by a constant value, $\epsilon_{n}$, within $z_{n}<z<z_{n+1}$. The matrices $M_{n}$ then become, for the $s$ and $p$ polarizations, and with $\delta_{n}=q_{n}\left(z_{n+1}-\right.$ $\left.z_{n}\right) \equiv q_{n} \delta z_{n}$,

$$
\left[\begin{array}{ll}
\cos \delta_{n} & q_{n}^{-1} \sin \delta_{n}  \tag{5}\\
-q_{n} \sin \delta_{n} & \cos \delta_{n}
\end{array}\right], \quad\left[\begin{array}{ll}
\cos \delta_{n} & Q_{n}^{-1} \sin \delta_{n} \\
-Q_{n} \sin \delta_{n} & \cos \delta_{n}
\end{array}\right]
$$

The numerical method based on these matrices taken to first order in $\delta z_{n}$ is equivalent to the Euler method of solving the differential equations (TR, Sec. 13-1). Natural improvements are to go to higher order in $\delta z_{n}$ and to allow a variable $\epsilon(z)$ within a layer. Law and Beaglehole ${ }^{3}$ took a linear variation in $\epsilon(z)$,

$$
\begin{equation*}
\epsilon(z)=\epsilon_{n}+\left(z-z_{n}\right) \delta \epsilon_{n} / \delta z_{n} \tag{6}
\end{equation*}
$$

( $\delta \epsilon_{n}=\epsilon_{n+1}-\epsilon_{n}$ ), and the corresponding matrix to first order in $\delta z_{n}$. In TR the linear approximation was taken to second order in $\delta z_{n}$. Here we derive expressions for matrices for linear and cubic variations in $\epsilon(z)$ taken up to third order in $\delta z_{n}$. But first we consider some general properties of such matrices.

## 2. GENERAL PROPERTIES OF THE LAYER MATRICES

The matrices in Eqs. (5) are unimodular (have unit determinants). Thus any approximate matrices derived from them will be unimodular, to the appropriate order of approximation. For example, the matrices corresponding to linear $\epsilon(z)$, and taken to second order in $\delta z_{n}$, will be unimodular to second order in $\delta z_{n}$.

The matrix $M_{n}$ takes ( $E_{n}, D_{n}$ ) into ( $E_{n+1}, D_{n+1}$ ) according to Eq. (1). For the moment, we write this matrix as $M(n, n+$ 1). The inverse matrix takes ( $\mathrm{E}_{n+1}, D_{n+1}$ ) into ( $E_{n}, D_{n}$ ). This is $M(n+1, n)$ so

$$
\begin{equation*}
M^{-1}(n, n+1)=M(n+1, n) \tag{7}
\end{equation*}
$$

In other words, taking the inverse of $M$ is equivalent to the exchange of $n$ and $n+1$. Now the inverse of a unimodular two-by-two matrix is

$$
\left[\begin{array}{ll}
m_{11} & m_{12}  \tag{8}\\
m_{21} & m_{22}
\end{array}\right]^{-1}=\left[\begin{array}{cc}
m_{22} & -m_{12} \\
-m_{21} & m_{11}
\end{array}\right]
$$

Thus we have two symmetries. First, we can obtain $m_{22}$ from $m_{11}$ by exchanging $n$ and $n+1$. Second, each of the off-diagonal elements is antisymmetric with respect to this interchange.
At normal incidence there is no physical distinction between $s$ and $p$ polarizations, and $r_{p}=r_{s}$. From Eqs. (3) and (4), on using the normal-incidence limiting values, $q_{a} \rightarrow n_{a} \omega /$ $c, q_{b} \rightarrow n_{b} \omega / c, Q_{a} \rightarrow n_{a}^{-1} \omega / c$, and $Q_{b} \rightarrow n_{b}^{-1} \omega / c$, where $n=\epsilon^{1 / 2}$ is the refractive index, we find the relationships

$$
\begin{array}{ll}
p_{11}=s_{22}, & p_{12}=-c^{2} / \omega^{2} s_{21}, \\
p_{21}=\omega^{2} / c^{2} s_{12}, & p_{22}=s_{11} . \tag{9}
\end{array}
$$

## 3. CALCULATION OF THE MATRIX <br> ELEMENTS

In this section we derive general expressions for the $s$ and $p$ matrix elements for an arbitrary profile. These expressions are then evaluated, to third order in $\delta z_{n}$, for the linear and cubic profiles.

Expressions up to the second order in $\delta z_{n}$ were derived in TR, Sec. $12-5$, by using matrix methods. An equivalent method that is due to Brekhovskikh ${ }^{4}$ (explained in Sec. 5-5 of TR) is somewhat simpler to apply and will be used here. The reflection amplitude $r_{s}$ for an inhomogeneity extending from $a$ to $b$ is calculated in the form

$$
\begin{equation*}
r_{s}=\exp \left(2 i q_{a} a\right) \frac{q_{a} u(a)-q_{b} v(a)}{q_{a} u(a)+q_{b} v(a)} \tag{10}
\end{equation*}
$$

where $u(z)$ and $v(z)$ satisfy the coupled integral equations
$u(z)=1-i q_{b} \int_{z}^{b} \mathrm{~d} \zeta v(\zeta), \quad v(z)=1-i{q_{b}}^{-1} \int_{z}^{b} \mathrm{~d} \zeta q^{2}(\zeta) u(\zeta)$.

These equations may be iterated to give $u=\sum u_{n}$ and $v=$ $\sum v_{n}$, starting with $u_{0}=1=v_{0}$. The $n$ th-order iterates are $n$th order in the interfacial thickness. They are given, for $n$ $\geq 1$, by

$$
\begin{align*}
& u_{n}(z)=-i q_{b} \int_{z}^{b} \mathrm{~d} \zeta v_{n-1}(\zeta) \\
& v_{n}(z)=-i q_{b}^{-1} \int_{z}^{b} \mathrm{~d} \zeta q^{2}(\zeta) u_{n-1}(\zeta) \tag{12}
\end{align*}
$$

To evaluate $r_{s}$ to third order we need $u_{n}(a)$ and $v_{n}(a)$ up to $n$ $=3$. The resulting $u(a)$ and $v(a)$ are

$$
\begin{align*}
u(a)= & 1-i q_{b}(b-a)-\int_{a}^{b} \mathrm{~d} z q^{2}(z)(z-a) \\
& +i q_{b} \int_{a}^{b} \mathrm{~d} z q^{2}(z)(z-a)(b-z)+\ldots  \tag{13}\\
v(a)= & 1-i / q_{b} \int_{a}^{b} \mathrm{~d} z q^{2}(z)-\int_{a}^{b} \mathrm{~d} z q^{2}(z)(b-z) \\
& +i / q_{b} \int_{a}^{b} \mathrm{~d} z q^{2}(z) \int_{a}^{z} \mathrm{~d} \zeta q^{2}(\zeta)(z-\zeta)+\ldots \tag{14}
\end{align*}
$$

When $\epsilon(z)$ is real (no absorption), so is $q^{2}=\epsilon \omega^{2} / c^{2}-K^{2}$, and thus for even $n$ all $u_{n}$ and $v_{n}$ are real, and for odd $n$ they are imaginary. We write $u(a)=u_{r}+i u_{i}$ and $v(a)=v_{r}+i v_{i}$, substitute into Eq. (10), and compare with Eq. (3). This leads to the identifications

$$
\begin{array}{ll}
s_{11}=v_{r}, & s_{12}=-u_{i} / q_{b}, \\
s_{21}=q_{b} v_{i}, & s_{22}=u_{r} . \tag{15}
\end{array}
$$

The $p$-polarization matrix elements may be obtained similarly. The reflection amplitude is calculated in the form

$$
\begin{equation*}
-r_{p}=\exp \left(2 i q_{a} a\right) \frac{Q_{a} U(a)-Q_{b} V(a)}{Q_{a} U(a)+Q_{b} V(a)}, \tag{16}
\end{equation*}
$$

where now $U(z)$ and $V(z)$ satisfy the coupled integral equations

$$
\begin{align*}
& U(z)=1-i Q_{b} \int_{z}^{b} \mathrm{~d} \zeta \epsilon(\zeta) V(\zeta) \\
& V(z)=1-i Q_{b}^{-1} \int_{z}^{b} \mathrm{~d} \zeta \epsilon^{-1}(\zeta) q^{2}(\zeta) U(\zeta) \tag{17}
\end{align*}
$$

The results of iterating up to third order in the thickness are

$$
\begin{align*}
U(a)= & 1-i Q_{b} \int_{a}^{b} \mathrm{~d} z \epsilon(z)-\int_{a}^{b} \mathrm{~d} z \epsilon(z) \\
& \times \int_{z}^{b} \mathrm{~d} \zeta q^{2}(\zeta) / \epsilon(\zeta)+i Q_{b} \int_{a}^{b} \mathrm{~d} z \epsilon(z) \\
& \times \int_{z}^{b} \mathrm{~d} \zeta q^{2}(\zeta) / \epsilon(\zeta) \int_{\zeta}^{b} \mathrm{~d} \xi \epsilon(\xi)+\ldots,  \tag{18}\\
V(a)= & 1-i Q_{b}^{-1} \int_{a}^{b} \mathrm{~d} z q^{2}(z) / \epsilon(z) \\
& -\int_{a}^{b} \mathrm{~d} z q^{2}(z) / \epsilon(z) \int_{z}^{b} \mathrm{~d} \zeta \epsilon(\zeta)+\ldots \\
& +i Q_{b}^{-1} \int_{a}^{b} \mathrm{~d} z q^{2}(z) / \epsilon(z) \int_{z}^{b} \mathrm{~d} \zeta \epsilon(\zeta) \\
& \times \int_{\zeta}^{b} \mathrm{~d} \zeta q^{2}(\xi) / \epsilon(\xi)+\ldots \tag{19}
\end{align*}
$$



Fig. 1. A stack of $N$ nonuniform layers bounded by media with dielectric constants $\epsilon_{a}$ and $\epsilon_{b}$. The $n$th layer extends from $z_{n}$ to $z_{n+1}$, and in this case the dielectric function within the $n$th layer is approximated by the line passing through $\epsilon\left(z_{n}\right)$ and $\epsilon\left(z_{n+1}\right)$ (linear fit). The cubic fit, discussed in Section 5, is indistinguishable from the exact $\epsilon(z)$ on this scale.

We again write $U(a)=U_{r}+i U_{i}, V(a)=V_{r}+i V_{i}$, substitute into Eq. (16), and compare with Eq. (4). This leads to

$$
\begin{array}{ll}
p_{11}=V_{r}, & p_{12}=-U_{i} / Q_{b} \\
p_{21}=Q_{b} V_{i}, & p_{22}=U_{r} \tag{20}
\end{array}
$$

## 4. THIRD-ORDER RESULTS FOR A LINEAR FIT TO $\epsilon(z)$

The above expressions are for a general stratification extending from $z=a$ to $z=b$. We now specialize to a profile that has $\epsilon(z)$ linear in $z$ [as given by Eq. (6)] and extends from $z_{n}$ to $z_{n+1}$. An arbitrary profile can then be approximated by a set of such layers, as illustrated in Fig. 1.
The matrix elements for the $s$ polarization are, to third order,

$$
\begin{align*}
s_{11}= & 1+\left(\delta z_{n}\right)^{2}\left[K^{2} / 2-\omega^{2} / c^{2}\left(2 \epsilon_{n}+\epsilon_{n+1}\right) / 6\right] \\
s_{12}= & \delta z_{n}+\left(\delta z_{n}\right)^{3}\left[K^{2} / 6-\omega^{2} / c^{2}\left(\epsilon_{n}+\epsilon_{n+1}\right) / 12\right] \\
s_{21}= & \delta z_{n}\left[K^{2}-\omega^{2} / c^{2}\left(\epsilon_{n}+\epsilon_{n+1}\right) / 2\right] \\
& +\left(\delta z_{n}\right)^{3}\left[K^{4} / 6-K^{2} \omega^{2} / c^{2}\left(\epsilon_{n}+\epsilon_{n+1}\right) / 6\right. \\
& +\omega^{4} / c^{4}\left(\epsilon_{n}^{2}+3 \epsilon_{n} \epsilon_{n+1}+\epsilon_{n+1}^{2} / 30\right] \\
s_{22}= & 1+\left(\delta z_{n}\right)^{2}\left[K^{2} / 2-\omega^{2} / c^{2}\left(\epsilon_{n}+2 \epsilon_{n+1}\right) / 6\right] \tag{21}
\end{align*}
$$

The corresponding results for the $p$ polarization are

$$
\begin{aligned}
p_{11}= & 1+\left(\delta z_{n}\right)^{2}\left\{K ^ { 2 } \left[2\left(\epsilon_{n+1}{ }^{2} / \delta \epsilon_{n}\right) \log \left(\epsilon_{n+1} / \epsilon_{n}\right)\right.\right. \\
& \left.\left.-\epsilon_{n}-\epsilon_{n+1}\right] / 4 \delta \epsilon_{n}-\omega^{2} / c^{2}\left(\epsilon_{n}+2 \epsilon_{n+1}\right) / 6\right\}, \\
p_{12}= & \delta z_{n}\left(\epsilon_{n}+\epsilon_{n+1}\right) / 2+\left(\delta z_{n}\right)^{3}\left\{K ^ { 2 } \left[\epsilon_{n+1}^{4}-\epsilon_{n}^{4}-4 \epsilon_{n}^{2} \epsilon_{n+1}^{2}\right.\right. \\
& \left.\times \log \left(\epsilon_{n+1} / \epsilon_{n}\right)\right] / 16\left(\delta \epsilon_{n}\right)^{3} \\
& \left.-\omega^{2} / c^{2}\left(\epsilon_{n}^{2}+3 \epsilon_{n} \epsilon_{n+1}+\epsilon_{n+1}^{2}\right) / 30\right\}, \\
p_{21}= & \delta z_{n}\left[K^{2} \log \left(\epsilon_{n+1} / \epsilon_{n}\right) / \delta \epsilon_{n}-\omega^{2} / c^{2}\right] \\
& +\left(\delta z_{n}\right)^{3}\left\{\omega^{4} / c^{4}\left(\epsilon_{n}+\epsilon_{n+1}\right) / 12+K^{2} \omega^{2} / c^{2}\right. \\
& \times\left[\delta \epsilon_{n}\left(\epsilon_{n}^{2}+10 \epsilon_{n} \epsilon_{n+1}+\epsilon_{n+1}^{2}\right)-6\left(\epsilon_{n}^{3}+\epsilon_{n+1}^{3}\right)\right. \\
& \left.\times \log \left(\epsilon_{n+1} / \epsilon_{n}\right)\right] / 36\left(\delta \epsilon_{n}\right)^{3}+K^{4}\left[\left(\epsilon_{n+1}^{2}+\epsilon_{n}^{2}\right) \log \left(\epsilon_{n+1} / \epsilon_{n}\right)\right. \\
& \left.\left.-\left(\epsilon_{n+1}^{2}-\epsilon_{n}^{2}\right)\right] / 4\left(\delta \epsilon_{n}\right)^{3}\right\},
\end{aligned}
$$

$$
\begin{align*}
p_{22}= & 1+\left(\delta z_{n}\right)^{2}\left\{K^{2}\left[\epsilon_{n}+\epsilon_{n+1}-\left(2 \epsilon_{n}^{2} / \delta \epsilon_{n}\right) \log \left(\epsilon_{n+1} / \epsilon_{n}\right)\right] / 4 \delta \epsilon_{n}\right. \\
& \left.-\omega^{2} / c^{2}\left(2 \epsilon_{n}+\epsilon_{n+1}\right) / 6\right\} \tag{22}
\end{align*}
$$

For numerical work it is faster and more accurate to replace the terms containing $\log \left(\epsilon_{n+1} / \epsilon_{n}\right)$ by the leading terms in the expansion in terms of $\delta \epsilon_{n} / \epsilon_{n}$. We obtain
$p_{11} \simeq 1+\left(\delta z_{n}\right)^{2}\left[K^{2}\left(2 \epsilon_{n}+\epsilon_{n+1}\right) / 6 \epsilon_{n}-\omega^{2} / c^{2}\left(\epsilon_{n}+2 \epsilon_{n+1}\right) / 6\right]$,
$p_{12} \simeq \delta z_{n}\left(\epsilon_{n}+\epsilon_{n+1}\right) / 2+\left(\delta z_{n}\right)^{3}\left[K^{2}\left(\epsilon_{n}+\epsilon_{n+1}\right) / 12\right.$
$\left.-\omega^{2} / c^{2}\left(\epsilon_{n}^{2}+3 \epsilon_{n} \epsilon_{n+1}+\epsilon_{n+1}^{2}\right) / 30\right]$,
$p_{21} \simeq \delta z_{n}\left[K^{2}\left(\epsilon_{n}{ }^{-1}+\epsilon_{n+1}{ }^{-1}\right) / 2-\omega^{2} / c^{2}\right]$
$+\left(\delta z_{n}\right)^{3}\left[\omega^{4} / c^{4}\left(\epsilon_{n}+\epsilon_{n+1}\right) / 12-K^{2}\left(\omega^{2} / c^{2}\right) / 3\right.$
$\left.+K^{4}\left(\epsilon_{n}{ }^{-1}+\epsilon_{n+1}{ }^{-1}\right) / 12\right]$,
$p_{22} \simeq 1+\left(\delta z_{n}\right)^{2}\left[K^{2}\left(\epsilon_{n}+2 \epsilon_{n+1}\right) / 6 \epsilon_{n+1}-\omega^{2} / c^{2}\left(2 \epsilon_{n}+\epsilon_{n+1}\right) / 6\right]$.

## 5. THIRD-ORDER RESULTS FOR A CUBIC FIT TO $\epsilon(Z)$

The linear fit to $\epsilon(z)$ in $\left[z_{n}, z_{n+1}\right]$ uses just $\epsilon_{n}$ and $\epsilon_{n+1}$. A more accurate fit can be obtained if the derivatives $\epsilon_{n}{ }^{\prime}$ and $\epsilon_{n+1}{ }^{\prime}$ are known. The four values $\epsilon_{n}, \epsilon_{n+1}, \epsilon_{n}{ }^{\prime}$, and $\epsilon_{n+1}{ }^{\prime}$ are sufficient for a cubic approximation to $\epsilon(z)$ [see TR, Eq. (13.13)]:

$$
\begin{align*}
\epsilon(z) \simeq & \epsilon_{n}+\left(z-z_{n}\right) \epsilon_{n}^{\prime}+\left(\frac{z-z_{n}}{\delta z_{n}}\right)^{2}\left[3 \delta \epsilon_{n}-\delta z_{n}\left(2 \epsilon_{n}^{\prime}+\epsilon_{n+1}^{\prime}\right)\right] \\
& +\left(\frac{z-z_{n}}{\delta z_{n}}\right)^{3}\left[\delta z_{n}\left(\epsilon_{n}^{\prime}+\epsilon_{n+1}^{\prime}\right)-2 \delta \epsilon_{n}\right] . \tag{24}
\end{align*}
$$

The resulting $s$ wave matrix elements may be found from Eqs. (13) and (14):

$$
\begin{align*}
s_{11}= & 1+\left(\delta z_{n}\right)^{2}\left\{K^{2} / 2-\omega^{2} / c^{2}\left[\left(7 \epsilon_{n}+3 \epsilon_{n+1}\right) / 20\right.\right. \\
& \left.\left.+\delta z_{n}\left(\epsilon_{n}^{\prime} / 20-\epsilon_{n+1}^{\prime} / 30\right)\right]\right\}, \\
s_{12}= & \delta z_{n}+\left(\delta z_{n}\right)^{3}\left\{K^{2} / 6-\omega^{2} / c^{2}\left[\left(\epsilon_{n}+\epsilon_{n+1}\right) / 12\right.\right. \\
& \left.\left.+\delta z_{n}\left(\epsilon_{n}^{\prime}-\epsilon_{n+1}^{\prime}\right) / 60\right]\right\}, \\
s_{21}= & \delta z_{n}\left\{K^{2}-\omega^{2} / c^{2}\left[\left(\epsilon_{n}+\epsilon_{n+1}\right) / 2\right.\right. \\
& \left.\left.+\delta z_{n}\left(\epsilon_{n}^{\prime}-\epsilon_{n+1}^{\prime}\right) / 12\right]\right\}+\left(\delta z_{n}\right)^{3}\left\{K^{4} / 6\right. \\
& -K^{2} \omega^{2} / c^{2}\left[\left(\epsilon_{n}+\epsilon_{n+1}\right) / 6+\delta z_{n}\left(\epsilon_{n}^{\prime}-\epsilon_{n+1}^{\prime}\right) / 40\right] \\
& +\omega^{4} / c^{4}\left[74\left(\epsilon_{n}+\epsilon_{n+1}\right)^{2}+124 \epsilon_{n} \epsilon_{n+1}\right. \\
& +\delta z_{n}\left(26 \epsilon_{n}^{\prime} \epsilon_{n}+37 \epsilon_{n}^{\prime} \epsilon_{n+1}-37 \epsilon_{n} \epsilon_{n+1}^{\prime}\right. \\
& \left.-26 \epsilon_{n+1}^{\prime} \epsilon_{n+1}\right)+\left(\delta z_{n}\right)^{2}\left(2 \epsilon_{n}^{\prime 2}-5 \epsilon_{n}^{\prime} \epsilon_{n+1}^{\prime}\right. \\
& \left.\left.\left.+2 \epsilon_{n+1}^{\prime 2}\right)\right] / 2520\right\}, \\
s_{22}= & 1+\left(\delta z_{n}\right)^{2}\left\{K^{2} / 2-\omega^{2} / c^{2}\left[\left(3 \epsilon_{n}+7 \epsilon_{n+1}\right) / 20\right.\right. \\
& \left.\left.+\delta z_{n}\left(\epsilon_{n}^{\prime} / 30-\epsilon_{n+1}^{\prime} / 20\right)\right]\right\} . \tag{25}
\end{align*}
$$

The elements $p_{i j}$ of the $p$-polarization matrices will not be given. They are complicated, and (as we explain in Section 6) the cubic fit to $\epsilon(z)$ gave results that were close to the simpler linear fit, except in one circumstance.

## 6. COMPARISON OF THE NUMERICAL TECHNIQUES

In Chap. 13 of TR comparison is made between L1 and L2, the linear approximations taken to first and second order in $\delta z_{n}$. Here we compare L1, L2, and L3. The cubic approximations, $\mathrm{C} 1-\mathrm{C} 3$, were found in general to be similar to the corresponding linear approximations L1-L3, except for profiles thin in comparison with the wavelength, i.e., for $(\omega / \mathrm{c}) \Delta z$ small. In that case only a small number of matrices is required, and the cubic approximation is more accurate. In general, however, we have found that a cubic fit to $\epsilon(z)$, which involves the calculation of the derivative of $\epsilon(z)$ at each boundary, is more trouble than it is worth.

The remainder of this section is restricted to comparison of the linear approximations. In all cases we give the fractional errors, with sign, expressed as parts per thousand, the quantity displayed being $10^{3}(A / E-1)$, where $A$ and $E$ are the approximate and the exact values, respectively. The dielectric constants $\epsilon_{a}=1$ and $\epsilon_{b}=(4 / 3)^{2}$ are used in all three tables. Table 1 compares L1, L2, and L3 for the Rayleigh profile, defined by $\epsilon=\epsilon_{a}$ for $z<a, \epsilon=\epsilon_{b}$ for $z>b$, and, for $a \leq$ $z \leq b$,

$$
\begin{equation*}
\epsilon(z)=\left[\left(\epsilon_{a}^{-1 / 2}+\epsilon_{b}^{-1 / 2}\right) / 2+(z-\bar{z}) \frac{\epsilon_{b}^{-1 / 2}-\epsilon_{a}^{-1 / 2}}{\Delta z}\right]^{-2}, \tag{26}
\end{equation*}
$$

where $\bar{z}=\left(z_{a}+z_{b}\right) / 2$ and $\Delta z=b-a$. Figures 2-15 and 5-4 of TR show the normal-incidence reflectivity for the exactly solvable Rayleigh profile.
The next two tables compare L2 and L3 for the exponential profile, given by $\epsilon=\epsilon_{a}$ for $z<a, \epsilon=\epsilon_{b}$ for $z>z_{b}$, and, for $z_{a} \leq z \leq z_{b}$,

$$
\begin{equation*}
\epsilon(z)=\left(\epsilon_{a} \epsilon_{b}\right)^{1 / 2} \exp \left[\frac{z-\bar{z}}{\Delta z} \log \frac{\epsilon_{b}}{\epsilon_{a}}\right], \tag{27}
\end{equation*}
$$

where $\bar{z}=(a+b) / 2$ and $\Delta z=b-a$. The $s$ and $p$ reflectivities and the ellipsometric ratio for the exponential profile are displayed in Figs. 6-4-6-6 of TR. Table 2 shows errors in

Table 1. Fractional Errors (parts per thousand) in the Normal-Incidence Reflectivity for the Rayleigh Profile as a Function of the Interface Thickness $\Delta z^{a}$

| $\frac{\omega \Delta z}{c}$ | L1 | L2 | L3 |
| :---: | :---: | :---: | :--- |
| 0.2 | -0.3 | 0.004 | 0.007 |
| 0.4 | -1 | -0.02 | 0.03 |
| 0.6 | -3 | -0.2 | 0.07 |
| 0.8 | -4 | -0.7 | 0.1 |
| 1.0 | -4 | -2 | 0.2 |
| 1.2 | -3 | -4 | 0.3 |
| 1.4 | 1 | -9 | 0.4 |
| 1.6 | 10 | -20 | 0.6 |
| 1.8 | 30 | -30 | 0.7 |
| 2.0 | 70 | -50 | 0.9 |

[^0]Table 2. Parts-per-Thousand Errors in the $s$ and $p$ Reflectivities for the Exponential Profile as a Function of the Angle of Incidence ${ }^{a}$

|  | $R_{s}$ |  | $R_{p}$ |  |  |
| :---: | ---: | :---: | :---: | :---: | :---: |
| $\theta_{a}(\mathrm{deg})$ | L 2 | L 3 |  | L2 | L3 |
| 0 | 40 | 0.4 | 40 | 0.4 |  |
| 15 | 40 | 0.1 | 40 | 0.2 |  |
| 30 | 4 | 0.0 | -30 | -0.7 |  |
| 45 | -10 | -0.02 | -10 | -1 |  |
| 60 | -4 | -0.004 | -1 | -0.7 |  |
| 75 | -1 | -0.0006 | -0.5 | -0.2 |  |
| 90 | 0 | 0 | 0 | 0 |  |

${ }^{a}$ The layer thickness is approximately one half of the wavelength in medi$\operatorname{um} a,(\omega / c) \Delta z=3$, and $N=30$.

Table 3. Parts-per-Thousand Errors in the Real and Imaginary Parts of $r_{p} / r_{s}$ at $45^{\circ}$, for the Exponential Profile at $(\omega / c) \Delta z=3$, as a Function of the Number of Layers, $\boldsymbol{N}$

| $N$ | L 2 | L 3 |
| :---: | :---: | :---: |
| 10 | $600,-20$ | $6,-5$ |
| 20 | $650,-3$ | $-0.2,-1$ |
| 30 | $70,-1$ | $-0.2,-0.6$ |
| 40 | $40,-1$ | $-0.2,-0.3$ |
| 50 | $20,-0.5$ | $-0.1,-0.2$ |

$R_{s}$ and $R_{p}$ as a function of angle of incidence for fixed thickness and number of layers. Table 3 compares errors in the real and imaginary parts of $r_{p} / r_{s}$, at fixed thickness and angle of incidence, as a function of $N$, the number of layers.

From the results shown here, and others like them, we conclude that the linear approximation taken to third order in the layer matrix thickness (L3) is generally much better than the previous best matrix approximation L2, which in turn was an improvement over L1. The increased accuracy is obtained at the expense of slightly more complex expressions to program [compare, for example, the $s_{12}$ and $s_{21}$ matrix elements in Eqs. (21), with and without the $\left(\delta z_{n}\right)^{3}$ terms]. There is a corresponding increase in computer running time: we found that for the same number of layers the L3 method took 30 to $40 \%$ longer to run than the L2. This cost in programming and computer time is offset many times over by the up-to- 2 -orders of magnitude increase in accuracy of the third-order results.

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[^0]:    ${ }^{a}$ The profile has been approximated by 10 layers, in each of which $\epsilon(z)$ varies linearly with $z$.

